Translation-Invariant Quantum Systems with effectively broken Symmetry

by

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December, 2022

A thesis submitted to the
Graduate School
of the
Institute of Science and Technology Austria
in partial fulfillment of the requirements
for the degree of
Doctor of Philosophy

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ISTA Thesis, ISSN: 2663-337X

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Abstract

The scope of this thesis is to study quantum systems exhibiting a continuous symmetry that is broken on the level of the corresponding effective theory. In particular we are going to investigate translation-invariant Bose gases in the mean field limit, effectively described by the Hartree functional, and the Fröhlich Polaron in the regime of strong coupling, effectively described by the Pekar functional. The latter is a model describing the interaction between a charged particle and the optical modes of a polar crystal. Regarding the former, we assume in addition that the particles in the gas are unconfined, and typically we will consider particles that are subject to an attractive interaction. In both cases the ground state energy of the Hamiltonian is not a proper eigenvalue due to the underlying translation-invariance, while on the contrary there exists a whole invariant orbit of minimizers for the corresponding effective functionals. Both, the absence of proper eigenstates and the broken symmetry of the effective theory, make the study significantly more involved and it is the content of this thesis to develop a frameworks which allows for a systematic way to circumvent these issues.

It is a well-established result that the ground state energy of Bose gases in the mean field limit, as well as the ground state energy of the Fröhlich Polaron in the regime of strong coupling, is to leading order given by the minimal energy of the corresponding effective theory. As part of this thesis we identify the sub-leading term in the expansion of the ground state energy, which can be interpreted as the quantum correction to the classical energy, since the effective theories under consideration can be seen as classical counterparts.

We are further going to establish an asymptotic expression for the energy-momentum relation of the Fröhlich Polaron in the strong coupling limit. In the regime of suitably small momenta, this asymptotic expression agrees with the energy-momentum relation of a free particle having an effectively increased mass, and we find that this effectively increased mass agrees with the conjectured value in the physics literature.

In addition we will discuss two unrelated papers written by the author during his stay at ISTA in the appendix. The first one concerns the realization of anyons, which are quasi-particles acquiring a non-trivial phase under the exchange of two particles, as molecular impurities. The second one provides a classification of those vector fields defined on a given manifold that can be written as the gradient of a given functional with respect to a suitable metric, provided that some mild smoothness assumptions hold. This classification is subsequently used to identify those quantum Markov semigroups that can be written as a gradient flow of the relative entropy.

Acknowledgements

Funding from the European Union's Horizon 2020 research and innovation programme under the ERC grant agreement No 694227 is gratefully acknowledged.

About the Author

Morris Brooks completed a MSc at the Technical University of Vienna before joining ISTA in September 2019. His research interests include the mathematical study of physical systems with a large or infinite number of degrees of freedom, especially of those arising in many body quantum physics, with an emphasize on establishing effective theories allowing for a simplified description of such models. Besides the papers written together with his supervisor Robert Seiringer presented in this thesis, Morris worked during his stay at ISTA together with the theoretical physics group of Mikhail Lemeshko on the realization of anyons, leading to a publication in Physical Review Letters, as well as together with Jan Maas on the classification of gradient flows with an application to quantum Markov semigroups.

List of Collaborators and Publications

The thesis contains the following papers that are published, respectively accepted for publication:

- M. Brooks and R. Seiringer. Validity of Bogoliubov's approximation for translation-invariant Bose gases. Accepted for publication in Probability and Mathematical Physics, published by Mathematical Sciences Publishers.
- M. Brooks, E. Yakaboylu, D. Lundholm and M. Lemeshko. Molecular impurities as a realization of anyons on the two-sphere. *Physical Review Letters* 126:015301. ©2021 by the American Physical Society.

as well as the following preprints:

- M. Brooks, and R. Seiringer. The Fröhlich Polaron at Strong Coupling – Part I: The Quantum Correction to the Classical Energy. *arXiv*: 2207.03156.
- M. Brooks, and R. Seiringer. The Fröhlich Polaron at Strong Coupling – Part II: Energy-Momentum Relation and effective Mass. *arXiv*: 2211.03353.
- M. Brooks and J. Maas. Characterisation of gradient flows for a given functional. *arXiv*: 2209.11149.

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CHAPTER 1

Introduction

It is a central observation that the fundamental physical laws are symmetric with respect to the basic transformations of space, or equivalently, according to Noether's theorem, that the total momentum as well as the total angular momentum are conserved under the time evolution. Historically, symmetries and conserved quantities have been an important tool in the mathematical analysis of physical systems, as they allow to reduce the available degrees of freedom. This is especially relevant when it comes to low dimensional systems, where symmetries have been used to identify exact solutions. In this thesis we are concerned with theories that posses a large or infinite number of degrees of freedom instead, where exact solutions are out of reach and effective theories gain relevance. In contrast to low dimensional theories, the presence of continuous symmetries seems to rather complicate the mathematical treatment of the physical systems under consideration, making novel techniques a necessity.

1.1 Translation-invariant Bose gases

The first physical system we shall discuss is an unconfined gas of interacting (bosonic) particles. In the absence of any confinement, like a box or a trapping potential, we will typically assume that the interaction is attractive in order to prevent the gas from diffusing over the whole available space $\mathbb{R}^d$. As a concrete example we will investigate a (bosonic) gas of gravitating particles, which can be considered as a model for a neutral (Bose) star. In quantum physics, a gas of N particles is described by a wave-function $\Psi \in L^2\big(\mathbb{R}^{N\times d}\big)$, where $x = \big(x^{(1)}, \dots, x^{(N)}\big) \in \mathbb{R}^{N\times d}$ contains the coordinate vectors $x^{(j)} \in \mathbb{R}^d$ of the various particles, together with a self-adjoint operator H_N on $L^2\big(\mathbb{R}^{N\times d}\big)$ that encodes the dynamical information of the theory, referred to as the Hamiltonian of the system. In the following we will consider Hamiltonians of the form

$$H_N := \sum_{j=1}^{N} (-\Delta)_j + \frac{1}{N-1} \sum_{j<k} v\left(x^{(j)} - x^{(k)}\right), \tag{1.1.1}$$

where $v : \mathbb{R}^d \longrightarrow \mathbb{R}$ is a given interaction potential and $(-\Delta)_j$ indicates that the Laplace operator Δ acts on the j-th particle in the tensor product $L^2\big(\mathbb{R}^{N\times d}\big) \cong L^2\big(\mathbb{R}^d\big)^{\otimes N}$. Typically we will take v to be negative with $v(x) \underset{|x|\to\infty}{\longrightarrow} 0$, describing an attractive interaction between the particles in the gas, and we use the non-relativistic kinetic energy $-\Delta$ for the sake of concreteness, even though our results are valid for a much larger class of translation invariant operators including the (pseudo) relativistic kinetic energy $\sqrt{m^2-\Delta}$. Due to the mean-field scaling factor $\frac{1}{N-1}$, the interaction term in Eq. (1.1.1) is of the same order of magnitude as the kinetic energy, which gives rise to complex phenomena as a consequence of the competition between the two contributions to the total energy. We further want to emphasize that the interaction term $\frac{1}{N-1}\sum_{j<k} v\left(x^{(j)}-x^{(k)}\right)$ in Eq. (1.1.1) only depends on the relative position of the particles to each other, and consequently H_N is invariant under the group of translations in space $(x^{(1)},\dots,x^{(N)})\mapsto(x^{(1)}+v,\dots,x^{(N)}+v)$, where $v\in\mathbb{R}^d$. Equivalently, the total momentum $\mathbb{P}:=\sum_{j=1}^N \frac{1}{i}\nabla_j$ commutes with the Hamiltonian H_N, i.e. $[H_N,\mathbb{P}]=0$, and is therefore conserved under the time evolution $U_t:=e^{itH_N}$.

Regarding Bose gases, we are primarily concerned with the behaviour of the ground state energy of the Hamiltonian H_N in the parameter regime where the number of particles N in the gas goes to infinity, i.e. we take an interested in the quantity

$$E_N:=\inf_{\Psi:\|\Psi\|=1}\langle H_N\rangle_\Psi\,, \tag{1.1.2}$$

in the limit $N\to\infty$. To be more precise we shall establish an asymptotic two term expansion of the form $E_N=Na+b+o_{N\to\infty}(1)$, where $a,b\in\mathbb{R}$ are (rather) explicit constants. Since the infimum in Eq. (1.1.2) is reached by permutation symmetric $\Psi:\mathbb{R}^{N\times d}\longrightarrow\mathbb{C}$ only, which we will refer to as bosonic wave-functions, we shall restrict ourself to such elements $\Psi\in L^2_{\mathrm{sym}}\big(\mathbb{R}^{N\times d}\big)\cong L^2\big(\mathbb{R}^d\big)^{\otimes_s N}$ in the following, where $\otimes_s$ denotes the symmetric tensor product. Based on the large dimension of the space $\mathbb{R}^{N\times d}$, finding an exact expression for the ground state energy E_N seems to be out of reach and it becomes necessary to introduce an effective theory. A suitable effective theory can be derived by restricting the test functions Ψ to a specific sub-manifold of $L^2_{\mathrm{sym}}(\mathbb{R}^{N\times d})$. In the case of a Bose gas, the most natural permutation symmetric N particle test functions are considered to be pure product states $\Psi:=u^{\otimes N}$ with $u\in L^2\big(\mathbb{R}^d\big)$ satisfying $\|u\|=1$. Due to the mean-field factor $\frac{1}{N-1}$ in front of the interaction v, and the absence of any scaling factor in the argument of v, the energy of such a test function is proportional to N, which leads to the definition of the Hartree functional

$$\mathcal{E}_{\mathrm{H}}[u]:=\frac{1}{N}\langle H_N\rangle_{u^{\otimes N}}=\int|\nabla_x u|^2\mathrm{d}x+\frac{1}{2}\int\int|u(x)|^2v(x-y)|u(y)|^2\mathrm{d}x\mathrm{d}y.$$

Clearly we obtain an upper bound on the ground state energy E_N by

$$\frac{1}{N}E_N\leqslant\inf_{u:\|u\|=1}\mathcal{E}_{\mathrm{H}}[u]=:e_{\mathrm{H}}.$$

A less trivial but well-established result is that the upper bound e_{H} is asymptotically correct in the regime of large N, i.e. it is known that the ground state energy E_N is to leading order given by $E_N=Ne_{\mathrm{H}}+o_{N\to\infty}(N)$, see [71]. In the presence of a confining box or trapping potential, it is even known that the ground state Ψ_{GS}, characterized (up to a phase) by $\langle H_N\rangle_\Psi=E_N$ and $\|\Psi_{\mathrm{GS}}\|=1$, is close to the pure product $\Psi_{\mathrm{GS}}\approx u_0^{\otimes N}$ in a suitable topology, where u_0 is characterized (up to a phase) by $\mathcal{E}_{\mathrm{H}}[u_0]=e_H$ and $\|u_0\|=1$. As we will argue in the subsequent paragraph, this picture is no longer valid in the translation invariant setting studied in this thesis.

In order to understand the action of a continuous symmetry group on a quantum theory, it is usually useful to find a fibre representation first, i.e. we want to find an identification

$L^2_{\mathrm{sym}}(\mathbb{R}^{N\times d}) \cong L^2\big(\mathbb{R}^d, \mathcal{H}_N\big)$, where $\mathcal{H}_N$ is a suitable Hilbert space, as well as a collection of operators $\{H_N(p) : p \in \mathbb{R}^d\}$ defined on $\mathcal{H}_N$, such that the action of H_N reads $(H_N\Psi)_p = H_N(p)\Psi_p$ and the action of the total momentum operator is given by $(\mathbb{P}\Psi)_p = p\Psi_p$. In the case of a N particle gas, such a fibration can naturally be realized using the vector space of relative coordinates $X_N := \big\{x \in \mathbb{R}^{N\times d} : \sum_{j=1}^N x^{(j)} = 0\big\}$. With the notation $\nabla_{j,k} := \nabla_j - \nabla_k$ at hand, we can rewrite H_N as

$$H_N = \frac{1}{N}\mathbb{P}^2 - \frac{1}{2N}\sum_{j,k=1}^N \nabla_{j,k}^2 + \frac{1}{N-1}\sum_{j<k} v\left(x^{(j)} - x^{(k)}\right),$$

where $-\frac{1}{2N}\sum_{j,k=1}^N \nabla_{j,k}^2 + \frac{1}{N-1}\sum_{j<k} v\left(x^{(j)} - x^{(k)}\right)$ can naturally be seen as an operator acting on $L^2_{\mathrm{sym}}(X_N)$. Defining an identification of the spaces $L^2_{\mathrm{sym}}(\mathbb{R}^{N\times d}) \cong L^2\big(\mathbb{R}^d, L^2_{\mathrm{sym}}(X_N)\big)$ as $\Psi_p(x^{(1)}, \ldots, x^{(N)}) := \left(\frac{\sqrt{N}}{2\pi}\right)^{\frac{d}{2}} \int_{\mathbb{R}^d} e^{-ipy}\Psi(x^{(1)} + y, \ldots, x^{(N)} + y)\,\mathrm{d}y$ therefore yields the desired fibration with the fibre Hamiltonian

$$H_N(p) := \frac{|p|^2}{N} - \frac{1}{2N}\sum_{j,k=1}^N \nabla_{j,k}^2 + \frac{1}{N-1}\sum_{j<k} v\left(x^{(j)} - x^{(k)}\right)$$

acting on $L^2_{\mathrm{sym}}(X_N)$. As an immediate consequence we observe that the joint spectrum $\sigma(\mathbb{P}, H_N)$ is given by the union of the parabolas $E = \frac{|p|^2}{N} + \lambda$ with $\lambda \in \sigma(H_N(0))$, a property which follows from the Galilean invariance of the non-relativistic kinetic energy. Furthermore, assuming that $H_N(0)$ has a ground state Ψ_{rel} in $L^2_{\mathrm{sym}}(X_N)$, the ground state of H_N in $L^2\big(\mathbb{R}^d, L^2_{\mathrm{sym}}(X_N)\big)$ is formally given by $p \mapsto \delta_0(p)\Psi_{\mathrm{rel}}$, which corresponds to the function $\Psi_{\mathrm{GS}}(x^{(1)}, \ldots, x^{(N)}) := \left(\frac{1}{2\pi}\right)^{\frac{d}{2}} \Psi_{\mathrm{rel}}\big(x^{(1)} - \bar{x}, \ldots, x^{(N)} - \bar{x}\big)$, with $\bar{x} := \frac{1}{N}\sum_{j=1}^N x^{(j)}$, according to our identification $L^2_{\mathrm{sym}}(\mathbb{R}^{N\times d}) \cong L^2\big(\mathbb{R}^d, L^2_{\mathrm{sym}}(X_N)\big)$. Clearly Ψ_{GS} is non-zero and translation invariant, i.e. $\Psi_{\mathrm{GS}}(x^{(1)} + y, \ldots, x^{(N)} + y) = \Psi_{\mathrm{GS}}(x^{(1)}, \ldots, x^{(N)})$ for all $y \in \mathbb{R}^d$, which in particular means that Ψ_{GS} does not have a finite L^2 norm and $\inf \sigma(H_N)$ is therefore not a proper eigenvalue. Furthermore this means that Ψ_{GS} cannot be close to a product state, since $u^{\otimes N}$, as an L^2 function, is localized in space while Ψ_{GS} is constant along every (non-compact) orbit $\{(x^{(1)} + y, \ldots, x^{(N)} + y) : y \in \mathbb{R}^d\}$.

Since the fiber Hamiltonian $H_N(0)$ contains all the spectral information of the original Hamiltonian H_N, it is tempting to analyse the operator $H_N(0)$ instead of H_N, especially when we consider that $H_N(0)$ might have a proper ground state and that we are effectively removing d degrees of freedom by freezing the total momentum coordinate $p = 0$. However we believe that the fibration in terms of relative coordinates is not beneficial when it comes to the large N asymptotics of the ground state energy, as we are not aware of a natural notion of products states in the L^2 space over the vector space of relative coordinates X_N, and therefore it is not even clear how to recover the leading order asymptotics $E_N \approx Ne_{\mathrm{H}}$, originally obtained by a restriction to pure products.

We have seen so far that there is no straightforward way of comparing the ground state Ψ_{GS}, respectively its fibre counterpart Ψ_{rel}, with the pure product state $u^{\otimes N}$. We circumvent this issue by relaxing our definition of a ground state, to be precise we say that a sequence of states Ψ_N is an approximate ground state in case $\langle H_N\rangle_{\Psi_N} = E_N + o_{N\to\infty}(1)$. Since we are interested in the two term expansion of the ground state energy $E_N = Ne_{\mathrm{H}} + b + o_{N\to\infty}(1)$, where $b \in \mathbb{R}$ is a (rather) explicit constant, our definition of an approximate ground state uses indeed the correct scale. In contrast to the exact ground state, it is possible to construct an approximate ground state which is close to the product state $u_0^{\otimes N}$, where u_0 is a minimizer of the Hartree functional $\mathcal{E}_{\mathrm{H}}$. By the translation-invariance of H_N, it is clear that the Hartree functional $\mathcal{E}_{\mathrm{H}}$ is translation-invariant as well and therefore $u_y \in L^2\big(\mathbb{R}^d\big)$ defined as $u_y(x) := u_0(x-y)$ is again a minimizer of $\mathcal{E}_H$. As a consequence we can assume w.l.o.g. that u_0 is centred around the origin in the sense that $\int_{x_i<0} |u_0(x)|^2 \mathrm{d}x = \int_{x_i>0} |u_0(x)|^2 \mathrm{d}x = \frac{1}{2}$ for all $i \in \{1, \dots, d\}$. In the following we will break the translation-invariance of the true ground state Ψ_{GS} in order to construct an approximate ground state Ψ_N that is confined around the origin as well.

In the light of the relative-coordinate fibration, it seems to be natural to construct an approximate ground state by localizing the center of mass coordinate $\bar{x} = \frac{1}{N}\sum_{j=1}^N x^{(j)}$, such that $|\bar{x}| \leqslant \kappa_N \ll 1$ for all $x \in \operatorname{supp}(\Psi_N)$. However it turns out that this property is insufficient to conclude $\Psi_N \approx u_0^{\otimes N}$, as we shall illustrate in the subsequent paragraph. Let us first specify the notion $\Psi_N \approx \widetilde{\Psi}_N$ as being equivalent to

$$\left|\big\langle B_k \otimes_s \mathbb{1}^{\otimes(N-k)}\big\rangle_{\Psi_N} - \big\langle B_k \otimes_s \mathbb{1}^{\otimes(N-k)}\big\rangle_{\widetilde{\Psi}_N}\right| \underset{N\to\infty}{\longrightarrow} 0$$

for all bounded k particle operators B_k. In case $\widetilde{\Psi}_N = u^{\otimes N}$, we will also refer to this as (complete) Bose-Einstein condensation with respect to u. In order to illustrate that a center of mass localization is insufficient, let us define the test function $\Psi_N(x^{(1)}, \dots, x^{(N)}) := u_t(x^{(1)}) \cdots u_t(x^{(N-1)}) g\left(\frac{\bar{x}}{\kappa_N}\right)$ for $t \neq 0$. Clearly the center of mass $\bar{x}$ is localized around the origin for $\kappa_N \ll 1$. However since Ψ_N contains a factor u_t in every component except the last one, it is easy to show that $\Psi_N \approx u_t^{\otimes N}$ as long as $\frac{1}{N} \ll \kappa_N$, which especially in particular means that Ψ_N cannot be close to $u_0^{\otimes N}$. We conclude that the center of mass is not the right statistical quantity for our localization procedure.

As it turns out, the median, respectively a hybrid between the median and the center of mass, is a more robust statistical quantity. In order to see this, let us assume $d = 1$ for the sake of simplicity and let Ψ_N be a (permutation symmetric) test function having a median localized around the origin. To be precise, let us assume that for any $x \in \operatorname{supp}(\Psi_N)$, there are at least $(\frac{1}{2} - \epsilon_N)N$ particles satisfying $x^{(j)} \leqslant \epsilon_N$ and at least $(\frac{1}{2} - \epsilon_N)N$ particles satisfying $x^{(j)} \geqslant -\epsilon_N$, where $\epsilon_N \ll 1$. As an immediate consequence we obtain $\lim_{N\to\infty} \langle \mathbb{1}_{x^{(1)}\leqslant\epsilon_N} \mathbb{1}_{x^{(2)}\geqslant-\epsilon_N}\rangle_{\Psi_N} = \frac{1}{4}$. This however means that Ψ_N cannot be close to $u_t^{\otimes N}$ for $t \neq 0$, since this would imply

$$\lim_{N\to\infty} \langle \mathbb{1}_{x^{(1)}\leqslant\epsilon_N} \mathbb{1}_{x^{(2)}\geqslant-\epsilon_N}\rangle_{\Psi_N} = \int_{x\leqslant t} |u_0(x)|^2 \mathrm{d}x \left(1 - \int_{x\leqslant t} |u_0(x)|^2 \mathrm{d}x\right) = \frac{1}{4}$$

and hence $\int_{x\leqslant t} |u_0(x)|^2 \mathrm{d}x = \frac{1}{2}$, which is a contradiction to our assumptions $t \neq 0$ and $\int_{x\leqslant 0} |u_0(x)|^2 \mathrm{d}x = \frac{1}{2}$, given that $u_0 > 0$. The concrete construction of a Ψ_N having a localized median, the corresponding estimate on the energy penalty and the proof that Ψ_N indeed satisfies Bose-Einstein condensation $\Psi_N \approx u_0^{\otimes N}$ can be found in Chapter 2. Having an approximate ground state Ψ_N at hand will be a central prerequisite in establishing the two term expansion $E_N = N e_{\mathrm{H}} + b + o_{N\to\infty}(1)$, as we shall explain in the following.

In order to identify the sub-leading term in the expansion of E_N it is useful to recast the Hamiltonian H_N in the language of second quantization. For this purpose let us define the Fock space over a given Hilbert space $\mathcal{H}$ as the direct sum $\mathcal{F}(\mathcal{H}) := \bigoplus_{n=0}^\infty \mathcal{H}^{\otimes_s n}$ and let us define for any element $f \in \mathcal{H}$ the creation operator $a^\dagger(f)$ on $\mathcal{F}(\mathcal{H})$ as

$$a^\dagger(f)\Psi := \sqrt{h(n+1)}\, f \otimes_s \Psi \tag{1.1.3}$$

for all $\Psi \in \mathcal{H}^{\otimes_s n}$, where $h > 0$ is a given constant. Furthermore we denote the adjoint operator as $a(f)$ and refer to it as the annihilation operator. It can easily be checked that creation and annihilation operators satisfy the (rescaled) canonical commutation relations $[a(f), a^\dagger(g)] = h \langle f|g\rangle_{\mathcal{H}}$. In the following we choose $\mathcal{H} := L^2\big(\mathbb{R}^d\big)$ and $h := \frac{1}{N}$, and we introduce the shorthand notation $a_j := a(f_j)$, where $\{f_j : j \in \mathbb{N}\}$ is a basis of $L^2\big(\mathbb{R}^d\big)$, which allows us to express the Hamiltonian H_N as

$$\frac{1}{N} H_N = \sum_{j,k=0}^{\infty} \langle f_j| - \Delta|f_k\rangle \, a_j^\dagger a_k + \frac{N}{2(N-1)} \sum_{i,j,k,\ell=0}^{\infty} \langle f_i \otimes f_j|\widehat{v}|f_k \otimes f_\ell\rangle \, a_i^\dagger a_j^\dagger a_k a_\ell,$$

where we denote $\widehat{v}$ as the two body multiplication operator by $v(x-y)$. Furthermore we can naturally express the fact that Ψ_N satisfies Bose-Einstein condensation $\Psi_N \approx u_0^{\otimes N}$ in the language of second quantization. For this purpose, let us assume that the first basis element is given by $f_0 := u_0$. Since $a_0^\dagger a_0$, restricted to $L^2\big(\mathbb{R}^d\big)^{\otimes_s N}$, is given by $|u_0\rangle\langle u_0| \otimes_s \mathbb{1}^{\otimes(N-1)}$, Bose-Einstein condensation immediately implies $\langle a_0^\dagger a_0\rangle_{\Psi_N} = 1 + o_{N\to\infty}(1)$ by definition, or equivalently $\langle \mathcal{N}_+\rangle_{\Psi_N} = o_{N\to\infty}(1)$ with $\mathcal{N}_+ := \sum_{j=1}^\infty a_j^\dagger a_j$. Heuristically, this means that we should think of the modes a_j with $j \geqslant 1$ as being small, while we do not have sufficient information to determine the value of a_0.

Making use of the fact that the number of particles

$$\mathcal{N} := \sum_{j=0}^{\infty} a_j^\dagger a_j \tag{1.1.4}$$

is fixed to $\mathcal{N} = N$ and the observation that H_N is gauge invariant, i.e. H_N stays invariant under the transformation $a_j \mapsto e^{i\theta} a_j$ with $\theta \in \mathbb{R}$, we see that one of the degrees of freedom in our problem is redundant. Following the approach presented in [72], we can make this statement rigorous by applying a unitary transformation U_N, referred to as the excitation map. This map removes the dependence of the Hamiltonian H_N on the zero mode a_0 by eliminating the particle number constraint, and it is defined as

$$U_N \left(u_0^{\otimes i_0} \otimes_{\mathrm{s}} u_1^{\otimes i_1} \otimes_{\mathrm{s}} \cdots \otimes_{\mathrm{s}} u_m^{\otimes i_m}\right) := u_1^{\otimes i_1} \otimes_{\mathrm{s}} \cdots \otimes_{\mathrm{s}} u_m^{\otimes i_m} \tag{1.1.5}$$

for non-negative integers $i_0 + \cdots + i_m = N$, mapping $L^2\big(\mathbb{R}^d\big)^{\otimes_s N}$ into the Fock space $\mathcal{F}\left(\{u_0\}^\perp\right)$ over modes orthogonal to u_0. It is an easy exercise to check that $\mathcal{N}_+$ stays invariant under the excitation map, and therefore Bose-Einstein condensation implies $\langle \mathcal{N}_+\rangle_{U_N \Psi_N} = o_{N\to\infty}(1)$.

Regarding the Hartree theory $\mathcal{E}_H$ we can get rid of the norm constraint $\|u\| = 1$ in a similar fashion, by making use of the map $z \mapsto \iota(z) := \sqrt{1 - \|z\|^2}\, u_0 + z$, defined for $z \in \{u_0\}^\perp$ satisfying $\|z\| \leqslant 1$, leading to the study of the transformed functional $z \mapsto \mathcal{E}_H[\iota(z)]$. Since $\iota(0) = u_0$ is a minimizer of $\mathcal{E}_H$, i.e. $\mathcal{E}_H[\iota(z)] = e_{\mathrm{H}}$, we obtain by a formal Taylor expansion

$$\mathcal{E}_H[\iota(z)] = e_{\mathrm{H}} + \sum_{j,k=1}^{\infty} \left(Q_{j,k}\overline{z}_j z_k + \overline{G}_{j,k} z_j z_k + G_{j,k}\overline{z}_j \overline{z}_k\right) + o\left(\sum_{j=1}^{\infty} \overline{z}_j z_j\right), \tag{1.1.6}$$

where $z_j := \langle f_j|z\rangle$, $Q_{j,k} := \frac{1}{2}\left(\partial_{\mathfrak{Re} z_j} - i\partial_{\mathfrak{Im} z_j}\right)\left(\partial_{\mathfrak{Re} z_k} + i\partial_{\mathfrak{Im} z_k}\right)|_{z=0}\mathcal{E}_H[\iota(z)]$ and $G_{j,k} := \frac{1}{2}\left(\partial_{\mathfrak{Re} z_j} - i\partial_{\mathfrak{Im} z_j}\right)\left(\partial_{\mathfrak{Re} z_k} - i\partial_{\mathfrak{Im} z_k}\right)|_{z=0}\mathcal{E}_H[\iota(z)]$. As we demonstrate in Chapter 2, the map ι and the excitation map U_N share similar properties, which enables us to use the same Taylor expansion as in Eq. (1.1.6) for the transformed operator $U_N H_N U_N^{-1}$ as well, i.e. one can verify that

$$\frac{1}{N} U_N H_N U_N^{-1} = e_{\mathrm{H}} + \sum_{j,k=1}^{\infty} \left(Q_{j,k} a_j^\dagger a_k + \overline{G}_{j,k} a_j a_k + G_{j,k} a_j^\dagger a_k^\dagger \right) + o\left(\sum_{j=1}^{\infty} a_j^\dagger a_j \right), \quad (1.1.7)$$

where $o\left(\sum_{j=1}^{\infty} a_j^\dagger a_j\right)$ is a symbolic expression for terms which are at least cubic in the operators $\{a_j : j \geqslant 1\}$. Since our approximate ground state satisfies Bose-Einstein condensation, i.e. since we think of the modes a_j as being small, we expect terms of higher order to be negligible, leading to the two term expansion of the energy $E_N \approx N e_{\mathrm{H}} + b$ with $b := \inf \sigma(\mathbb{H})$ and the Bogoliubov operator defined as $\mathbb{H} := N \sum_{j,k=1}^{\infty} \left(Q_{j,k} a_j^\dagger a_k + \overline{G}_{j,k} a_j a_k + G_{j,k} a_j^\dagger a_k^\dagger \right)$. Note that $\mathbb{H}$ is indeed independent of N due to the scaling in the commutation relations $[a(f), a^\dagger(g)] = \frac{1}{N} \langle f | g \rangle$. This approach of establishing the two term expansion of the ground state energy has been carried out in [72] for Bose gases that are confined by a box or a trapping potential.

A central tool in [72] is an operator inequality of the form $\sum_{j=1}^{\infty} a_j^\dagger a_j \lesssim \frac{1}{N} \mathbb{H}$, which allows one to absorb the error term $o\left(\sum_{j=1}^{\infty} a_j^\dagger a_j\right)$ in Eq. (1.1.7) by the quadratic part $\mathbb{H}$. In the translation-invariant setting such an operator inequality is no longer possible, since the quadratic part $\mathbb{H}$ is degenerate in the directions $f_1 := \frac{\partial_{x_1} u_0}{\|\partial_{x_1} u_0\|}, \dots, f_d := \frac{\partial_{x_d} u_0}{\|\partial_{x_d} u_0\|}$ and therefore we can only absorb terms which are small compared to $\sum_{j=d+1}^{\infty} a_j^\dagger a_j$. We circumvent this issue by applying yet another unitary transformation $\mathcal{W}_N$ to our Hamiltonian as well as a corresponding transformation F to our effective theory. Essentially, F flattens the manifold of minimizers corresponding to $z \mapsto \mathcal{E}_{\mathrm{H}}[\iota(z)]$, which leads to the improved Taylor expansion

$$\mathcal{E}_H[\iota(F(z))] = e_{\mathrm{H}} + \sum_{j,k=1}^{\infty} \left(Q_{j,k} \overline{z}_j z_k + \overline{G}_{j,k} z_j z_k + G_{j,k} \overline{z}_j \overline{z}_k \right) + o\left(\sum_{j=d+1}^{\infty} \overline{z}_j z_j \right).$$

Again, $\mathcal{W}_N$ and F share similar properties, which we use in order to obtain an improved Taylor expansion of the Hamiltonian

$$\frac{1}{N} \mathcal{W}_N U_N H_N U_N^{-1} \mathcal{W}_N^{-1} = e_{\mathrm{H}} + \frac{1}{N} \mathbb{H} + o\left(\sum_{j=d+1}^{\infty} a_j^\dagger a_j \right).$$

Absorbing the residuum $o\left(\sum_{j=d+1}^{\infty} a_j^\dagger a_j\right)$ by the quadratic part $\mathbb{H}$, then allows us to establish the two term expansion of the ground state energy $E_N = N e_{\mathrm{H}} + \inf \sigma(\mathbb{H}) + o_{N \to \infty}(1)$.

1.2 The Fröhlich Polaron at Strong Coupling

The second physical system we shall discuss is the Fröhlich Polaron, which is a model for a charged particle, say an electron, interacting with a polarizable medium. The medium itself is a crystal made of initially neutral particles, which become dipoles due to the electric field of the charged particle travelling through the crystal. In the Fröhlich theory, the lattice spacing is assumed to be vanishingly small, allowing for a continuous description of the crystal by a polarization field $y \mapsto \Phi(y)$, which measures the electric dipole moment of the medium at a given point in space $y \in \mathbb{R}^3$. Mathematically the Fröhlich polaron, which is a quasiparticle consisting of the electron and a cloud of excitations of the polarization field attached to it, is described by the Hamiltonian

$$\mathbb{H} := -\Delta_x + \mathcal{N} - a\left(w_x\right) - a^\dagger\left(w_x\right) \tag{1.2.1}$$

acting on the Hilbert space $L^2(\mathbb{R}^3) \otimes \mathcal{F}\left(L^2(\mathbb{R}^3)\right)$, where Δ_x is the Laplace operator on the Hilbert space of the electron $L^2(\mathbb{R}^3)$ and x is the position of the electron, the creation and annihilation operators a and $a^\dagger$ are defined in Eq. (1.1.3) with $h := \frac{1}{\alpha^2}$ acting on the Hilbert space $\mathcal{F}\left(L^2(\mathbb{R}^3)\right)$, the corresponding particle number operator $\mathcal{N}$ is defined in Eq. (1.1.4) and the interaction $w_x : \mathbb{R}^3 \longrightarrow \mathbb{R}$ is given by $w_x(y) := \frac{1}{\pi^{\frac{3}{2}}|y-x|^2}$. Regarding the physical interpretation, $-\Delta_x$ is the kinetic energy of the electron and the particle number operator $\mathcal{N}$ represents the internal energy of the polarization field $\Phi(x) := \frac{1}{2}\left(a_x + a_x^\dagger\right)$, where a_x is a symbolic expression for the distribution $a(f) = \int_{\mathbb{R}^3} \overline{f(x)} a_x \mathrm{d}x$. The last terms in Eq. (1.2.1) model the interaction between the electron, living in the Hilbert space $L^2(\mathbb{R}^3)$, and the polarization field, living in the Hilbert space $\mathcal{F}\left(L^2(\mathbb{R}^3)\right)$, where the constant $\alpha > 0$ appearing in the canonical commutation relations $[a(f), a^\dagger(g)] = \frac{1}{\alpha^2}\langle f|g\rangle$ is interpreted as the interaction strength between the charged particle and the medium. We want to emphasize that the interaction

$$a\left(w_x\right) + a^\dagger\left(w_x\right) = \frac{2}{\pi^{\frac{3}{2}}} \int_{\mathbb{R}^3} \frac{\Phi(y)}{|x-y|^2} \mathrm{d}y$$

only depends on the relative position between the electron and the argument y of the field operator $\Phi(y)$, and consequently the operator $\mathbb{H}$ is invariant under the group of translations in space $\{\mathcal{T}_y : y \in \mathbb{R}^3\}$, characterized (up to a phase) by the transformation laws $x \mapsto x + y$, $\frac{1}{i}\nabla_x \mapsto \frac{1}{i}\nabla_x$ and $a_x \mapsto a_{x-y}$, which in particular implies $\Phi(x) \mapsto \Phi(x-y)$. Since the group of translations is generated by the total momentum operators $\mathbb{P} = (\mathbb{P}_1, \mathbb{P}_2, \mathbb{P}_3)$ defined as

$$\mathbb{P} := \frac{1}{i}\nabla + \alpha^2 \int_{\mathbb{R}^3} k\, a_k^\dagger a_k \mathrm{d}k,$$

where we use the standard notation $\int_{\mathbb{R}^3} g(k) a_k^\dagger a_k \mathrm{d}k$ as a symbolic expression for the operator $\sum_{n,m=1}^\infty \left\langle f_n \middle| g\left(\frac{1}{i}\nabla\right) \middle| f_m \right\rangle a^\dagger(f_n) a(f_m)$ and $\{f_n : n \geqslant 1\}$ is an orthonormal basis of $L^2(\mathbb{R}^3)$, the translation invariance of the Hamiltonian $\mathbb{H}$ can equivalently be expressed as $[\mathbb{H}, \mathbb{P}] = 0$, making the total momentum $\mathbb{P}$ a conserved quantity under the time evolution generated by $\mathbb{H}$.

Regarding the polaron we are primarily interested in the low energy properties of $\mathbb{H}$ in the regime of large coupling α between the electron and the polarizable medium. The first main result, presented in Chapter 3, identifies the two term expansion of the ground state energy $E_\alpha := \inf \sigma(\mathbb{H})$ in the asymptotics of large α and the second main result, presented in Chapter 4, establishes an asymptotic expression for the energy-momentum relation $E_\alpha(P)$, defined as $E_\alpha(P) := \inf \sigma|_{\mathbb{P}=P}(\mathbb{H})$ with $\sigma|_{\mathbb{P}=P}(\mathbb{H}) := \{E : (P, E) \in \sigma(\mathbb{P}, \mathbb{H})\}$. Since the translation group is shifting the electron as well as the polarization field, but not the medium itself, our theory is not fully Galilean invariant and therefore one can not expect the joint spectrum $\sigma(\mathbb{P}, \mathbb{H})$ to consist of parabolas, as it was the case for the translation-invariant (non-relativistic) Bose gas, making it an interesting object to study. In particular we confirm that, asymptotically, the energy-momentum relation $E_\alpha(P)$ of a polaron coincides with the one of a free particle having an effectively increased mass which scales like α^4 in the limit of large α, which is a well known conjecture from 1948 in the physics literature due to Landau and Pekar [63], however a rigorous mathematical proof has so far been out of reach.

Again our methods rely on the usage of an effective theory that arises as a restriction to a suitable manifold of test functions. In the case of the polaron, a suitable manifold is given by states of the form $\Psi = \psi \otimes \Omega_\varphi$, where $\psi \in L^2(\mathbb{R}^3)$ is an electron wave-function satisfying $\|\psi\| = 1$ and Ω_φ is a coherent state with basis $\varphi \in L^2(\mathbb{R}^3)$ characterized (up to a phase) by $a(f)\Omega_\varphi = \langle f|\varphi\rangle \Omega_\varphi$ and $\|\Omega_\varphi\| = 1$, i.e. Ω_φ is an eigenvector of the annihilation operator $a(f)$ to the eigenvalue $\langle f|\varphi\rangle$. The expectation value of $\mathbb{H}$ with respect to such a state turns out to be independent of α, leading us to the definition of the Pekar energy functional

$$\mathcal{E}(\psi,\varphi) := \langle \mathbb{H}\rangle_{\psi\otimes\Omega_\varphi} = \int_{\mathbb{R}^3} |\nabla_x \psi|^2 \mathrm{d}x + \int_{\mathbb{R}^3} |\varphi(y)|^2 \mathrm{d}y - \frac{2}{\pi^{\frac{3}{2}}} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|\psi(x)|^2 \mathfrak{Re}\varphi(y)}{|x-y|^2} \mathrm{d}y\mathrm{d}x.$$

We clearly have the upper bound $E_\alpha \leqslant \inf_\varphi \inf_{\psi:\|\psi\|=1} \mathcal{E}(\psi,\varphi) =: e^{\mathrm{Pek}}$. Furthermore it has been established in [1, 29, 79] that this upper bound is sharp in the asymptotics of large α, i.e. we have $E_\alpha = e^{\mathrm{Pek}} + o_{\alpha\to\infty}(1)$.

In order to identify the subleading term in the energy expansion $E_\alpha = e^{\mathrm{Pek}} + o_{\alpha\to\infty}(1)$ we first introduce a finite dimensional version of $\mathbb{H}$ as

$$\mathbb{H}_{\mathrm{fin}} := -\Delta_x + \sum_{n=1}^N a_n^\dagger a_n - \sum_{n=1}^N \langle f_n|w_x\rangle \left(a_n + a_n^\dagger\right),$$

where $\{f_n : n \in \{1,\dots,N\}\}$ is a real-valued orthonormal basis of a suitable finite dimensional subspace $X_{\mathrm{fin}} \subseteq L^2(\mathbb{R}^3)$ and we define $a_n := a(f_n)$ as usual. Due to the ultraviolet regularization techniques developed in [40] we have $|E_\alpha - E_{\alpha,\mathrm{fin}}| \ll \alpha^{-2}$ with $E_{\alpha,\mathrm{fin}} := \inf \sigma(\mathbb{H}_{\mathrm{fin}})$, and hence it is enough to establish the two term expansion for the energy $E_{\alpha,\mathrm{fin}}$ of the regularized model. Following the methods in [40] we can furthermore eliminate the electronic degrees of freedom for a lower bound. Let us first identify the Fock space $\mathcal{F}(X_{\mathrm{fin}})$ over the finite collection of modes $a_1,\dots,a_N$ with $L^2\left(\mathbb{R}^N\right)$ such that the annihilation operators read $a_n = \lambda_n + \frac{1}{2\alpha^2}\partial_{\lambda_n}$ with $\lambda = (\lambda_1,\dots,\lambda_N) \in \mathbb{R}^N$. According to this identification we obtain

$$\begin{aligned}\mathbb{H}_{\mathrm{fin}} &= -\Delta_x + V_\lambda(x) + \sum_{n=1}^N a_n^\dagger a_n \geqslant \inf\sigma\left(-\Delta + V_\lambda\right) + \sum_{n=1}^N a_n^\dagger a_n \\ &= -\frac{1}{4\alpha^4}\sum_{n=1}^N \partial_{\lambda_n}^2 + \inf\sigma\left(-\Delta + V_\lambda\right) + \sum_{n=1}^N \lambda_n^2 - \frac{N}{2\alpha^2}\end{aligned} \tag{1.2.2}$$

with $V_\lambda(x) := -2\sum_{n=1}^N \langle f_n|w_x\rangle \lambda_n$, where we have used that $\lambda_n = \frac{1}{2}\left(a_n + a_n^\dagger\right)$. Similarly we can eliminate the dependence on the electronic degrees of freedom in the effective energy functional $\mathcal{E}$, leading to the study of the Pekar functional

$$\mathcal{F}^{\mathrm{Pek}}(\varphi) := \inf_{\|\psi\|=1} \mathcal{E}(\psi,\varphi) = \inf\sigma\left(-\Delta + V_\lambda\right) + \int_{\mathbb{R}^3} |\varphi(x)|^2 \mathrm{d}x$$

with $\lambda_n := \frac{1}{2}\left(\varphi_n + \overline{\varphi}_n\right)$ and $\varphi_n := \langle f_n|\varphi\rangle$. In order to emphasize the structural similarity between the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$ and the right hand side of Eq. (1.2.2) note that we can write $\int_{\mathbb{R}^3} |\varphi(x)|^2 \mathrm{d}x = \sum_{n=1}^N \lambda_n^2$ for $\varphi = \sum_{n=1}^N \lambda_n f_n$, and by a (formal) Taylor expansion of $\mathcal{F}^{\mathrm{Pek}}$ around a minimizer φ^{Pek} we obtain

$$\mathcal{F}^{\mathrm{Pek}}(\varphi) = e^{\mathrm{Pek}} + \sum_{i,j=1}^N H_{i,j}^{\mathrm{Pek}}(\lambda_i - \lambda_i^{\mathrm{Pek}})(\lambda_j - \lambda_j^{\mathrm{Pek}}) + o\left(|\lambda - \lambda^{\mathrm{Pek}}|^2\right)$$

with $H_{i,j}^{\mathrm{Pek}} := \frac{1}{2}\partial_{\mathfrak{Re}\varphi_i}\partial_{\mathfrak{Re}\varphi_j}\mathcal{F}^{\mathrm{Pek}}$ and $\lambda_j^{\mathrm{Pek}} := \langle f_j|\varphi^{\mathrm{Pek}}\rangle$. Consequently we have, at least formally, the lower bound

$$\mathbb{H}_{\mathrm{fin}} \geqslant e^{\mathrm{Pek}} - \frac{1}{4\alpha^4}\sum_{n=1}^{N}\partial_{\lambda_n}^2 + \sum_{i,j=1}^{N} H_{i,j}^{\mathrm{Pek}}(\lambda_i - \lambda_i^{\mathrm{Pek}})(\lambda_j - \lambda_j^{\mathrm{Pek}}) - \frac{N}{2\alpha^2} + o\left(|\lambda - \lambda^{\mathrm{Pek}}|^2\right). \quad (1.2.3)$$

Since the operator $-\frac{1}{4\alpha^4}\sum_{n=1}^{N}\partial_{\lambda_n}^2 + \sum_{i,j=1}^{N} H_{i,j}^{\mathrm{Pek}}(\lambda_i - \lambda_i^{\mathrm{Pek}})(\lambda_j - \lambda_j^{\mathrm{Pek}}) - \frac{N}{2\alpha^2}$ is, up to a shift in λ, a collection of harmonic oscillators, we can identify its ground state energy explicitly as $-\frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right]$, leading to the conjectured two term expansion of the ground state energy $E_\alpha = e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + o_{\alpha\to\infty}\left(\frac{1}{\alpha^2}\right)$.

In order to verify this conjecture, we have to make sure that the residuum $o\left(|\lambda - \lambda^{\mathrm{Pek}}|^2\right)$ is small compared to the quadratic part in Eq. (1.2.3), i.e. we need the a priori information that λ is close to λ^{Pek}. Following the strategy previously developed for the mathematical treatment of translation-invariant Bose gases, we first construct an approximate ground state Ψ_α that is confined around the origin. In this context we call a family of states $\{\Psi_\alpha : \alpha > 0\}$ an approximate ground state in case $\langle\mathbb{H}\rangle_{\Psi_\alpha} = E_\alpha + o_{\alpha\to\infty}\left(\frac{1}{\alpha^2}\right)$. The confinement is achieved by localizing a regularized version of the median, i.e. for any $x \in \mathrm{supp}(\Psi_{\alpha,n}) \subseteq \mathbb{R}^{n\times 3}$, where $\Psi_\alpha = \bigoplus_{n=0}^{\infty}\Psi_{\alpha,n}$ with $\Psi_{\alpha,n} \in L^2(\mathbb{R}^3)^{\otimes_s n}$, there are at least $(\frac{1}{2} - \epsilon_\alpha)n$ particles satisfying $x_k^{(j)} \leqslant \epsilon_\alpha$ and at least $(\frac{1}{2} - \alpha)n$ particles satisfying $x_k^{(j)} \geqslant -\epsilon_\alpha$, where $k \in \{1,2,3\}$ and $\epsilon_\alpha \ll 1$. As we demonstrate in Chapter 3, such a state is necessarily close to the coherent state $\Omega_{\varphi^{\mathrm{Pek}}}$ where φ^{Pek} is a minimizer of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$, in the sense that Ψ_α is an approximate eigenstate of the annihilation operators a_n with respect to the eigenvalue λ_n^{Pek}. This implies in particular that $\lambda_n - \varphi_n^{\mathrm{Pek}}$ is a small quantity, allowing us to absorb the error term $o\left(|\lambda - \lambda^{\mathrm{Pek}}|^2\right)$ in Eq. (1.2.3) by the quadratic part $-\frac{1}{4\alpha^4}\sum_{n=1}^{N}\partial_{\lambda_n}^2 + \sum_{i,j=1}^{N} H_{i,j}^{\mathrm{Pek}}(\lambda_i - \lambda_i^{\mathrm{Pek}})(\lambda_j - \lambda_j^{\mathrm{Pek}}) - \frac{N}{2\alpha^2}$, at least after a suitable unitary transformation, which is similar to the unitary $\mathcal{W}_N$ used in Section 1.1.

The corresponding upper bound $E_\alpha \leqslant e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + o_{\alpha\to\infty}\left(\frac{1}{\alpha^2}\right)$ has been established in [40, 91] by construction of a suitable test function. Combining lower and upper bound then yields the two term expansion of the ground state energy

$$E_\alpha = e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + o_{\alpha\to\infty}\left(\frac{1}{\alpha^2}\right).$$

Finally we shall derive a similar expression for the conditional ground state energy $E_\alpha(P) := \inf\sigma|_{\mathbb{P}=P}(\mathbb{H})$. By using the method of Lagrange multiplier, we will first eliminate the momentum restriction leading to a global minimization problem, which we will treat similarly to the previous problem of finding an asymptotic expansion for the (unconditional) ground state energy E_α. Clearly we have

$$\inf\sigma\big(\mathbb{H} + \lambda(P - \mathbb{P})\big) = \inf_{P' \in \mathbb{R}^3}\Big\{E_\alpha(P') + \lambda(P - P')\Big\},$$

where $\lambda \in \mathbb{R}^3$ is the Lagrange multiplier with which we multiply the momentum constraint $\mathbb{P} = P$, leading to the lower bound on the conditional ground state energy

$$E_\alpha(P) \geqslant \inf\sigma\big(\mathbb{H} + \lambda(P - \mathbb{P})\big) \quad (1.2.4)$$

in terms of the global minimum of $\mathbb{H} + \lambda(P - \mathbb{P})$. As it turns out, the lower bound in Eq. (1.2.4) is insufficient, since $\mathbb{H} + \lambda(P - \mathbb{P})$ is unbounded from below for $\lambda \neq 0$. This issue can be avoided by introducing an ultraviolet cut-off in the Hamiltonian $\mathbb{H}$ as well as in the total momentum operator $\mathbb{P}$, leading to the study of the regularized operators $\mathbb{H}_{\mathrm{reg}}$ and $\mathbb{P}_{\mathrm{reg}}$ defined as the restriction (in the sense of quadratic forms) of the operators $\mathbb{H}$ and $\mathbb{P}$ to $\mathcal{F}(X_\Lambda)$, which can naturally be seen as a subspace of $\mathcal{F}(L^2(\mathbb{R}^3))$, with X_Λ being defined as the space of all functions φ which have their Fourier transformation supported in the ball $B_\Lambda(0)$. Making the optimal choice $\lambda := \frac{P}{m\alpha^4}$, and choosing a suitable $\Lambda > 0$, we shall verify in Chapter 4 the lower bound $\mathbb{H}_{\mathrm{reg}} + \lambda(P - \mathbb{P}_{\mathrm{reg}}) \gtrsim e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \frac{|P|^2}{2m\alpha^4}$ with $m := \frac{2}{3}\|\nabla\varphi^{\mathrm{Pek}}\|^2$, leading to the (asymptotically sharp) lower bound

$$\inf \sigma|_{\mathbb{P}_{\mathrm{reg}}=P}(\mathbb{H}_{\mathrm{reg}}) \gtrsim e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \frac{|P|^2}{2m\alpha^4}. \tag{1.2.5}$$

In order to compare the energy-momentum relation of the regularized model $E_{\alpha,\mathrm{reg}}(P)$ with $E_\alpha(P)$, we apply the result in [40], respectively [97], which provide the estimate $\mathbb{H} \gtrsim \mathbb{H}_{\mathrm{reg}} + \mathcal{N}^\perp$ for a suitable choice of the regularization parameter Λ, where $\mathcal{N}^\perp$ is the particle number operator on the Fock space $\mathcal{F}(X_\Lambda^\perp)$. This yields

$$E_\alpha(P) \gtrsim \inf \sigma|_{\mathbb{P}=P}\left(\mathbb{H}_{\mathrm{reg}} + \mathcal{N}^\perp\right) = \inf_{P' \in \mathbb{R}^3}\left\{\inf \sigma|_{\mathbb{P}_{\mathrm{reg}}=P'}(\mathbb{H}_{\mathrm{reg}}) + \inf \sigma|_{\mathbb{P}^\perp = P - P'}(\mathcal{N}^\perp)\right\},$$

where $\mathbb{P}^\perp := \mathbb{P} - \mathbb{P}_{\mathrm{reg}}$ is the restriction of $\mathbb{P}$ to $\mathcal{F}(X_\Lambda^\perp)$, which can naturally be seen as a subspace of $\mathcal{F}(L^2(\mathbb{R}^3))$. Using the elementary fact that $\inf \sigma|_{\mathbb{P}^\perp = P - P'}(\mathcal{N}^\perp) = \frac{1}{\alpha^2}\delta_{P,P'}$, where $\delta_{P,P'} := 1$ for $P = P'$ and $\delta_{P,P'} := 0$ otherwise, we obtain according to Eq. (1.2.5)

$$\begin{aligned} E_\alpha(P) &\gtrsim \inf_{P' \in \mathbb{R}^3}\left\{e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \frac{|P'|^2}{2m\alpha^4} + \frac{1}{\alpha^2}\delta_{P,P'}\right\} \\ &= e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \min\left\{\frac{|P|^2}{2m\alpha^4}, \frac{1}{\alpha^2}\right\}. \end{aligned} \tag{1.2.6}$$

By the upper bound $E_\alpha(P) \leqslant e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \min\left\{\frac{|P|^2}{2m\alpha^4}, \frac{1}{\alpha^2}\right\} + o_{\alpha\to\infty}\left(\frac{1}{\alpha^2}\right)$ derived in [91], our lower bound in Eq. (1.2.6) is asymptotically sharp, leading to the main result of Chapter 4

$$E_\alpha(P) = e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \min\left\{\frac{|P|^2}{2m\alpha^4}, \frac{1}{\alpha^2}\right\} + o_{\alpha\to\infty}\left(\frac{1}{\alpha^2}\right).$$

For momenta P below the critical value $P_{\mathrm{crit}} := \sqrt{2m}\alpha$ we obtain in particular that the energy-momentum relation of a polaron $E_\alpha(P) - E_\alpha(0) \approx \frac{|P|^2}{2m\alpha^4}$ coincides with the energy-momentum relation of a (non-relativistic) free particle having mass $m\alpha^4$. In this sense we confirm the celebrated conjecture by Landau and Pekar, claiming that the effective mass of a polaron is given by $M_{\mathrm{eff}} = m\alpha^4$.

1.3 Main novel contributions of the Thesis.

In Chapter 2 we provide a two term expansion for the ground state energy E_N of a translation-invariant, mean-field, Bose gas in Theorem 2.1.4, given that the mild Assumptions 2.1.1 and

2.1.3 hold. As an intermediate result we confirm the existence of approximate ground states satisfying Bose-Einstein condensation in Theorem 2.1.2.

In Chapter 3 we establish a lower bound on the ground state energy E_α of the Fröhlich Hamiltonian in Theorem 3.1.1, which is asymptotically sharp up to the subleading order in the limit of large coupling $\alpha \to \infty$. While our result concerns the Fröhlich polaron in $\mathbb{R}^3$, corresponding results have been obtained previously for the Fröhlich polaron in a bounded region of space, see [40], as well as for the Fröhlich polaron on the three dimensional torus, see [37].

In Chapter 4 we provide a lower bound on the ground state energy $E_\alpha(P)$ of the Fröhlich Hamiltonian as a function of the total momentum in Theorem 4.1.1, which is asymptotically sharp up to the subleading order in the limit of large coupling $\alpha \to \infty$. Together with the corresponding upper bound derived in [91] and the results of Chapter 3, we obtain an asymptotic expression for the energy-momentum increment $E_\alpha(P) - E_\alpha(0)$, which is a quantity related to the effective mass of a polaron.

Appendix A is the output of a first year rotation project in the group of Mikhail Lemeshko, where we provide a numerical computation of the full low-energy spectrum of two anyons on the sphere in Figure A.1. Furthermore we show that a system of quasiparticles with anyonic statistics can be realized in terms of linear molecules exchanging angular momentum with a many-particle bath.

Appendix B is the output of a first year rotation project in the group of Jan Maas, where we classify those vector fields which can be written as the gradient flow of a given functional with respect to some smooth metric in Theorem B.1.1, given that the regularity Assumption B.2.1 holds. Subsequently we use this classification in Theorem B.1.2, to show that any ergodic quantum Markov semigroup defined on a finite dimensional C^*-algebra can be written as the gradient of the relative entropy, given that it respects a certain scalar product.

CHAPTER 2

Validity of Bogoliubov's approximation for translation-invariant Bose gases

Abstract. We verify Bogoliubov's approximation for translation-invariant Bose gases in the mean field regime, i.e. we prove that the ground state energy E_N is given by $E_N = Ne_{\mathrm{H}} + \inf \sigma(\mathbb{H}) + o_{N\to\infty}(1)$, where N is the number of particles, e_{H} is the minimal Hartree energy and $\mathbb{H}$ is the Bogoliubov Hamiltonian. As an intermediate result we show the existence of approximate ground states Ψ_N, i.e. states satisfying $\langle H_N \rangle_{\Psi_N} = E_N + o_{N\to\infty}(1)$, exhibiting complete Bose–Einstein condensation with respect to one of the Hartree minimizers.

2.1 Introduction and Main Results

We study the Hamiltonian H_N acting on the Hilbert space $L^2_{\mathrm{sym}}(\mathbb{R}^{N\times d}) \simeq \bigotimes_{\mathrm{s}}^N L^2(\mathbb{R}^d)$ of N identical bosons in $\mathbb{R}^d$ for $d \geqslant 1$, given by

$$H_N := \sum_{i=1}^N T_i + \frac{1}{N-1}\sum_{i<j} v(x_i - x_j), \tag{2.1.1}$$

where T is a non-negative and translation-invariant operator defined on the single particle space $L^2(\mathbb{R}^d)$ and the interaction potential v is an even function. Typically we will think of T as the non-relativistic energy $T = -\Delta$ or the pseudo relativistic energy $T = \sqrt{m^2 - \Delta} - m$, and of the interaction v as being attractive. The most prominent features of this model are the mean field scaling $\frac{1}{N-1}$ of the interaction energy and the invariance of H_N under translations, which especially means that the Hamiltonian H_N describes an unconfined system of N bosons. By choosing a product state $\Psi := u^{\otimes^N}$ as a test function, we obtain the trivial upper bound on the ground state energy $E_N := \inf \sigma(H_N)$ per particle

$$N^{-1}E_N \leqslant N^{-1}\langle H_N \rangle_\Psi = \langle T \rangle_u + \frac{1}{2}\int\int |u(x)|^2 v(x-y)|u(y)|^2 \mathrm{d}x\mathrm{d}y =: \mathcal{E}_{\mathrm{H}}[u],$$

where $\mathcal{E}_{\mathrm{H}}[u]$ is referred to as the Hartree energy functional. This upper bound is independent of the particle number N due to the scaling by $\frac{1}{N-1}$ of the interaction. It is known under quite general assumptions on v and T that the upper bound

$$e_{\mathrm{H}} := \inf_{\|u\|=1} \mathcal{E}_{\mathrm{H}}[u] \tag{2.1.2}$$

on the ground state energy per particle is asymptotically correct in the mean field limit $N \to \infty$, see [71]. Furthermore, the Bogoliubov approximation [13] predicts that the next order term in the approximation $E_N \approx N\, e_{\mathrm{H}}$ is of order one and given by the ground state energy of the corresponding Bogoliubov Hamiltonian $\mathbb{H}$, which is formally the second quantization of the Hessian $\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}$ at a minimizer u_0. In the past decade, this conjecture has been proven for a variety of mean field models [48, 72, 99, 115], and also for systems with more singular interactions [27, 11, 12, 14, 15, 100]. However, the rigorous verification of Bogoliubov's approximation has so far been restricted to confined systems only. In the case of translation-invariant models, we face the problem that minimizers of the Hartree energy functional $\mathcal{E}_{\mathrm{H}}$ are not unique and that the Hessian $\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}$ at a minimizer u_0 does not exhibit a gap, i.e. we do not have an inequality of the form $\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}} \geqslant c$ with $c > 0$. Novel ideas and techniques are required in order to deal with these translation-invariance specific problems, which we will develop in the course of this paper allowing us to verify Bogoliubov's prediction $E_N = N\, e_{\mathrm{H}} + \inf \sigma(\mathbb{H}) + o_N(1)$ for translation-invariant systems. As an intermediate step, we will construct a sequence of approximate ground states Ψ_N satisfying complete Bose–Einstein condensation, which we believe to be of independent interest.

Note that the situation is different for time-dependent problems, where it is already well-known that fluctuations around a product state $u^{\otimes^N}$ evolve according to a (time-dependent) Bogoliubov operator, even for translation-invariant systems [74].

Due to the translation-invariance, it is clear that H_N has no ground state and therefore we have to restrict our attention to sequences of approximate ground states Ψ_N. We will use the convention that states Ψ are normed Hilbert space elements, i.e. $\|\Psi\| = 1$. In our first result we show the existence of a sequence of approximate ground states Ψ_N, with the property that Ψ_N is close to a product state $u_0^{\otimes^N}$ where u_0 minimizes the Hartree energy $\mathcal{E}_{\mathrm{H}}$. In this context, close means that the sequence Ψ_N satisfies complete Bose–Einstein condensation with respect to the state u_0, i.e. the corresponding one particle density matrices $\gamma_N^{(1)}$ satisfy $\langle \gamma_N^{(1)} \rangle_{u_0} \underset{N\to\infty}{\longrightarrow} 1$. In general we define the k-particle density matrix $\gamma_\Psi^{(k)}$ corresponding to a state $\Psi \in \bigotimes_{\mathrm{s}}^N L^2(\mathbb{R}^d)$ by the equation $\mathrm{Tr}\left[\gamma_\Psi^{(k)}\, B\right] = \langle B \otimes 1 \otimes \cdots \otimes 1 \rangle_\Psi$ for all bounded k-particle operators B. This means in particular that we use the normalization convention $\mathrm{Tr}\left[\gamma_N^{(k)}\right] = 1$. In order to prove complete Bose–Einstein condensation, we need certain assumptions concerning the kinetic energy operator T and the Hartree theory, as well as a relative bound of the interaction potential v in terms of the kinetic energy.

Assumption 2.1.1. *The kinetic energy is given by $T := (m^2 - \Delta)^s - m^{2s}$ with $m > 0$ and $s \in (0, 1]$, the interaction potential v satisfies $\lim_{|x|\to\infty} v(x) = 0$ and the chain of inequalities*

$$-\lambda T - \Lambda \leqslant v \leqslant |v| \leqslant \Lambda(T + 1) \tag{2.1.3}$$

for some $\lambda \in (0, 2)$ and $\Lambda \in (0, \infty)$. Furthermore, the Hartree energy defined in Eq. (2.1.2) is strictly negative, i.e. $e_{\mathrm{H}} < 0$, and there exists a real-valued function $u_0 \in L^2(\mathbb{R}^d)$ that minimizes the Hartree energy, i.e. $e_{\mathrm{H}} = \mathcal{E}_{\mathrm{H}}[u_0]$, and satisfies $\int_{[x_r \leqslant t]} |u_0(x)|^2\, \mathrm{d}x = \frac{1}{2}$ if and only if $t = 0$, where x_r is the r-th component of the vector $x \in \mathbb{R}^d$. Up to a complex phase, all other Hartree minimizers are given by translations of u_0, i.e. all minimizers are of the form $e^{i\theta} u_{0,t}$ with $\theta \in [0, 2\pi), t \in \mathbb{R}^d$ and $u_{0,t}(x) := u_0(x - t)$.

By the translation-invariance of the Hartree energy, any shift of a Hartree minimizer $u_0(x-t)$ is again a minimizer. Therefore, we can always choose the Hartree minimizer such that it is centered around zero, i.e. such that $\int_{[x_r \leqslant 0]} |u_0(x)|^2 \, \mathrm{d}x = \frac{1}{2}$ for all $r \in \{1, \ldots, d\}$. In particular, in case the minimizers u of $\mathcal{E}_H$ satisfy $u > 0$, the existence of a u_0 satisfying $\int_{[x_r \leqslant t]} |u_0(x)|^2 \, \mathrm{d}x = \frac{1}{2}$ if and only if $t = 0$ is always granted. Furthermore, most of our proofs do not depend on the concrete structure $T = (m^2 - \Delta)^s - m^{2s}$ of the kinetic energy, and it is sufficient to assume instead that the operator T is of the translation-invariant form $T = t(i\nabla)$ for some t with $t(p) \underset{|p| \to \infty}{\longrightarrow} \infty$ such that the Hartree approximation $\frac{1}{N} E_N \underset{N \to \infty}{\longrightarrow} e_{\mathrm{H}}$ as well as the IMS localization formula in Lemma 2.2.2 hold.

With Assumption 2.1.1 at hand, we obtain our first main result Theorem 2.1.2, which we will prove in Section 2.2.

Theorem 2.1.2. *Given Assumption 2.1.1, there exists a sequence of states $\Psi_N \in \bigotimes_{\mathrm{s}}^N L^2(\mathbb{R}^d)$ with $\langle H_N \rangle_{\Psi_N} = E_N + o_{N \to \infty}(1)$, exhibiting complete Bose–Einstein condensation with respect to the state u_0, i.e.*

$$\langle \gamma_N^{(1)} \rangle_{u_0} \underset{N \to \infty}{\longrightarrow} 1. \tag{2.1.4}$$

Since Assumption 2.1.1 implies the validity of the Hartree approximation in the form $\frac{1}{N} E_N \underset{N \to \infty}{\longrightarrow} e_{\mathrm{H}}$, see [71], it is clear that the product state $u_0^{\otimes N}$, which trivially satisfies perfect Bose–Einstein condensation, approximates the ground state energy to leading order, i.e. $\langle H_N \rangle_{u_0^{\otimes N}} = E_N + o_{N \to \infty}(N)$. In Theorem 2.1.2 we improve this result by constructing a Bose–Einstein condensate that approximates E_N even up to terms $o_{N \to \infty}(1)$. Note, however, that Theorem 2.1.2 claims nothing about the rate of convergence in Eq. (2.1.4). One can improve this result a posteriori by using the trial states in our proof of the upper bound in Theorem 2.1.4, which yields for any given sequence $c_N \underset{N \to \infty}{\longrightarrow} \infty$ a sequence of approximate ground states $\widetilde{\Psi}_N$ satisfying

$$|\langle \widetilde{\gamma}_N^{(1)} \rangle_{u_0} - 1| \leqslant \frac{c_N}{N}.$$

It follows from our proof of the lower bound in Theorem 2.1.4 that this result is optimal in the sense that any sequence with $|\langle \widetilde{\gamma}_N^{(1)} \rangle_{u_0} - 1| = O_{N \to \infty}\left(\frac{1}{N}\right)$ cannot be a sequence of approximate ground states.

Furthermore it follows from the proof of Theorem 2.1.2 that for any sequence $c_N \underset{N \to \infty}{\longrightarrow} \infty$, there exist states Ψ'_N exhibiting complete Bose–Einstein condensation with $\langle H_N \rangle_{\Psi'_N} \leqslant E_N + \frac{c_N}{N}$. Again it is a consequence of our proof of the lower bound that this result is optimal in the sense that any sequence with $\langle H_N \rangle_{\Psi'_N} = E_N + O_{N \to \infty}\left(\frac{1}{N}\right)$ does not satisfy complete Bose–Einstein condensation.

Proof strategy of Theorem 2.1.2. With Assumption 2.1.1 at hand, we can apply the results in [71] which tell us that the Hartree asymptotics $\frac{1}{N} E_N \underset{N \to \infty}{\longrightarrow} e_{\mathrm{H}}$ holds true and that any sequence of approximate ground states Ψ_N has a subsequence such that the k-particle density matrices converge weakly to a mixture of not necessarily normed Hartree minimizers. This means that there exists a probability measure μ supported on functions u with $\|u\| \leqslant 1$

and $\mathcal{E}_{\mathrm{H}}[u] = \inf_{\|v\|=\|u\|} \mathcal{E}_{\mathrm{H}}[v]$, such that the k-particle density matrix of the subsequence Ψ_{N_j} satisfies

$$\mathrm{Tr}\left[\gamma_{N_j}^{(k)}\, K\right] \underset{j\to\infty}{\longrightarrow} \int \mathrm{Tr}\left[\left(|u\rangle\langle u|\right)^{\otimes^k} K\right] \mathrm{d}\mu(u) \tag{2.1.5}$$

for any compact k particle operator K. The proofs in [71] rely on the quantum de Finetti theorem (see also [120, 55]), which identifies states on the infinite symmetric tensor product as the convex hull of product states. In order to prove Theorem 2.1.2, we have to construct a sequence of approximate ground states Ψ_N such that the corresponding measure μ in Eq. (2.1.5) is equal to the delta measure δ_{u_0}. In particular this means that μ has to be supported on the set of normed elements $\|u\| = 1$, or equivalently we have to make sure that mass cannot escape to infinity. For confined systems satisfying a binding inequality, it has been shown in [71] that μ is always supported on normed elements. For translation-invariant systems this is no longer the case, since one can always find $y_N \in \mathbb{R}^d$ such that $\widetilde{\Psi}_N \underset{N\to\infty}{\rightharpoonup} 0$ where

$$\widetilde{\Psi}_N\left(x^{(1)}, \dots, x^{(N)}\right) := \Psi_N\left(x^{(1)} - y_N, \dots, x^{(N)} - y_N\right)$$

for all $\left(x^{(1)}, \dots, x^{(N)}\right) \in \mathbb{R}^{N\times d}$, and therefore the corresponding measure is supported on $\{0\}$ only. While one could circumvent this issue by factoring out the center-of-mass variable, we avoid doing this since there is no straightforward analogue of product states and Bose–Einstein condensation in the space of relative coordinates. Alternatively we overcome this problem by localizing a sequence of approximate ground states Ψ_N only to configurations that are centered around zero. It turns out that the median of a configuration $x = \left(x^{(1)}, \dots, x^{(N)}\right) \in \mathbb{R}^{N\times d}$, respectively a regularized version of the median, is the right statistical quantity to measure whether a configuration is centered around the origin or not. Furthermore, we will energetically rule out configurations where the mass is split up in two or multiple parts, e.g. we will rule out configurations where $\frac{N}{2}$ particles are very far from the other $\frac{N}{2}$ particles. We conclude that the mass is concentrated at the origin and therefore it does not escape to infinity.

In order to identify the support of the measure μ in Eq. (2.1.5), note that all Hartree minimizers are up to a complex phase translations of the minimizer u_0, which is a function centered around zero. Consequently, up to this complex phase, u_0 is the only minimizer with the property of being centered around zero. Using the support property of Ψ_N, this already suggests that the measure μ should be supported on states of the form $\{e^{i\theta}u_0 : \theta \in [0, 2\pi)\}$ only. Since $|e^{i\theta}u_0\rangle\langle e^{i\theta}u_0| = |u_0\rangle\langle u_0|$ defines the same density matrix for all complex phases $e^{i\theta}$, this support property of the measure μ implies the convergence of the density matrix $\gamma_N^{(k)}$ to a single condensate $\left(|u_0\rangle\langle u_0|\right)^{\otimes^k}$.

Having a sequence of approximate ground states at hand that satisfies complete Bose–Einstein condensation is a crucial prerequisite in identifying the sub-leading term in the energy asymptotics $E_N = N\, e_{\mathrm{H}} + o(N)$. In the following, let $u_0, u_1, \dots, u_d, u_{d+1}, \dots$ be a real orthonormal basis of $L^2\left(\mathbb{R}^d\right)$, where u_0 is the Hartree minimizer from Assumption 2.1.1 and $u_1, \dots, u_d$ a basis of the vector space spanned by the partial derivatives $\langle \partial_{x_1} u_0, \dots, \partial_{x_d} u_0\rangle$. Since the functional $\mathcal{E}_{\mathrm{H}}$ is invariant under a phase change $u \mapsto e^{i\theta}u$, we can restrict ourself to states u with $\langle u_0, u\rangle \geqslant 0$. Then, the Hessian $\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}$ of the Hartree energy is a real quadratic form defined on $\{u_0\}^\perp \subset L^2\left(\mathbb{R}^d\right)$, and consequently there exist coefficients $Q_{i,j}, G_{i,j} \in \mathbb{C}$, $i, j \in \mathbb{N}$, such that $\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}[z] = \sum_{i,j=1}^{\infty}\left(Q_{i,j}\overline{z}_i z_j + \overline{G}_{i,j} z_i z_j + G_{i,j}\overline{z}_i\overline{z}_j\right)$, where z_i are the coordinates of $z \in \{u_0\}^\perp$. In order to define the Bogoliubov operator $\mathbb{H}$, let $a_i, a_i^\dagger$ be the annihilation/creation operators corresponding to the state $u_i \in L^2\left(\mathbb{R}^d\right)$. Following [72] we formally define $\mathbb{H}$ as the second quantization of the Hessian $\mathrm{Hess}|_{u_0}\mathcal{E}_\mathrm{H}$, i.e.

$$\mathbb{H} := \sum_{i,j=1}^{\infty} \left(Q_{i,j}\ a_i^\dagger a_j + \overline{G}_{i,j}\ a_i a_j + G_{i,j}\ a_i^\dagger a_j^\dagger \right). \tag{2.1.6}$$

For a rigorous construction see Definition 2.4.3.

Note that due to the translation-invariance, the Hessian $\mathrm{Hess}|_{u_0}\mathcal{E}_\mathrm{H}$ is degenerate in the directions u_j for $j \in \{1, \ldots, d\}$, i.e. $\mathrm{Hess}|_{u_0}\mathcal{E}_\mathrm{H}[u_j] = 0$. The following Assumption makes sure that $\mathrm{Hess}|_{u_0}\mathcal{E}_\mathrm{H}$ is non-degenerate in all other directions.

Assumption 2.1.3. *The partial derivatives of u_0 are in the form domain of T, and there exists a constant $\eta > 0$ such that*

$$\mathrm{Hess}|_{u_0}\mathcal{E}_\mathrm{H}[z] \geqslant \eta \left\| z \right\|^2 \tag{2.1.7}$$

for all z of the form $z = i\sum_{j=1}^d s_j u_j + z_{>d}$ with $s_j \in \mathbb{R}$ and $z_{>d} \in \{u_0, \partial_{x_1}u_0, \ldots, \partial_{x_d}u_0\}^\perp$. Furthermore, the Hartree minimizer u_0 is an element of $H^2(\mathbb{R}^d)$.

With the Assumption 2.1.3 at hand, we arrive at our second main Theorem, which identifies the sub-leading term in the energy asymptotics as the ground state energy $\inf \sigma\left(\mathbb{H}\right)$ of the Bogoliubov operator $\mathbb{H}$.

Theorem 2.1.4. *Let E_N be the ground state energy of the Hamiltonian H_N defined in Eq. (2.1.1), e_H the Hartree energy defined in Eq. (2.1.2) and let $\mathbb{H}$ be the Bogoliubov operator defined in Eq. (2.1.6). Given Assumption 2.1.1 and Assumption 2.1.3, we have*

$$E_N = N\, e_\mathrm{H} + \inf \sigma\left(\mathbb{H}\right) + o_{N\to\infty}\left(1\right). \tag{2.1.8}$$

Examples of systems satisfying both Assumptions 2.1.1 and 2.1.3, and hence our Theorem 2.1.4 applies to, are as follows.

Example (I). Let us first consider a system of N non-relativistic bosons in $\mathbb{R}^3$ interacting with each other via a Newtonian potential

$$H_N := -\sum_{i=1}^N \Delta_i - \frac{g}{N-1}\sum_{i<j}\frac{1}{|x_i - x_j|}$$

with $g > 0$. Existence and uniqueness of the Hartree minimizer u_0, in the sense of Assumption 2.1.1, have been shown in [76]. Moreover, u_0 is strictly positive and smooth, hence satisfies all the other requirements of Assumptions 2.1.1 and 2.1.3. The non-degeneracy of the Hessian follows from the results in [69] by standard arguments, see for instance [41]. Furthermore, it is clear by a scaling argument that $e_\mathrm{H} < 0$ and that we can bound the interaction energy in terms of the kinetic energy by $\frac{1}{|x|} \leqslant -\epsilon\Delta + \frac{1}{4\epsilon}$ for all $\epsilon > 0$.

Example (II). As a second example let us consider a system of N pseudo-relativistic bosons in $\mathbb{R}^3$ with positive mass $m > 0$, interacting with each other via a Newtonian potential

$$H_N := \sum_{i=1}^{N} \left(\sqrt{m^2 - \Delta_i} - m \right) - \frac{g}{N-1} \sum_{i<j} \frac{1}{|x_i - x_j|},$$

where we assume that the coupling strength satisfies $g \in (0, g_*)$ for a suitable positive constant $g_* > 0$. It has been shown in [81] that there exists a Hartree minimizer u_0 as long as the coupling g is below a critical value, in which case the Hartree approximation $\lim_{N\to\infty} N^{-1} E_N = e_{\mathrm{H}}$ holds true. The chain of operator inequalities in Assumption 2.1.1 holds as long as the coupling is below the critical value $\frac{4}{\pi}$, see [54, 58]. By restricting the attention to possibly smaller couplings $g \in (0, g_*)$ it has been shown in [69, 51] that minimizers u_0 are unique in the sense of Assumption 2.1.1. Furthermore it follows from the results in [69, 51] that the Hessian is non-degenerate in the sense of Assumption 2.1.3 for couplings g below a critical value. We will verify this explicitly in Appendix 2.6, using an argument similar to the one in [41] for non-relativistic systems. (The argument in [41] is based on scaling the coordinates and hence not directly applicable in the pseudo-relativistic case.)

Example (III). As a third example let us consider the exactly solvable model of N non-relativistic bosons on the real line $\mathbb{R}$, interacting with each other via an attractive delta potential

$$H_N := -\sum_{i=1}^{N} \partial_i^2 - \frac{\lambda}{N-1} \sum_{i<j} \delta(x_i - x_j),$$

where $\lambda > 0$, see [87] for an explicit expression of the ground state energy. In this case the Hartree energy $\mathcal{E}_{\mathrm{H}}$ is given by

$$\mathcal{E}_{\mathrm{H}}[u] = \int_{-\infty}^{\infty} |u'(x)|^2 \mathrm{d}x - \frac{\lambda}{2} \int_{-\infty}^{\infty} |u(x)|^4 \mathrm{d}x.$$

For $d = 1$ we have $\delta \leqslant -\epsilon\, \partial^2 + \frac{1}{4\epsilon}$ for all $\epsilon > 0$ in the sense of quadratic forms, and therefore Eq. (2.1.3) in Assumption 2.1.1 holds. By a scaling argument it is clear that $e_{\mathrm{H}} < 0$ and minimizers of the Hartree energy are unique in the sense of Assumption 2.1.1, see [62] where the uniqueness of solutions to the corresponding Euler-Lagrange equation is verified. Furthermore the coercivity assumption in Eq. (2.1.7) is a consequence of the slightly different coercivity result in [129] (arguing, e.g., as in Appendix 2.6).

We remark that in Examples (I) and (III), the value of the coupling constant, and hence also the factor $1/(N-1)$ in front of the interaction term, is irrelevant, since it can be replaced by any other value by a simple scaling of the coordinates. This does not apply to Example (II), however.

Proof strategy of Theorem 2.1.4. We will verify the upper bound in our main result (2.1.8) analogously to the proof of the energy asymptotics for confined systems in [72]. The more difficult lower bound will be based on the correspondence between the Hartree energy

$\mathcal{E}_{\mathrm{H}}$ and the Hamiltonian H_N. This correspondence becomes evident when we rewrite H_N in the language of second quantization. For this purpose, let us define the rescaled creation operators $b_j^\dagger := \frac{1}{\sqrt{N}} a_{u_j}^\dagger$, where we suppress the N dependence in our notation for simplicity. Then we can write

$$N^{-1} H_N = \sum_{i,j=0}^{\infty} T_{i,j}\ b_i^\dagger b_j + \frac{N}{N-1}\frac{1}{2}\sum_{ij,k\ell} \hat{v}_{ij,k\ell}\ b_i^\dagger b_j^\dagger b_k b_\ell, \tag{2.1.9}$$

where $T_{i,j}$ are the matrix entries of the operator T with respect to the basis $\{u_i : i \in \mathbb{N}_0\}$ and $\hat{v}_{ij,k\ell}$ are the ones of the two body multiplication operator $\hat{v} = v(x-y)$ with respect to the basis $\{u_i \otimes u_j : i, j \in \mathbb{N}_0\}$. Up to the factor $\frac{N}{N-1}$, the Hartree energy $\mathcal{E}_{\mathrm{H}}[u]$

$$\mathcal{E}_{\mathrm{H}}[u] = \sum_{i,j=0}^{\infty} T_{i,j}\ \overline{c_i}\ c_j + \frac{1}{2}\sum_{ij,k\ell} \hat{v}_{ij,k\ell}\ \overline{c_i}\ \overline{c_j}\ c_k\ c_\ell$$

is represented by the same symbolic expression as in Eq. (2.1.9), i.e. we plug in the complex numbers c_i instead of the operators b_i. Before investigating the next order term in the energy asymptotics, let us discuss the next order expansion of the commutative counterpart $\mathcal{E}_{\mathrm{H}}[u] = e_{\mathrm{H}} + o(\|u - u_0\|)$, which is given by the Hessian of the functional $\mathcal{E}_{\mathrm{H}}$. Since the Hartree energy is defined on the infinite dimensional manifold $\{u \in L^2(\mathbb{R}^d) : \|u\| = 1, \langle u_0, u\rangle \geqslant 0\} \subset L^2(\mathbb{R}^d)$, it is convenient to introduce the embedding

$$\iota : \begin{cases} \{z \in \{u_0\}^\perp : \|z\| \leqslant 1\} \longrightarrow \{u \in L^2(\mathbb{R}^d) : \|u\| = 1, \langle u_0, u\rangle \geqslant 0\}, \\ \quad z \mapsto \iota(z) := \sqrt{1 - \|z\|^2}\ u_0 + z. \end{cases} \tag{2.1.10}$$

Using the chart ι, we can express the Hessian as $\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}} = D^2|_0(\mathcal{E}_{\mathrm{H}} \circ \iota)$ and the second order expansion at $z = 0$ is given by

$$\mathcal{E}_{\mathrm{H}}[\iota(z)] = e_{\mathrm{H}} + \mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}[z] + o\left(\|z\|^2\right).$$

In contrast to confined systems, the Hessian for translation-invariant systems is always degenerate in the directions $u_1, \ldots, u_d$, i.e. $\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}[u_j] = 0$ for $j \in \{1, \ldots, d\}$. It is important to observe that the manifold of minimizers $\mathcal{M} := \{z : \mathcal{E}_{\mathrm{H}}[\iota(z)] = e_{\mathrm{H}}\}$ is not contained in the null space of the Hessian $\{z : \mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}[z] = 0\}$. Therefore, we do not have the crucial estimate $\mathcal{E}_{\mathrm{H}}[\iota(z)] \geqslant e_{\mathrm{H}} + (1-\epsilon)\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}[z]$, $0 < \epsilon < 1$, not even in an arbitrary small neighborhood of zero. In order to obtain such an inequality, we will introduce yet another transformation F on the ball $\{z \in \{u_0\}^\perp : \|z\| \leqslant 1\}$, such that $D|_0 F$ is the identity and such that F flattens the manifold of minimizers $\mathcal{M}$, i.e. $\mathcal{E}_{\mathrm{H}}\left[(\iota \circ F)\left(\sum_{j=1}^d t_j u_j\right)\right] = e_{\mathrm{H}}$ for all $t_j \in \mathbb{R}$. For a concrete construction of F see Eq. (2.4.7) in Section 2.4. Under the assumption that the Hessian is only degenerate in the directions u_j, see Assumption 2.1.3, we obtain for any fixed $\epsilon > 0$ and z small enough the important estimate

$$\mathcal{E}_{\mathrm{H}}[(\iota \circ F)(z)] \geqslant e_{\mathrm{H}} + (1-\epsilon)\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}[z]. \tag{2.1.11}$$

Returning to the Hamiltonian H_N, we will introduce non-commutative counterparts to the embedding ι and the transformation F. The counterpart to ι is the excitation map U_N introduced in [72], where it has already been used to verify the next order approximation of the ground state energy for confined systems. It is defined as

$$U_N\left(u_0^{\otimes i_0} \otimes_{\mathrm{s}} u_1^{\otimes i_1} \otimes_{\mathrm{s}} \cdots \otimes_{\mathrm{s}} u_m^{\otimes i_m}\right) := u_1^{\otimes i_1} \otimes_{\mathrm{s}} \cdots \otimes_{\mathrm{s}} u_m^{\otimes i_m} \tag{2.1.12}$$

for non-negative integers $i_0 + \cdots + i_m = N$, mapping the N particle space $\bigotimes_{\mathrm{s}}^N L^2\left(\mathbb{R}^d\right)$ into the truncated Fock space $\mathcal{F}_{\leqslant N}\left(\{u_0\}^\perp\right) := \bigoplus_{n\leqslant N} \bigotimes_{\mathrm{s}}^n \{u_0\}^\perp$ over modes orthogonal to u_0, where the symmetric tensor product $\otimes_{\mathrm{s}}$ is defined as

$$\psi_k \otimes_s \psi_\ell\Big(x^{(1)}, \ldots, x^{(k+\ell)}\Big) := \frac{1}{\sqrt{\ell! k! (k+\ell)!}} \sum_{\sigma \in S_{k+\ell}} \psi_k\Big(x^{(\sigma_1)}, \ldots, x^{(\sigma_k)}\Big) \psi_\ell\Big(x^{(\sigma_{k+1})}, \ldots, x^{(\sigma_{k+\ell})}\Big)$$

for $\psi_k \in \bigotimes_{\mathrm{s}}^k L^2(\mathbb{R}^3)$ and $\psi_\ell \in \bigotimes_{\mathrm{s}}^\ell L^2(\mathbb{R}^3)$, and S_n is the set of permutations on $\{1, \ldots, n\}$. Regarding the transformation F, we construct the counterpart $\mathcal{W}_N$ in Definition 2.4.8 as a certain transformation reminiscent of the Gross transformation in [49, 102], operating on the space $\mathcal{F}\left(\{u_0\}^\perp\right)$. Based on these correspondences and the observation that the Bogoliubov operator is the non-commutative analogue of the Hessian $\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}$, we obtain the following inequality analogous to Eq. (2.1.11)

$$\left(\mathcal{W}_N U_N\right) N^{-1} H_N \left(\mathcal{W}_N U_N\right)^{-1} \gtrsim e_{\mathrm{H}} + (1-\epsilon) N^{-1} \mathbb{H}. \tag{2.1.13}$$

We write $\gtrsim$ for two reasons: There are errors of order $o\left(\frac{1}{N}\right)$ coming from the non-commutative nature of H_N; moreover Eq. (2.1.13) only holds for states Ψ that satisfy a strengthened version of Bose–Einstein condensation of the form $U_N \Psi \in \mathcal{F}_{\leqslant M_N}\left(\{u_0\}^\perp\right)$ with $M_N \ll N$, which corresponds to the fact that Inequality (2.1.11) only holds for small z. The rigorous verification of inequality (2.1.13) will be the content of Sections 2.4 and 2.5.

Our construction of $\mathcal{W}_N$ and the proof of Inequality (2.1.13) do not rely on the specific structure of H_N or $L^2(\mathbb{R}^d)$, and they can be generalized for various mean field models with continuous symmetries. The essential assumption is that the dimension of the symmetry group agrees with the nullity of the Hessian, i.e. the Hessian is as non-degenerate as possible in the presence of a continuous symmetry, see Assumption 2.1.3.

Outline. The paper is structured as follows. In Section 2.2 we construct a sequence of approximate ground states satisfying complete Bose–Einstein condensation, which verifies our first main Theorem 2.1.2. The methods and results of Section 2.2 can be read independently of the rest of the paper, which is dedicated to the proof of our second main Theorem 2.1.4. In Section 2.3, we will introduce the relevant Fock spaces as well as a useful notation for second quantized operators, which we believe to be intuitive and natural for our problem. With the basic notions at hand, we will follow the strategy in [72] and reformulate our problem in a Fock space language using the excitation map U_N. In Section 2.4 we will discuss the energy asymptotics of H_N, starting with a precise definition of the Bogoliubov operator $\mathbb{H}$ in Subsection 2.4.1, the verification of the upper bound in Subsection 2.4.2 and the proof of the lower bound in Subsection 2.4.3, up to the proof of the main technical inequality Eq. (2.1.13). The proof of the latter is the content of Section 2.5.

2.2 Bose–Einstein Condensation of Ground States

In this section we will prove Theorem 2.1.2 by constructing a sequence Ψ_N of approximate ground states satisfying complete Bose–Einstein condensation. The concrete construction of Ψ_N will be part of Subsection 2.2.1, where we introduce a suitable localization method and verify that mass does not escape to infinity. In the following Subsection 2.2.2, we will use this to verify complete Bose–Einstein condensation of the sequence Ψ_N.

2.2.1 Localization of the Ground State

In the following we are constructing a sequence of states Ψ_N, i.e. elements satisfying $\|\Psi_N\| = 1$, localized only to configurations $x \in \mathbb{R}^{N\times d}$ centered at zero, such that $\langle H_N\rangle_{\Psi_N} = E_N + o_{N\to\infty}(1)$. For such a sequence we will verify that mass cannot escape to infinity. As it turns out, the regularized median M_N, which we will define in the subsequent Definition 2.2.1, is the right statistical quantity to measure the center

$$x_{\text{center}} := \left(M_{N,k}\left(x_1^{(1)},\dots,x_1^{(N)}\right),\dots,M_{N,k}\left(x_d^{(1)},\dots,x_d^{(N)}\right)\right) \in \mathbb{R}^d$$

of a configuration $x = \left(x^{(1)},\dots,x^{(N)}\right) \in \mathbb{R}^{N\times d}$, where $x^{(j)} = \left(x_1^{(j)},\dots,x_d^{(j)}\right) \in \mathbb{R}^d$ is the coordinate vector of the j-th particle.

Definition 2.2.1 (Localization)**.** Given $N \in \mathbb{N}$ and k such that $k + \frac{N}{2} \in \mathbb{N}$, we define the regularized median $M_{N,k} : \mathbb{R}^N \longrightarrow \mathbb{R}$ as the unique permutation-invariant function that is defined for all $x^{(1)} \leqslant \dots \leqslant x^{(N)}$ as

$$M_{N,k}\left(x^{(1)},\dots,x^{(N)}\right) := \frac{1}{2k+1}\sum_{j=\frac{N}{2}-k}^{\frac{N}{2}+k} x^{(j)}.$$

In the IMS-type estimate of the following Lemma 2.2.2, which has been proven in [70, Lemma 7], we will make use of the specific structure of the operator $T = (m^2-\Delta)^s - m^{2s}$. Note that this is the only place where the specific structure is relevant for us.

Lemma 2.2.2. *Let $T = (m^2-\Delta)^s - m^{2s}$ be as in Assumption 2.1.1 and let $\{\chi_i : i \in I\}$ be a family of $W^{1,\infty}(\mathbb{R}^d)$ functions with $\sum_i \chi_i^2 = 1$. With the definition $C := m^{2(s-1)}s$ we have for all states $u \in L^2\left(\mathbb{R}^d\right)$*

$$\sum_{i\in I}\langle T\rangle_{\chi_i u} \leqslant \langle T\rangle_u + C\left\|\sum_{i\in I}|\nabla\chi_i|^2\right\|_\infty.$$

Lemma 2.2.3. *Let E_N denote the ground state energy of H_N and let k_N be a sequence with $\sqrt{N} \ll k_N \ll N$ such that $k_N + \frac{N}{2} \in \mathbb{N}$. Then there exists a sequence of states Ψ_N in $L^2_{\text{sym}}\left(\mathbb{R}^{N\times d}\right)$ with $\langle H_N\rangle_{\Psi_N} - E_N \underset{N\to\infty}{\longrightarrow} 0$ and a sequence $0 < \alpha_N \ll 1$, such that*

$$\left|M_{N,k_N}\left(x_r^{(1)},\dots,x_r^{(N)}\right)\right| \leqslant \alpha_N$$

for all $x \in \operatorname{supp}(\Psi_N) \subset \mathbb{R}^{N\times d}$ and $r \in \{1,\dots,d\}$.

Proof. Let $0 < \alpha_N \leqslant 1$ be a sequence with $\frac{\sqrt{N}}{k_N} \ll \alpha_N \ll 1$ and let $\nu_\ell : \mathbb{R} \to \mathbb{R}$, $\ell \in \mathbb{Z}$, be a family of C^∞ functions with $\sum_{\ell\in\mathbb{Z}} \nu_\ell^2 = 1$, $\operatorname{supp}(\nu_\ell) \subset (\ell-1,\ell+1)$ and $\nu_\ell(x) = \nu_0(x-\ell)$. Then we define the family of functions $\chi_{\ell,r} : \mathbb{R}^{N\times d} \longrightarrow \mathbb{R}$ with $\ell \in \mathbb{Z}$ and $r \in \{1,\dots,d\}$ as

$$\chi_{\ell,r}(x) := \nu_\ell\left(\frac{1}{\alpha_N}M_{N,k_N}\left(x_r^{(1)},\dots,x_r^{(N)}\right)\right)$$

and for $\ell = (\ell_1,\dots,\ell_d) \in \mathbb{Z}^d$ we define $\chi_\ell := \chi_{\ell_1,1}\dots\chi_{\ell_d,d}$. First of all $\sum_{\ell\in\mathbb{Z}^d}\chi_\ell^2 = \left(\sum_{\ell_1\in\mathbb{Z}}\chi_{\ell_1,1}^2\right)\dots\left(\sum_{\ell_d\in\mathbb{Z}}\chi_{\ell_d,d}^2\right) = 1$. Furthermore, for any $x \in \mathbb{R}^{N\times d}$ the family of smooth functions $\{\chi_\ell : \ell \in \mathbb{Z}^d\}$ satisfies $\#\{\ell \in \mathbb{Z}^d : \chi_\ell(x) \neq 0\} = \# \prod_{r=1}^d \{z \in \mathbb{Z} : \chi_{z,r}(x) \neq 0\} \leqslant 2^d$. With the definition $C_d := 2^d C$, where C is the constant from Lemma 2.2.2, we obtain any state $\Psi \in L^2\left(\mathbb{R}^{N\times d}\right)$

$$\sum_{j=1}^N \langle T_j \rangle_\Psi \geqslant \sum_{j=1}^N \sum_{\ell \in \mathbb{Z}^d} \langle T_j \rangle_{\chi_\ell \Psi} - C_d \sum_{j=1}^N \sup_{\ell \in \mathbb{Z}^d} \left\| |\nabla_j \chi_\ell|^2 \right\|_\infty \geqslant \sum_{j=1}^N \sum_{\ell \in \mathbb{Z}^d} \langle T_j \rangle_{\chi_\ell \Psi} - N \frac{C_d d}{\alpha_N^2 k_N^2} \|\nu_0'\|_\infty^2,$$

where we used the fact that $|\nabla_j \chi_\ell|^2 \leqslant \sum_{r=1}^d |\partial_j \chi_{\ell_r, r}|^2 \leqslant \sum_{r=1}^d \frac{1}{\alpha_N^2} \|\nu_{\ell_r}'\|_\infty^2 \|\partial_j M_{N,k_N}\|_\infty^2$, $\|\partial_j M_{N,k_N}\|_\infty \leqslant \frac{1}{k_N}$ and $\|\nu_z'\|_\infty = \|\nu_0'\|_\infty$ for any $z \in \mathbb{Z}$. By our choice of α_N it is clear that $\epsilon_N := N \frac{C_d d}{\alpha_N^2 k_N^2} \|\nu_0'\|_\infty^2 \underset{N\to\infty}{\longrightarrow} 0$. In the following let Φ_N be a sequence of states with $\langle H_N \rangle_{\Phi_N} - E_N \underset{N\to\infty}{\longrightarrow} 0$, and let us define $\rho_{N,\ell} := \|\chi_\ell \Phi_N\|^2$ as well as $\Phi_{N,\ell} := \rho_{N,\ell}^{-\frac{1}{2}} \chi_\ell \Phi_N$. Since Φ_N is a state, it is clear that $\sum_\ell \rho_{N,\ell} = 1$. We have the estimate

$$\sum_{\ell \in \mathbb{Z}^d} \rho_{N,\ell} \langle H_N \rangle_{\Phi_{N,\ell}} \leqslant \sum_{j=1}^N \langle T_j \rangle_{\Phi_N} + \epsilon_N + \frac{1}{N-1} \sum_{i<j} \langle v(x_i - x_j) \rangle_{\Phi_N} = \langle H_N \rangle_{\Phi_N} + \epsilon_N,$$

and therefore there exists at least one $l \in \mathbb{Z}^d$ such that $\langle H_N \rangle_{\Phi_{N,\ell}} \leqslant \langle H_N \rangle_{\Phi_N} + \epsilon_N$. We can finally define $\Psi_N\left(x^{(1)}, \ldots, x^{(N)}\right) := \Phi_{N,\ell}\left(x^{(1)} + \xi, \ldots, x^{(N)} + \xi\right)$ with $\xi := \alpha_N \ell$. By translation-invariance of H_N, we have $\langle H_N \rangle_{\Psi_N} \leqslant \langle H_N \rangle_{\Phi_N} + \epsilon_N$ and consequently $\langle H_N \rangle_{\Psi_N} - E_N \underset{N\to\infty}{\longrightarrow} 0$. Furthermore, $\Psi_N\left(x^{(1)}, \ldots, x^{(N)}\right) \neq 0$ implies for all $r \in \{1, \ldots, d\}$

$$\frac{1}{\alpha_N} M_{N,k_N}\left(x_r^{(1)} + \xi_r, \ldots, x_r^{(N)} + \xi_r\right) = \frac{1}{\alpha_N} M_{N,k_N}\left(x_r^{(1)}, \ldots, x_r^{(N)}\right) + \ell_r \in \operatorname{supp}(\nu_{\ell_r}),$$

and therefore $M_{N,k_N}\left(x_r^{(1)}, \ldots, x_r^{(N)}\right) \in (-\alpha_N, \alpha_N)$. ∎

Recall the inequality $-(\lambda T + \Lambda) \leqslant v \leqslant |v| \leqslant \Lambda(T+1)$ from Assumption 2.1.1. Let us denote with $\hat{v} := v(x-y)$ the two body multiplication operator associated to the interaction potential v. Due to the translation-invariance of T, we can promote the one body operator inequality from above to the two body operator inequality

$$-(\lambda T + \Lambda) \otimes 1_{L^2(\mathbb{R}^d)} \leqslant \hat{v} \leqslant |\hat{v}| \leqslant \Lambda(T+1) \otimes 1_{L^2(\mathbb{R}^d)}.$$

As an immediate consequence of this inequality we have the following Lemma.

Lemma 2.2.4. *Given Assumption 2.1.1, there exist constants c and $\delta > 0$ such that*

$$\delta \sum_{j=1}^N (T_j - c) \leqslant H_N \leqslant \delta^{-1} \sum_{j=1}^N (T_j + c),$$

as well as $\frac{1}{N-1} \sum_{i<j} |v(x_i - x_j)| \leqslant c\,(H_N + N)$.

Definition 2.2.5. Let us define $n_{N,r,L} : \mathbb{R}^{N\times d} \longrightarrow \mathbb{R}$ as the density of particles $x^{(j)} \in \mathbb{R}^d$ that satisfy $x_r^{(j)} \geqslant L$, i.e. for a configuration $x = \left(x^{(1)}, \ldots, x^{(N)}\right) \in \mathbb{R}^{N\times d}$ with $x^{(j)} = \left(x_1^{(j)}, \ldots, x_d^{(j)}\right) \in \mathbb{R}^d$ we define

$$n_{N,r,L}(x) := \frac{1}{N} \sum_{j=1}^N \mathbb{1}_{[L,\infty)}\left(x_r^{(j)}\right).$$

Furthermore, let $\Omega_{N,r,L,\delta}$ be the set of all $x \in \mathbb{R}^{N\times d}$ that satisfy $n_{N,r,L}(x) \geqslant \delta$ and $M_{N,k_N}\left(x_r^{(1)},\dots,x_r^{(N)}\right) \leqslant \xi_0$, where k_N is the sequence introduced in Lemma 2.2.3 and ξ_0 is some fixed positive number. Let $E_{N,r,L,\delta}$ denote the ground state energy of H_N restricted to states Φ with $\mathrm{supp}(\Phi) \subset \Omega_{N,r,L,\delta}$.

Lemma 2.2.6. *Given Assumption 2.1.1, there exist for all $\delta > 0$ constants $\gamma_\delta > 0$, $L_0(\delta)$ and $N_0(\delta)$, such that for all $r \in \{1,\dots,d\}$, $L \geqslant L_0(\delta)$ and $N \geqslant N_0(\delta)$*

$$E_{N,r,L,\delta} \geqslant E_N + \gamma_\delta N. \tag{2.2.1}$$

Proof. According to Definition 2.2.5, for any configuration $x = \left(x^{(1)},\dots,x^{(N)}\right) \in \Omega_{N,r,L,\delta}$ there are at least $\frac{N}{2} - k_N$ particles $x^{(j)}$ such that $x_r^{(j)} \leqslant \xi_0$ and at least δN particles $x^{(k)}$ such that $x_r^{(k)} \geqslant L$. Heuristically, this means that $\frac{N}{2}$ particles do not interact with δN particles in case $L - \xi_0$ is large compared to the range of the interaction v. Since the interaction in Eq. (2.1.1) scales like $\frac{1}{N}$, the absence of $\frac{N}{2} \times \delta N$ interaction pairs corresponds to an increase in energy of order N. In order to make this rigorous, i.e. in order to verify Eq. (2.2.1), we will apply the ideas of geometric localization from [73, 71]. In the first step, we decompose the energy $\langle H_N\rangle_\Psi$ of a state Ψ into a term E_- covering contributions from the left side $x_r^{(j)} \leqslant \xi + R$ with $\xi > \xi_0$ and $\xi + R < L$, a term E_+ covering contributions from the right side $x_r^{(j)} \geqslant \xi$ and a localization error depending on the length R of the overlap $[\xi, \xi+R]$ of the two regions, which can be neglected for large separations $R \gg 1$. In the second step, we will verify that the sum of the local energies $E_- + E_+$ is indeed larger than the ground state energy E_N by a contribution of order N, which corresponds to the observation that $E_- + E_+$ does not involve any interactions between particles on the left side and particles on the right side.

In the following let us fix an $r \in \{1,\dots,d\}$, and let $f_-, f_+ : \mathbb{R} \longrightarrow [0,1]$ be smooth functions with $f_-^2 + f_+^2 = 1$, $f_-(t) = 1$ for $t \leqslant 0$ and $f_+(t) = 1$ for $t \geqslant 1$. Then we define for $\xi \in \mathbb{R}$ and $R > 0$ the functions $f_{\xi,R,\pm} : \mathbb{R}^d \longrightarrow [0,1]$ as $f_{\xi,R,\pm}(x) := f_\pm\left(\frac{x_r - \xi}{R}\right)$. This family of functions clearly satisfies $f_{\xi,R,-}(x) = 1$ for $x_r \leqslant \xi$, $f_{\xi,R,-}(x) = 0$ for $x_r \geqslant \xi + R$, $f_{\xi,R,+}(x) = 1$ for $x_r \geqslant \xi + R$ and $f_{\xi,R,+}(x) = 0$ for $x_r \leqslant \xi$. Furthermore, there exists a constant $k > 0$ such that $|\nabla f_{\xi,R,\pm}|^2 \leqslant \frac{k}{R^2}$. By Lemma 2.2.2 we have the IMS localization formula $T \geqslant f_{\xi,R,-} T f_{\xi,R,-} + f_{\xi,R,+} T f_{\xi,R,+} - \frac{K}{R^2}$, $K := 2kC$. For a state $\Psi \in \bigotimes_{\mathrm{s}}^N L^2\left(\mathbb{R}^d\right)$, let us denote with $\gamma^{(k)}$ its reduced density matrices and with $\rho^{(k)}$ the corresponding density functions, and let us further define the localized objects $\gamma^{(k)}_{\xi,R,\pm} := f_{\xi,R,\pm}^{\otimes^k} \gamma^{(k)} f_{\xi,R,\pm}^{\otimes^k}$ and the corresponding density functions $\rho^{(k)}_{\xi,R,\pm}(x_1,\dots,x_k) := \rho^{(k)}(x_1,\dots,x_k) f_{\xi,R,\pm}(x_1)^2 \dots f_{\xi,R,\pm}(x_k)^2$. Then,

$$\begin{aligned}
\frac{1}{N}\langle H_N\rangle_\Psi &= \mathrm{Tr}\left[\gamma^{(1)}\, T\right] + \frac{1}{2}\int\int \rho^{(2)}(x,y) v(x-y)\mathrm{d}x\mathrm{d}y \\
&= \mathrm{Tr}\left[\gamma^{(1)} T\right] + \frac{1}{2}\int\int \rho^{(2)}(x,y)\left[f_{\xi,R,-}^2 + f_{\xi,R,+}^2\right](x)\left[f_{\xi,R,-}^2 + f_{\xi,R,+}^2\right](y)\; v(x-y)\mathrm{d}x\mathrm{d}y \\
&\geqslant E_- + E_+ + \int\int \rho^{(2)}(x,y) f_{\xi,R,-}(x)^2 f_{\xi,R,+}(y)^2 v(x-y)\mathrm{d}x\mathrm{d}y - \frac{K}{R^2},
\end{aligned}$$

where we define

$$E_\pm = \mathrm{Tr}\left[\gamma^{(1)}_{\xi,R,\pm}\, T\right] + \frac{1}{2}\int\int \rho^{(2)}_{\xi,R,\pm}(x,y) v(x-y)\mathrm{d}x\mathrm{d}y. \tag{2.2.2}$$

Note that we have $v_R := \sup_{|x|\geqslant R} |v(x)| \underset{R\to\infty}{\longrightarrow} 0$ by Assumption 2.1.1, and therefore we can estimate the localization error $\left|\iint \rho^{(2)}(x,y) f_{\xi,R,-}(x_r)^2 f_{\xi,R,+}(y_r)^2 v(x-y)\right|$ by

$$\int\int_{[|x_r-y_r|<R]} \rho^{(2)}(x,y) f_{\xi,R,-}(x)^2 f_{\xi,R,+}(y)^2 |v(x-y)| \mathrm{d}x\mathrm{d}y + v_R \int\int \rho^{(2)}(x,y)\mathrm{d}x\mathrm{d}y$$
$$\leqslant \int\int_{[|x_r-\xi|<R]} \rho^{(2)}(x,y)|v(x-y)|\mathrm{d}x\mathrm{d}y + v_R,$$

where we used the fact that $x \in \operatorname{supp}(f_{\xi,R,-})$, $y \in \operatorname{supp}(f_{\xi,R,+})$ and $|x_r - y_r| < R$ is only possible in case $|x_r - \xi| < R$. Let us now define for $n \in \mathbb{N}$ and $m \leqslant n$ the points $\xi_m := \xi_0 + 2Rm$. Clearly, the intervals $[|x_r - \xi_m| < R]$ are disjoint and therefore Lemma 2.2.4 yields

$$\sum_{m=1}^{n} \int\int_{[|x_r-\xi_m|<R]} \rho^{(2)}(x,y)|v(x-y)|\mathrm{d}x\mathrm{d}y \leqslant \int\int \rho^{(2)}(x,y)|v(x-y)|\mathrm{d}x\mathrm{d}y \leqslant \frac{2c}{N}\langle H_N\rangle_\Psi + 2c.$$

Hence, there exists an $m_* \leqslant n$ such that $\iint_{[|x_r-\xi_{m_*}|<R]} \rho^{(2)}(x,y)|v(x-y)| \leqslant \frac{2c}{nN}\langle H_N\rangle_\Psi + \frac{2c}{n}$. We conclude that for $n \in \mathbb{N}$, there exists a ξ with $\xi_0 \leqslant \xi \leqslant \xi_0 + 2nR$ such that

$$\frac{1+\frac{2c}{n}}{N}\langle H_N\rangle_\Psi \geqslant E_- + E_+ - \frac{K}{R^2} - v_R - \frac{2c}{n}. \tag{2.2.3}$$

Let us now investigate the local energy contributions $E_\pm$. As a first step, we follow the framework in [71] and define the mixed ℓ particle states

$$G_{\ell,\pm} = \binom{N}{\ell} \mathrm{Tr}_{\ell+1\to N}\left[f_{\xi,R,\pm}^{\otimes \ell} \otimes f_{\xi,R,\mp}^{\otimes N-\ell} \;\; |\Psi\rangle\langle\Psi| \;\; f_{\xi,R,\pm}^{\otimes \ell} \otimes f_{\xi,R,\mp}^{\otimes N-\ell}\right],$$

where we used the notion $\mathrm{Tr}_{\ell+1\to N}[\;.\;]$ for the partial trace over the indices $\ell+1,\ldots,N$. These mixed states satisfy $\mathrm{Tr}[G_{\ell,-}] = \mathrm{Tr}[G_{N-\ell,+}]$ as well as $\sum_{\ell=0}^N \mathrm{Tr}[G_{\ell,-}] = 1$. Furthermore, it was shown in [71] that we can use these mixed states to express the localized density matrices as

$$f_{\xi,R,\pm}^{\otimes k}\;\gamma^{(k)}\;f_{\xi,R,\pm}^{\otimes k} = \binom{N}{k}^{-1}\sum_{\ell=k}^{N}\binom{\ell}{k} G_{\ell,\pm}^{(k)}, \tag{2.2.4}$$

where $G_{\ell,\pm}^{(k)}$ is the k-th reduced density matrix of $G_{\ell,\pm}$. In the following, let us assume that the state Ψ satisfies $\operatorname{supp}(\Psi) \subset \Omega_{N,r,L_0,\delta}$ with $\delta > 0$ and $L_0 > \xi_0 + R$, i.e. all $x \in \operatorname{supp}(\Psi)$ satisfy $M_{N,k_N}(x) \leqslant \xi_0$ and $n_{N,r,L_0}(x) \geqslant \delta$. The first condition $M_{N,k_N}(x) \leqslant \xi_0$ implies that at most $\frac{N}{2} + k_N$ indices j satisfy $x_r^{(j)} > \xi_0$ and the second condition $n_{N,r,L_0}(x) \geqslant \delta$ is equivalent to the fact that at most $\lceil (1-\delta)N \rceil$ indices satisfy $x_r^{(j)} < L_0$. Let us denote $N_*(N) := \max\left(\frac{N}{2} + k_N, \lceil (1-\delta)N\rceil\right)$. From the support properties of $f_{\xi,R,\pm}$ we obtain for all ξ with $\xi_0 < \xi < L_0 - R$ and $x \in \operatorname{supp}(\Psi)$, that $f_{\xi,R,+}\left(x^{(1)}\right)\ldots f_{\xi,R,+}\left(x^{(\ell)}\right) = 0$ for all $\ell > N_*(N)$ and $f_{\xi,R,-}\left(x^{(\ell+1)}\right)\ldots f_{\xi,R,-}\left(x^{(N)}\right) = 0$ for all $N - \ell > N_*(N)$. Hence, we obtain for all ℓ with either $\ell > N_*(N)$ or $\ell < N - N_*(N)$, and ξ with $\xi_0 < \xi < L_0 - R$

$$\binom{N}{\ell}^{-1}\mathrm{Tr}\left[G_{\ell,+}\right] = \mathrm{Tr}\left[f_{\xi,R,+}^{\otimes \ell}\otimes f_{\xi,R,-}^{\otimes N-\ell}\;\;|\Psi\rangle\langle\Psi|\;\;f_{\xi,R,+}^{\otimes \ell}\otimes f_{\xi,R,-}^{\otimes N-\ell}\right]$$
$$= \int_{\operatorname{supp}(\Psi)} f_{\xi,R,+}\left(x^{(1)}\right)^2\ldots f_{\xi,R,+}\left(x^{(\ell)}\right)^2 f_{\xi,R,-}\left(x^{(\ell+1)}\right)^2\ldots f_{\xi,R,-}\left(x^{(N)}\right)^2|\Psi|^2\,\mathrm{d}x = 0,$$

and since $G_{\ell,+} \geqslant 0$ this implies $G_{\ell,+} = 0$ for all such ℓ. Using $\mathrm{Tr}[G_{\ell,-}] = \mathrm{Tr}[G_{N-\ell,+}]$, we also obtain $G_{\ell,-} = 0$ for all ℓ with $\ell > N_*(N)$, respectively $\ell < N - N_*(N)$.

Let us define rescaled versions $H_\ell^{(\lambda)} := \sum_{j=1}^{\ell} T_j + \frac{1}{\ell-1}\sum_{i<j}^{\ell} \lambda v(x_i - x_j)$ of the Hamiltonian H_N and let us denote the corresponding ground state energy by $E_\ell^{(\lambda)} := \inf \sigma\left(H_\ell^\lambda\right)$. Note that there exists a δ-dependent $\kappa_\delta < 1$ and $N_1 \in \mathbb{N}$, such that $\frac{N_*(N)-1}{N-1} \leqslant \kappa_\delta$ for all $N \geqslant N_1$. Applying Eq. (2.2.4) together with the identity $\mathrm{Tr}\left[G_{\ell,\pm}^{(1)}\, T\right] + \frac{l-1}{N-1}\frac{1}{2}\mathrm{Tr}\left[G_{\ell,\pm}^{(2)}\, \hat{v}\right] = \mathrm{Tr}\left[\frac{1}{\ell} H_\ell^{\left(\frac{\ell-1}{N-1}\right)}\, G_{\ell,\pm}\right]$ yields for all $N \geqslant N_1$ and ξ with $\xi_0 < \xi < L_0 - R$

$$\begin{aligned} E_\pm &= \mathrm{Tr}\left[\gamma_{\xi,R,\pm}^{(1)}\, T\right] + \frac{1}{2}\int\int \rho_{\xi,R,\pm}^{(2)}(x,y) v(x-y)\mathrm{d}x\mathrm{d}y = \frac{1}{N}\sum_{\ell=N-N_*(N)}^{N_*(N)} \mathrm{Tr}\left[H_\ell^{\left(\frac{\ell-1}{N-1}\right)}\, G_{\ell,\pm}\right] \\ &\geqslant \frac{1}{N}\sum_{\ell=N-N_*(N)}^{N_*(N)} E_\ell^{\left(\frac{l-1}{N-1}\right)}\, \mathrm{Tr}\left[G_{\ell,\pm}\right] \geqslant \frac{1}{N}\sum_{l=N-N_*(N)}^{N} \kappa_\delta E_\ell\, \mathrm{Tr}\left[G_{\ell,\pm}\right] \\ &\geqslant \kappa_\delta \min_{\ell \geqslant N-N_*(N)} \left(\frac{1}{\ell}E_\ell\right) \frac{1}{N}\sum_{l=0}^{N} \ell\, \mathrm{Tr}\left[G_{\ell,\pm}\right], \end{aligned}$$

where we used $H_k^{(\lambda_1)} \geqslant \frac{\lambda_1}{\lambda_2} H_k^{(\lambda_2)}$ for all $\lambda_1 \leqslant \lambda_2$ as well as the fact that $E_\ell = E_\ell^{(1)} < 0$, which is a direct consequence of the assumption $e_{\mathrm{H}} < 0$. Observe that

$$\frac{1}{N}\sum_{l=0}^{N} \ell\, \mathrm{Tr}\left[G_{\ell,-}\right] + \frac{1}{N}\sum_{l=0}^{N} \ell\, \mathrm{Tr}\left[G_{\ell,+}\right] = \frac{1}{N}\sum_{l=0}^{N} \ell\, \mathrm{Tr}\left[G_{\ell,-}\right] + \frac{1}{N}\sum_{l=0}^{N}(N-\ell)\, \mathrm{Tr}\left[G_{\ell,-}\right] = 1,$$

and consequently we obtain for all $N \geqslant N_1$ and ξ with $\xi_0 < \xi < L_0 - R$ the estimate

$$E_- + E_+ \geqslant \kappa_\delta \min_{\ell \geqslant N-N_*(N)} \frac{1}{\ell} E_\ell, \tag{2.2.5}$$

where $E_\pm$ is defined in Eq. (2.2.2). Furthermore, Assumption 2.1.1 enables us to apply the results in [71], which tell us that $\lim_\ell \frac{1}{\ell}E_\ell = e_{\mathrm{H}}$, and since $N - N_*(N) \underset{N\to\infty}{\longrightarrow} \infty$, we obtain that $\min_{\ell\geqslant N-N_*(N)} \frac{1}{\ell}E_\ell \underset{N\to\infty}{\longrightarrow} e_{\mathrm{H}}$ as well. For $R > 0$ and $n \in \mathbb{N}$, let us define $L_0 := \xi_0 + (2n+1)R$. Combining Inequalities (2.2.3) and (2.2.5), we obtain

$$\liminf_{N\to\infty} \frac{1}{N}\left[\left(1 + \frac{2c}{n}\right) E_{N,r,L_0,\delta} - E_N\right] \geqslant (\kappa_\delta - 1)e_{\mathrm{H}} - \frac{K}{R^2} - v_R - \frac{2c}{n}.$$

Since $\kappa_\delta < 1$ and $e_{\mathrm{H}} < 0$, we can choose R_δ and n_δ large enough, such that $\beta_\delta := (\kappa_\delta - 1)e_{\mathrm{H}} - \frac{K}{R_\delta^2} - v_{R_\delta} - \frac{2c}{n_\delta} > 0$. With the choice $L_0(\delta) := \xi_0 + (2n_\delta + 1)R_\delta$ we conclude

$$\begin{aligned} \liminf_{N\to\infty} \frac{1}{N}\left[E_{N,r,L_0(\delta),\delta} - E_N\right] &\geqslant \liminf_{N\to\infty} \frac{1}{N}\left(\min\left[\left(1 + \frac{2c}{n_\delta}\right) E_{N,r,L_0(\delta),\delta},\ 0\right] - E_N\right) \\ &\geqslant \min\left(\beta_\delta, -e_{\mathrm{H}}\right) > 0. \end{aligned}$$

■

Corollary 2.2.7. *Let Assumption 2.1.1 hold and Ψ_N be a sequence as in Lemma 2.2.3. Then,*

$$\lim_{L\to\infty} \limsup_{N\to\infty} \langle n_{N,r,L}\rangle_{\Psi_N} = 0$$

for any $r \in \{1, \ldots, d\}$.

Proof. In the following, let $\chi : \mathbb{R} \longrightarrow [0,1]$ be a function with $\chi(x) = 0$ for $x \leqslant 1$ and $\chi(x) = 1$ for $x \geqslant 2$, such that χ and $\sqrt{1-\chi^2}$ are C^∞. Then we define

$$f_{N,r,L,\delta}(x) := \chi\left(\frac{1}{\delta N}\sum_{j=1}^{N}\chi\left(\frac{2x_r^{(j)}}{L}\right)\right),$$

$g_{N,r,L,\delta}(x) := \sqrt{1-f_{N,r,L,\delta}^2}$ and $\alpha := \|\chi'\|_\infty^2\left(\|\chi'\|_\infty^2 + \|\sqrt{1-\chi^2}'\|_\infty^2\right)$. Note that we have $\operatorname{supp}(f_{N,r,L,\delta}\Psi_N) \subset \Omega_{N,r,\frac{L}{2},\delta}$. Therefore the localization formula from Lemma 2.2.2 and the result from Lemma 2.2.6 tell us that there exists a $\gamma_\delta > 0$ such that for all $L \geqslant 2L_0(\delta)$ and $N \geqslant N_0(\delta)$

$$\begin{aligned}\langle H_N\rangle_{\Psi_N} &\geqslant \langle H_N\rangle_{f_{N,r,L,\delta}\Psi_N} + \langle H_N\rangle_{g_{N,r,L,\delta}\Psi_N} - \frac{4C}{\delta^2 N L^2}\alpha\\ &\geqslant (E_N + \gamma_\delta N)\|f_{N,r,L,\delta}\Psi_N\|^2 + E_N\left(1-\|f_{N,r,L,\delta}\Psi_N\|^2\right) - \frac{4C}{\delta^2 N L^2}\alpha.\end{aligned}$$

Consequently, $0 \leqslant \|f_{N,r,L,\delta}\Psi_N\|^2 \leqslant \frac{\langle H_N\rangle_{\Psi_N} - E_N + \frac{4C}{\delta^2 N L^2}\alpha}{\gamma_\delta N} \underset{N\to\infty}{\longrightarrow} 0$. Furthermore, note that $x \in \operatorname{supp}(g_{N,r,L,\delta})$ implies $n_{N,r,L}(x) \leqslant \frac{1}{N}\sum_{j=1}^N \chi\left(\frac{2x_r^{(j)}}{L}\right) \leqslant 2\delta$ and therefore

$$0 \leqslant \langle n_{N,r,L}\rangle_{\Psi_N} = \langle n_{N,r,L}\rangle_{f_{N,r,L,\delta}\Psi_N} + \langle n_{N,r,L}\rangle_{g_{N,r,L,\delta}\Psi_N} \leqslant \|f_{N,r,L,\delta}\Psi_N\|^2 + 2\delta \underset{N\to\infty}{\longrightarrow} 2\delta$$

for all $L \geqslant 2L(\delta)$. Hence $\lim_{L\to\infty}\limsup_{N\to\infty}\langle n_{N,r,L}\rangle_{\Psi_N} = 0$. ∎

2.2.2 Convergence to a Single Condensate

It was shown in [71] that under quite general assumptions, including ours, on the decay and regularity of the interaction potential v, there exists for any sequence of states Φ_N with $\langle H_N\rangle_{\Phi_N} = E_N + o(N)$ a probability measure ν supported on the set of (not necessarily normed) Hartree minimizers $\{u \in \mathcal{H} : \mathcal{E}_{\mathrm{H}}[u] = e_{\mathrm{H}}(\|u\|)\}$, where $e_{\mathrm{H}}(s) := \inf_{\|v\|=s}\mathcal{E}_{\mathrm{H}}[v]$, such that a subsequence of the sequence $\gamma_{\Phi_N}^{(k)}$ converges weakly to the state $\int \left(|u\rangle\langle u|\right)^{\otimes^k}\mathrm{d}\nu(u)$ for all $k \in \mathbb{N}$, i.e.

$$\operatorname{Tr}\left[\gamma_{\Phi_{N_j}}^{(k)} B\right] \underset{j\to\infty}{\longrightarrow} \int \operatorname{Tr}\left[\left(|u\rangle\langle u|\right)^{\otimes^k} B\right]\mathrm{d}\nu(u) \tag{2.2.6}$$

for any compact k particle operator B. In Lemma 2.2.8, we will lift this weak convergence to a strong one for the sequence of approximate ground states Ψ_N constructed in Lemma 2.2.3, by using the fact that mass cannot escape to infinity as a consequence of Corollary 2.2.7. In this context, strong convergence means that Eq. (2.2.6) holds for all bounded k particle operators B, and not only compact ones. In particular, $\|u\| = 1$ on the support of ν.

Lemma 2.2.8 (Strong Convergence). *Let Ψ_N be the sequence from Lemma 2.2.3 and let $\gamma_N^{(k)}$ denote the corresponding reduced density matrices. Given Assumption 2.1.1, there exists a probability measure μ supported on $\mathbb{R}^d$ and a subsequence N_j, such that for any bounded k particle operator B*

$$\operatorname{Tr}\left[\gamma_{N_j}^{(k)} B\right] \underset{j\to\infty}{\longrightarrow} \int_{\mathbb{R}^d} \operatorname{Tr}\left[\left(|u_{0,t}\rangle\langle u_{0,t}|\right)^{\otimes^k} B\right]\mathrm{d}\mu(t),$$

where $u_{0,t}$ is defined in Assumption 2.1.1.

Proof. As was shown in [71], any sequence of approximate ground states, such as Ψ_N, has a subsequence N_j that converges weakly to a convex combination of product states over Hartree minimizers, i.e. there exists a probability measure ν supported on the set of Hartree minimizers u with $\|u\| \leqslant 1$, such that Eq. (2.2.6) holds for any compact k particle operator B. As the central step of this proof, we will verify that the measure ν satisfies the identity $\int \|u\|^2 \mathrm{d}\nu(u) = 1$. By Corollary 2.2.7, we know that

$$\lim_{L\to\infty} \limsup_{j\to\infty} \mathrm{Tr}\left[\gamma^{(1)}_{N_j}\ \mathbb{1}_{[x_r>L]}\right] = \lim_{L\to\infty} \limsup_{j\to\infty} \langle n_{N_j,r,L}\rangle_{\Psi_{N_j}} = 0.$$

Since the reflected states $x \mapsto \Psi_N(-x)$ still satisfy the conditions of Corollary 2.2.7, we obtain $\lim_{L\to\infty} \limsup_{j\to\infty} \mathrm{Tr}\left[\gamma^{(1)}_{N_j}\ \mathbb{1}_{[x_r<-L]}\right] = 0$ as well. Consequently,

$$\lim_{L\to\infty} \liminf_{j\to\infty} \mathrm{Tr}\left[\gamma^{(1)}_{N_j}\ \mathbb{1}_{[-L,L]^d}\right] = 1.$$

Since the operator $\mathbb{1}_{[-L,L]^d}$ is not compact, we cannot immediately apply the convergence (2.2.6) for $B := \mathbb{1}_{[-L,L]^d}$. In order to obtain a convergence in a stronger sense, note that by Lemma 2.2.4 we have a uniform bound on the kinetic energy of $\gamma^{(1)}_{N_j}$, i.e. there exists a constant $C < \infty$, such that

$$\mathrm{Tr}\left[(T+1)^{\frac{1}{2}}\ \gamma^{(1)}_{N_j}\ (T+1)^{\frac{1}{2}}\right] \leqslant C$$

for all $j \in \mathbb{N}$. Since the trace class operators are the dual space of the compact operators, there exists by the Banach-Alaoglu theorem a trace class operator γ and a subsequence, which we will still denote by N_j for the sake of readability, such that for any compact one particle operator K

$$\mathrm{Tr}\left[(T+1)^{\frac{1}{2}}\ \gamma^{(1)}_{N_j}\ (T+1)^{\frac{1}{2}}\ K\right] \underset{j\to\infty}{\longrightarrow} \mathrm{Tr}\left[\gamma\ K\right].$$

This in particular yields $\mathrm{Tr}\left[\gamma^{(1)}_{N_j}\ B\right] \underset{j\to\infty}{\longrightarrow} \mathrm{Tr}\left[(T+1)^{-\frac{1}{2}}\ \gamma\ (T+1)^{-\frac{1}{2}}\ B\right]$ for any compact B, and consequently $(T+1)^{-\frac{1}{2}}\ \gamma\ (T+1)^{-\frac{1}{2}} = \int |u\rangle\langle u|\, \mathrm{d}\nu(u)$ by Eq. (2.2.6). Since the kinetic energy is of the form $T = t\,(i\nabla)$ with $t(p) \underset{|p|\to\infty}{\longrightarrow} \infty$, the operator $K := (T+1)^{-\frac{1}{2}}\ \mathbb{1}_{[-L,L]^d}\ (T+1)^{-\frac{1}{2}}$ is compact. Collecting all the results we have obtained so far yields

$$\begin{aligned}
1 &= \lim_{L\to\infty} \liminf_{j\to\infty} \mathrm{Tr}\left[\gamma^{(1)}_{N_j}\ \mathbb{1}_{[-L,L]^d}\right] = \lim_{L\to\infty} \liminf_{j\to\infty} \mathrm{Tr}\left[(T+1)^{\frac{1}{2}}\ \gamma^{(1)}_{N_j}\ (T+1)^{\frac{1}{2}}\ K\right] \\
&= \lim_{L\to\infty} \mathrm{Tr}\left[(T+1)^{-\frac{1}{2}}\ \gamma\ (T+1)^{-\frac{1}{2}}\ \mathbb{1}_{[-L,L]^d}\right] = \lim_{L\to\infty} \int \mathrm{Tr}\left[|u\rangle\langle u|\ \ \mathbb{1}_{[-L,L]^d}\right] \mathrm{d}\nu(u) \\
&= \int \mathrm{Tr}\big[\,|u\rangle\langle u|\,\big] \mathrm{d}\nu(u) = \int \|u\|^2 \mathrm{d}\nu(u).
\end{aligned}$$

As an immediate consequence we obtain that ν is supported on Hartree minimizers u with $\|u\| = 1$. By Assumption 2.1.1, we know that all such Hartree minimizers are given by $e^{i\theta}u_{0,t}$ with $\theta \in [0, 2\pi)$ and $t \in \mathbb{R}^d$. Recall that $|e^{i\theta}u_{0,t}\rangle\langle e^{i\theta}u_{0,t}| = |u_{0,t}\rangle\langle u_{0,t}|$ defines the same density matrix for all complex phases $e^{i\theta}$. Therefore, defining the measure $\mu(A) := \nu\big(\{u_{0,t} : t \in A, \theta \in [0, 2\pi)\}\big)$ yields

$$\mathrm{Tr}\left[\gamma^{(k)}_{N_j}\ B\right] \underset{j\to\infty}{\longrightarrow} \int_{\mathbb{R}^d} \mathrm{Tr}\left[\big(|u_{0,t}\rangle\langle u_{0,t}|\big)^{\otimes^k} B\right] \mathrm{d}\mu(t) \qquad (2.2.7)$$

for all compact operators B. Since $\lim_j \mathrm{Tr}\left[\gamma_{N_j}^{(1)}\right] = 1 = \int_{\mathbb{R}^d} \mathrm{Tr}\left[\, |u_{0,t}\rangle\langle u_{0,t}|\,\right] \mathrm{d}\mu(t)$, this convergence holds even in the strong sense, see [128], i.e. the convergence (2.2.6) holds for all bounded operator B. ∎

Lemma 2.2.9. *Let Ψ_N be the sequence from Lemma 2.2.3. For any $\epsilon > 0$ and $r \in \{1, \ldots, d\}$, consider the bounded two particle operator $B_{\epsilon,r} := \mathbb{1}_{[x_r \leqslant \epsilon]}\, \mathbb{1}_{[y_r \geqslant -\epsilon]} + \mathbb{1}_{[y_r \leqslant \epsilon]}\, \mathbb{1}_{[x_r \geqslant -\epsilon]}$. Then*

$$\liminf_{N\to\infty} \mathrm{Tr}\left[\gamma_N^{(2)}\ B_{\epsilon,r}\right] \geqslant \frac{1}{2}.$$

Proof. With the help of the function $f_{N,\epsilon,r} := \frac{2}{N(N-1)} \sum_{i\neq j} \mathbb{1}_{\left[x_r^{(i)} \leqslant \epsilon\right]} \mathbb{1}_{\left[x_r^{(j)} \geqslant -\epsilon\right]}$ we have

$$\mathrm{Tr}\left[\gamma_N^{(2)} B_{\epsilon,r}\right] = \int_{\mathbb{R}^{N\times d}} f_{N,\epsilon,r}(x) |\Psi_N|^2 \mathrm{d}x.$$

Let α_N and k_N be the sequences introduced in Lemma 2.2.3 and let N be large enough such that $\alpha_N < \epsilon$. Then, $\left|M_{N,k_N}\left(x_r^{(1)}, \ldots, x_r^{(N)}\right)\right| < \epsilon$ for all $x \in \mathrm{supp}\,(\Psi_N)$, and therefore at least $\frac{N}{2} - k_N$ particles satisfy $x_r \leqslant \epsilon$ and at least $\frac{N}{2} - k_N$ particles satisfy $-\epsilon \leqslant x_r$. Consequently

$$f_{N,\epsilon,r}(x) \geqslant \frac{2}{N(N-1)} \left(\frac{N}{2} - k_N\right)^2 \underset{N\to\infty}{\longrightarrow} \frac{1}{2},$$

and therefore $\liminf_{N\to\infty} \int_{\mathbb{R}^{N\times d}} f_{N,\epsilon,r}(x) |\Psi_N|^2\ \mathrm{d}x \geqslant \frac{1}{2}$. ∎

Lemma 2.2.10. *The measure μ from Lemma 2.2.8 is supported on $\{0\} \subset \mathbb{R}^d$, i.e. $\mu = \delta_0$.*

Proof. Let us define the density function $\rho(x) := |u_0(x)|^2$, as well as the marginal density function $\rho_r(x_r) := \int \rho(x)\ \mathrm{d}x_1 \ldots \mathrm{d}x_{r-1} \mathrm{d}x_{r+1} \ldots \mathrm{d}x_d$ and the marginal measure $\mu_r(A) := \mu\left([x_r \in A]\right)$. Note that the two particle density function corresponding to $\left(|u_{0,t}\rangle\langle u_{0,t}|\right)^{\otimes 2}$ is given by $\rho(x-t)\rho(y-t)$, and therefore Lemmata 2.2.8 and 2.2.9 imply

$$\begin{aligned}
\frac{1}{2} &\leqslant \lim_j \mathrm{Tr}\left[\gamma_{N_j}^{(2)}\ B_{\epsilon,r}\right] = \int_{\mathbb{R}^d} \mathrm{Tr}\left[\left(|u_{0,t}\rangle\langle u_{0,t}|\right)^{\otimes 2} B_{\epsilon,r}\right] \mathrm{d}\mu(t) \\
&= 2\int_{\mathbb{R}} \left(\int_{-\infty}^{t_r+\epsilon} \rho_r(x_r)\mathrm{d}x_r\right)\left(\int_{t_r-\epsilon}^{\infty} \rho_r(x_r)\mathrm{d}x_r\right) \mathrm{d}\mu_r(t_r) \\
&= 2\int_{\mathbb{R}} f_r\left(t_r+\epsilon\right)\left(1 - f_r\left(t_r-\epsilon\right)\right)\ \mathrm{d}\mu_r(t_r) \underset{\epsilon\to 0}{\longrightarrow} 2\int_{\mathbb{R}} f_r(t_r)\left(1 - f_r(t_r)\right)\ \mathrm{d}\mu_r(t_r)
\end{aligned}$$

with the definition $f_r(s) := \int_{-\infty}^{s} \rho_r(x_r)\ \mathrm{d}x_r$, where we have used dominated convergence and continuity of f_r. Hence we obtain the inequality

$$\int_{\mathbb{R}} f_r(t_r)\left(1 - f_r(t_r)\right)\ \mathrm{d}\mu_r(t_r) \geqslant \frac{1}{4}.$$

Since the function $h(q) := q(1-q)$ is bounded by $\frac{1}{4}$ and attains its maximum only for $q = \frac{1}{2}$, we conclude $f_r(s) = \frac{1}{2}$ μ_r-almost everywhere. On the other hand, by Assumption 2.1.1 we know that $\int_{-\infty}^{s} \rho_r(x_r)\ \mathrm{d}x_r = \frac{1}{2}$ if and only if $s = 0$ and therefore $f_r(s) \neq \frac{1}{2}$ for all $s \neq 0$. This together with the fact $f_r(s) = \frac{1}{2}$ μ_r-almost everywhere, implies $\mu_r = \delta_0$. Since this holds for all marginal measures μ_r with $r \in \{1, \ldots, d\}$, we conclude $\mu = \delta_0$. ∎

By choosing the bounded one particle operator B as the projection onto the state u_0, Theorem 2.1.2 is a direct consequence of Lemmata 2.2.8 and 2.2.10.

2.3 Fock Space Formalism

In order to prove Theorem 2.1.4, we will make use of the correspondence between the Hartree energy $\mathcal{E}_{\mathrm{H}}$ and the Hamiltonian H_N. For a rigorous treatment of this correspondence, we first need to formulate our problem in the language of second quantization. In the subsequent Definition 2.3.1 we will define the necessary formalism including the relevant Fock spaces with the corresponding creation and annihilation operators. Following [72], we will use the excitation map U_N in order to arrive at an operator $U_N H_N U_N^{-1}$ that only depends on modes a_i, $i > 0$, describing excitations, and not on the mode a_0 corresponding to the condensate u_0. The usefulness of this stems from the fact that all the modes a_i, $i > 0$, can be thought of as being small due to Bose–Einstein condensation.

Before we start introducing the Fock space formalism, let us fix some notation. In the following we will repeatedly use the notation $A \cdot B$ for the composition of an operator $B : \mathcal{H}_1 \longrightarrow \mathcal{H}_2$ with an operator $A : \mathcal{H}_2 \longrightarrow \mathcal{H}_3$, especially when we want to stress that the involved operators map different Hilbert spaces. In order to have a consistent notation, we will occasionally write expectation values as operator products by identifying an element $u \in L^2(\mathbb{R})$ with a linear map $\mathbb{C} \longrightarrow L^2(\mathbb{R})$, e.g. we write $u^\dagger \cdot T \cdot u$ for the expectation value $\langle T \rangle_u$. Furthermore, recall the real orthonormal basis $u_0, u_1, \ldots, u_d, u_{d+1}, \ldots$ from the introduction, where u_0 is the Hartree minimizer from Assumption 2.1.1 and $u_1, \ldots, u_d$ form a basis of the vector space spanned by the partial derivatives $\partial_{x_1} u_0, \ldots, \partial_{x_d} u_0$. Moreover, let us define the spaces

$$\mathcal{H} : = L^2\big(\mathbb{R}^d\big),$$
$$\mathcal{H}_0 : = \{u_0\}^\perp \subset \mathcal{H}.$$

Definition 2.3.1. Let us denote with $a_j := a_{u_j}$ the annihilation operator corresponding to $u_j \in \mathcal{H}$ and $\mathcal{N}_{\geqslant k} := \sum_{j=k}^\infty a_j^\dagger a_j$. In the following, we will repeatedly use the Fock spaces $\mathcal{F} := \mathcal{F}(\mathcal{H})$, $\mathcal{F}_0 := \mathcal{F}(\mathcal{H}_0)$ and $\mathcal{F}_{\leqslant M} := \mathbb{1}_{[\mathcal{N} \leqslant M]} \mathcal{F}_0 \subset \mathcal{F}_0$, where $\mathcal{N} := \mathcal{N}_{\geqslant 1}$. For any $k \in \mathbb{N}_0$ we define the operator $a_{\geqslant k} : \mathrm{dom}\left(\sqrt{\mathcal{N}_{\geqslant k}}\right) \longrightarrow \mathcal{F} \otimes \mathcal{H}$ as

$$a_{\geqslant k} := \sum_{j=k}^\infty a_j \otimes u_j,$$

as well as the re-scaled operator $b_{\geqslant k} := \sum_{j=k}^\infty b_j \otimes u_j := \frac{1}{\sqrt{N}} a_{\geqslant k}$, and the re-scaled and restricted operator $\mathbb{L} := \frac{1}{N} \mathcal{N}\big|_{\mathcal{F}_{\leqslant N}} : \mathcal{F}_{\leqslant N} \longrightarrow \mathcal{F}_{\leqslant N}$, where we suppress the N dependence of $b_{\geqslant k}$ and $\mathbb{L}$ in our notation. Furthermore, given two operators $X = \sum_{i=0}^\infty X_i \otimes u_i$: $\mathrm{dom}(X) \longrightarrow \mathcal{F} \otimes \mathcal{H}$ and $Y = \sum_{i=0}^\infty Y_i \otimes u_i : \mathrm{dom}(Y) \longrightarrow \mathcal{F} \otimes \mathcal{H}$ defined on subsets $\mathrm{dom}(X), \mathrm{dom}(Y) \subset \mathcal{F}$, we define the product operator $X \underline{\otimes} Y : \mathcal{D} \longrightarrow \mathcal{F} \otimes \mathcal{H} \otimes \mathcal{H}$, with $\mathcal{D} := \{\Psi \in \mathcal{F} : \sum_{i,j=0}^\infty \|X_i Y_j \Psi\|^2 < \infty\}$, as

$$X \underline{\otimes} Y := X \otimes 1_{\mathcal{H}} \cdot Y = \sum_{i,j=0}^\infty (X_i Y_j) \otimes u_i \otimes u_j,$$

where we use the convention that tensor products are performed before operator products, i.e. $X \otimes 1_{\mathcal{H}} \cdot Y := (X \otimes 1_{\mathcal{H}}) \cdot Y$.

Remark 2.3.2. Recall that T is an operator acting on the one particle space $\mathcal{H}$ and $\hat{v} := v(x-y)$ is an operator acting on the two particle space $\mathcal{H} \otimes \mathcal{H}$. Then, $1_{\mathcal{F}} \otimes T$ is an operator on $\mathcal{F} \otimes \mathcal{H}$ and $1_{\mathcal{F}} \otimes \hat{v}$ operates on $\mathcal{F} \otimes \mathcal{H} \otimes \mathcal{H}$. With this, we have a convenient way to express double and four fold sums of creation and annihilation operators

$$b^\dagger_{\geqslant 0} \cdot\ 1_{\mathcal{F}} \otimes T \cdot b_{\geqslant 0} = \sum_{i,j=0}^{\infty} T_{i,j}\ b_i^\dagger b_j,$$
$$\left(b_{\geqslant 0} \underline{\otimes}\, b_{\geqslant 0}\right)^\dagger \cdot 1_{\mathcal{F}} \otimes \hat{v} \cdot b_{\geqslant 0} \underline{\otimes}\, b_{\geqslant 0} = \sum_{ij,k\ell=0}^{\infty} \hat{v}_{ij,k\ell}\ b_i^\dagger b_j^\dagger b_k b_\ell.$$

In order to avoid issues with operator domains, we will define products of the form $\left(b_{\geqslant 0} \underline{\otimes}\, b_{\geqslant 0}\right)^\dagger \cdot 1_{\mathcal{F}} \otimes \hat{v} \cdot b_{\geqslant 0} \underline{\otimes}\, b_{\geqslant 0}$ as quadratic forms, i.e. we define the quadratic form

$$\left\langle \left(b_{\geqslant 0} \underline{\otimes}\, b_{\geqslant 0}\right)^\dagger \cdot\ \left(1_{\mathcal{F}} \otimes \hat{v}\right) \cdot \left(b_{\geqslant 0} \underline{\otimes}\, b_{\geqslant 0}\right) \right\rangle_{\Psi} := \left\langle 1_{\mathcal{F}} \otimes \hat{v} \right\rangle_{b_{\geqslant 0} \underline{\otimes} b_{\geqslant 0} \Psi}.$$

For the sake of readability, we will suppress the tensor with the identity in our notation, i.e. we will simply write $b^\dagger_{\geqslant 0} \cdot\ T \cdot b_{\geqslant 0}$ and $\left(b_{\geqslant 0} \underline{\otimes}\, b_{\geqslant 0}\right)^\dagger \cdot\ \hat{v} \cdot b_{\geqslant 0} \underline{\otimes}\, b_{\geqslant 0}$.

In the following, we will make use of the fact that we can express the Hamiltonian in Eq. (2.1.1) in terms of the rescaled creation and annihilation operators as

$$N^{-1} H_N = b^\dagger_{\geqslant 0} \cdot\ T \cdot b_{\geqslant 0} + \frac{N}{2(N-1)} \left(b_{\geqslant 0} \underline{\otimes}\, b_{\geqslant 0}\right)^\dagger \cdot\ \hat{v} \cdot b_{\geqslant 0} \underline{\otimes}\, b_{\geqslant 0}. \tag{2.3.1}$$

Since the Hamiltonian H_N is only defined on the subset $\bigotimes_{\mathrm{s}}^N \mathcal{H} \subset \mathcal{F}$, the equation above only holds in this subspace of fixed particle number N. In order to focus on excitations above the condensate, we follow the strategy in [72] and map the Hamiltonian H_N to an operator which acts on the truncated Fock space $\mathcal{F}_{\leqslant N}$ of modes orthogonal to u_0 with the help of the excitation map U_N. We will think of this map U_N as the quantum counterpart to the embedding of the disc $\{z \in \{u_0\}^\perp : \|z\| \leqslant 1\}$ into the sphere $\{u \in \mathcal{H} : \|u\| = 1\}$ via the map ι defined in Eq. (2.1.10). The proof of the following properties of U_N is elementary and is left to the reader.

Lemma 2.3.3. *Recall the definition of the operator $\mathbb{L}$ in Definition 2.3.1 and the excitation map $U_N : \bigotimes_{\mathrm{s}}^N \mathcal{H} \longrightarrow \mathcal{F}_{\leqslant N}$ from Eq. (2.1.12)*

$$U_N \left(u_0^{\otimes i_0} \otimes_{\mathrm{s}} u_1^{\otimes i_1} \otimes_{\mathrm{s}} \cdots \otimes_{\mathrm{s}} u_m^{\otimes i_m} \right) := u_1^{\otimes i_1} \otimes_{\mathrm{s}} \cdots \otimes_{\mathrm{s}} u_m^{\otimes i_m},$$

for non-negative integers $i_0 + \cdots + i_m = N$. Under conjugation with this unitary map U_N, we have for all $i, j \geqslant 1$ the following transformation laws

$$U_N\, b_0^\dagger b_0\, U_N^{-1} = 1 - \mathbb{L},$$
$$U_N\, b_j^\dagger b_0\, U_N^{-1} = b_j^\dagger \sqrt{1 - \mathbb{L}},$$
$$U_N\, b_j^\dagger b_i\, U_N^{-1} = b_j^\dagger b_i.$$

We can summarize the transformation laws from Lemma 2.3.3 as follows: In any product of the form $b_i^\dagger b_j$ we exchange b_0 with the operator $\sqrt{1-\mathbb{L}}$. In analogy to this, the zero component of the embedding $\iota(z)$ defined in Eq. (2.1.10) is given by $u_0^\dagger \cdot \iota(z) = \sqrt{1-\|z\|^2}$. In order to express $U_N H_N U_N^{-1}$, let us first compute

$$\begin{aligned} U_N\left(b_{\geqslant 0}^\dagger \cdot T \cdot b_{\geqslant 0}\right) U_N^{-1} &= U_N\, \mathfrak{Re}\left[T_{0,0}\ b_0^\dagger b_0 + 2\sum_{i=1}^{\infty} T_{i,0}\ b_i^\dagger b_0 + \sum_{i,j=1}^{\infty} T_{i,j}\ b_i^\dagger b_j\right] U_N^{-1} \\ &= \mathfrak{Re}\left[T_{0,0}\ (1-\mathbb{L}) + 2\sum_{i=1}^{\infty} T_{i,0}\ b_i^\dagger \sqrt{1-\mathbb{L}} + \sum_{i,j=1}^{\infty} T_{i,j}\ b_i^\dagger b_j\right] \\ &= \mathfrak{Re}\left[u_0^\dagger \cdot T \cdot u_0\ (1-\mathbb{L}) + 2\ b_{\geqslant 1}^\dagger \cdot T \cdot u_0 \cdot \sqrt{1-\mathbb{L}} + b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1}\right], \end{aligned}$$

where the real part of an operator is defined as $\mathfrak{Re}\,[X] := \frac{X+X^\dagger}{2}$. Similarly, we can express the transformed operator $U_N\left(\frac{N}{2(N-1)}\left(b_{\geqslant 0} \otimes b_{\geqslant 0}\right)^\dagger \cdot\ \hat{v} \cdot b_{\geqslant 0} \otimes b_{\geqslant 0}\right) U_N^{-1}$ as

$$\begin{aligned} \mathfrak{Re}\Big[&\frac{1}{2}\big(u_0 \otimes u_0\big)^\dagger \cdot \hat{v} \cdot u_0 \otimes u_0\ f_0(\mathbb{L}) + 2\ \big(b_{\geqslant 1} \otimes u_0\big)^\dagger \cdot \hat{v} \cdot u_0 \otimes u_0\, f_1(\mathbb{L}) \\ &+ \big(b_{\geqslant 1} \otimes b_{\geqslant 1}\big)^\dagger \cdot \hat{v} \cdot u_0 \otimes u_0\, f_2(\mathbb{L}) + \big(b_{\geqslant 1} \otimes u_0\big)^\dagger \cdot \hat{v} \cdot b_{\geqslant 1} \otimes u_0\, f_3(\mathbb{L}) \\ &+ \big(u_0 \otimes b_{\geqslant 1}\big)^\dagger \cdot \hat{v} \cdot b_{\geqslant 1} \otimes u_0\, f_4(\mathbb{L}) + 2\ \big(b_{\geqslant 1} \otimes b_{\geqslant 1}\big)^\dagger \cdot \hat{v} \cdot b_{\geqslant 1} \otimes u_0\, f_5(\mathbb{L}) \\ &+ \frac{1}{2}\big(b_{\geqslant 1} \otimes b_{\geqslant 1}\big)^\dagger \cdot \hat{v} \cdot b_{\geqslant 1} \otimes b_{\geqslant 1}\, f_6(\mathbb{L})\Big], \end{aligned} \tag{2.3.2}$$

with $f_0(x) := \frac{N}{N-1}(1-x)(1-x-N^{-1})$, $f_1(x) := \frac{N}{N-1}(1-x-N^{-1})\sqrt{1-x}$, $f_2(x) := \frac{N}{N-1}\sqrt{1-x-N^{-1}}\sqrt{1-x}$, $f_3(x) := f_4(x) := \frac{N}{N-1}(1-x)$, $f_5(x) := \frac{N}{N-1}\sqrt{1-x}$ and $f_6(x) := \frac{N}{N-1}$. In order to keep the notation compact, let us name the essential building blocks involved in the expressions above.

Definition 2.3.4. We define $A_0 := u_0^\dagger \cdot T \cdot u_0$, $A_1 := 2\ b_{\geqslant 1}^\dagger \cdot T \cdot u_0$ and $A_2 := b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1}$, as well as $B_0 := \frac{1}{2}\big(u_0 \otimes u_0\big)^\dagger \cdot \hat{v} \cdot u_0 \otimes u_0$ and

$$\begin{aligned} B_1 &:= 2\ \big(b_{\geqslant 1} \otimes u_0\big)^\dagger \cdot \hat{v} \cdot u_0 \otimes u_0, & B_4 &:= \big(u_0 \otimes b_{\geqslant 1}\big)^\dagger \cdot \hat{v} \cdot b_{\geqslant 1} \otimes u_0, \\ B_2 &:= \big(b_{\geqslant 1} \otimes b_{\geqslant 1}\big)^\dagger \cdot \hat{v} \cdot u_0 \otimes u_0, & B_5 &:= 2\ \big(b_{\geqslant 1} \otimes b_{\geqslant 1}\big)^\dagger \cdot \hat{v} \cdot b_{\geqslant 1} \otimes u_0, \\ B_3 &:= \big(b_{\geqslant 1} \otimes u_0\big)^\dagger \cdot \hat{v} \cdot b_{\geqslant 1} \otimes u_0, & B_6 &:= \frac{1}{2}\big(b_{\geqslant 1} \otimes b_{\geqslant 1}\big)^\dagger \cdot \hat{v} \cdot b_{\geqslant 1} \otimes b_{\geqslant 1}. \end{aligned}$$

With these building blocks at hand, we can express the transformed Hamiltonian as

$$U_N N^{-1} H_N U_N^{-1} = \sum_{r=0}^{2} \mathfrak{Re}\left[A_r \sqrt{1-\mathbb{L}}^{\,2-r}\right] + \sum_{r=0}^{6} \mathfrak{Re}\left[B_r f_r(\mathbb{L})\right]. \tag{2.3.3}$$

In the subsequent Lemma 2.3.5 we will derive estimates for operator expressions of the form $B_r\, f(\mathbb{L})$. Such estimates will be useful for the identification of lower order terms in the energy asymptotics in Eq. (2.1.8).

Lemma 2.3.5. *Let us denote with π_M the orthogonal projection onto $\mathcal{F}_{\leqslant M}$. Given Assumption 2.1.1, there exists a constant c such that for functions $f : [0,1] \longrightarrow \mathbb{R}$*

$$\pm \pi_M\, \mathfrak{Re}\left[B_1 f(\mathbb{L})\right] \pi_M \leqslant c \sup_{x \leqslant \frac{M}{N}} |f(x)| \sqrt{\frac{M}{N}} \tag{2.3.4}$$

for all $M \leqslant N$, and for all $t > 0$ and $i \in \{2,3,4\}$ we have

$$\pm\pi_M \,\mathfrak{Re}\left[B_i f\left(\mathbb{L}\right)\right]\pi_M \leqslant c \sup_{x\leqslant \frac{M}{N}} |f(x)| \sqrt{\frac{M}{N}} \left(t + t^{-1}\, b_{\geqslant 1}^\dagger \cdot (T+1)\cdot b_{\geqslant 1}\right),$$
$$\pm\pi_M \,\mathfrak{Re}\left[B_5 f\left(\mathbb{L}\right)\right]\pi_M \leqslant c \sup_{x\leqslant \frac{M}{N}} |f(x)| \,\frac{M}{N} \left(t + t^{-1}\, b_{\geqslant 1}^\dagger \cdot (T+1)\cdot b_{\geqslant 1}\right),$$
$$-\frac{M}{2N}\, b_{\geqslant 1}^\dagger \cdot (\lambda\, T + \Lambda)\cdot b_{\geqslant 1} \leqslant \pi_M \,\mathfrak{Re}\left[B_6\right]\pi_M \leqslant \frac{M}{2N} b_{\geqslant 1}^\dagger \cdot (\Lambda T + \Lambda)\cdot b_{\geqslant 1},$$

where the constants λ, Λ are as in Assumption 2.1.1.

Proof. Using the Cauchy–Schwarz inequality as in Lemma 2.8.1 with $Q := 1_{\mathcal{F}_0} \otimes \hat{v}$, $A := b_{\geqslant 1} \underline{\otimes}\, u_0\, \pi_M$ and $B := 2u_0 \underline{\otimes}\, u_0\, f\left(\mathbb{L}\right)\pi_M$, and defining $k := \left(u_0 \otimes u_0\right)^\dagger \cdot |\hat{v}| \cdot u_0 \otimes u_0$, we obtain for any $s > 0$

$$\begin{aligned}\pm\pi_M \,\mathfrak{Re}\left[B_1 f\left(\mathbb{L}\right)\right]\pi_M &= \pm\mathfrak{Re}\left[A^\dagger \cdot Q \cdot B\right] \leqslant s\, A^\dagger \cdot |Q| \cdot A + s^{-1}\, B^\dagger \cdot |Q| \cdot B\\ &= s\, \pi_M \left(b_{\geqslant 1} \underline{\otimes}\, u_0\right)^\dagger \cdot |\hat{v}| \cdot b_{\geqslant 1} \underline{\otimes}\, u_0\, \pi_M + s^{-1} 4k\, \pi_M f\left(\mathbb{L}\right)^2 \pi_M.\end{aligned}$$

By Assumption 2.1.1, $|\hat{v}| \leqslant \Lambda\; 1_{\mathcal{H}} \otimes (T+1)$. Let $K := \Lambda\; u_0^\dagger \cdot (T+1)\cdot u_0$, then

$$\pi_M \left(b_{\geqslant 1} \underline{\otimes}\, u_0\right)^\dagger \cdot |\hat{v}| \cdot b_{\geqslant 1} \underline{\otimes}\, u_0 \cdot \pi_M \leqslant K\; \pi_M\, b_{\geqslant 1}^\dagger \cdot b_{\geqslant 1}\, \pi_M \leqslant K\, \frac{M}{N}.$$

Using $\pi_M f\left(\mathbb{L}\right)^2 \pi_M \leqslant \left(\sup_{x\leqslant \frac{M}{N}} |f(x)|\right)^2$ and choosing $s := \sqrt{\frac{N}{M}} \sup_{x\leqslant \frac{M}{N}} |f(x)|$ yields Eq. (2.3.4). The other inequalities can be derived similarly. ∎

The following two Lemmata will be useful tools in the verification of the lower bound of the energy asymptotics in Theorem 2.4.13.

Lemma 2.3.6. *There exist constants $c, \delta > 0$, such that for $N \geqslant 2$*

$$\delta\; b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1} - c \leqslant U_N N^{-1} H_N U_N^{-1} \leqslant c\left(b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1} + 1\right). \tag{2.3.5}$$

Let us further denote with P_n the orthogonal projection onto $\mathbb{1}_{[\mathcal{N}=n]}\mathcal{F}_0$. Then there exists a constant k, such that for $N \geqslant 2$

$$\sum_{n=0}^{N} P_n \left(U_N N^{-1} H_N U_N^{-1}\right) P_n \leqslant k\left(U_N N^{-1} H_N U_N^{-1} + k\right).$$

Proof. Recall from Lemma 2.2.4 that $N^{-1} H_N \geqslant \frac{\delta}{N}\sum_{j=1}^N T_j - \delta c = \delta\; b_{\geqslant 0}^\dagger \cdot T \cdot b_{\geqslant 0} - \delta c$. Therefore we have the estimate

$$\begin{aligned}U_N N^{-1} H_N U_N^{-1} &\geqslant \delta\left(u_0 \cdot \sqrt{1-\mathbb{L}} + b_{\geqslant 1}\right)^\dagger \cdot T \cdot \left(u_0 \cdot \sqrt{1-\mathbb{L}} + b_{\geqslant 1}\right) - \delta c\\ &\geqslant \frac{\delta}{2} b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1} - \delta u_0^\dagger \cdot T \cdot u_0 \left(1-\mathbb{L}\right) - \delta c \geqslant \widetilde{\delta} b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1} - \widetilde{c},\end{aligned}$$

with $\widetilde{\delta} := \frac{\delta}{2}$ and $\widetilde{c} := \delta u_0^\dagger \cdot T \cdot u_0 + \delta c$. The upper bound in Eq. (2.3.5) follows analogously. In order to verify the second inequality note that the map $A \mapsto \sum_n P_n A P_n$ is monotone and $\sum_n P_n \left(b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1}\right) P_n = b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1} \sum_n P_n^2 = b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1}$. Hence,

$$\sum_{M=0}^{N} P_n \left(U_N N^{-1} H_N U_N^{-1}\right) P_n \leqslant \sum_{M=0}^{N} P_n \left(c\, b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1} + c\right) P_n$$
$$= c\, b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1} + c \leqslant \delta^{-1} c\, U_N N^{-1} H_N U_N^{-1} + (c + \delta^{-1} c^2).$$

■

In the subsequent Lemma we are going to verify that we can exchange the N-dependent functions f_i in Eq. (2.3.3) with N-independent functions $\sqrt{1-x}^{\,\beta_i}$, for suitable β_i, without changing the operator substantially. This will be convenient in the lower bound of the energy asymptotics, since there we have to verify an operator Taylor approximation, which will be more convenient to do for the functions $\sqrt{1-x}^{\,\beta_i}$ than for the functions f_i.

Lemma 2.3.7. *Let $\beta_0 := 4, \beta_1 := 3$, $\beta_2 := \beta_3 := \beta_4 := 2$, $\beta_5 := 1$ and $\beta_6 := 0$, and let us define the operators $\widetilde{A}_N$ and $\widetilde{B}_N$ acting on $\mathcal{F}_0$ as*

$$\widetilde{A}_N := \sum_{r=0}^{2} \mathfrak{Re}\left[A_r \sqrt{1-\mathbb{L}}^{2-r}\right], \tag{2.3.6}$$

$$\widetilde{B}_N := \sum_{r=0}^{6} \mathfrak{Re}\left[B_r \sqrt{1-\mathbb{L}}^{\beta_r}\right]. \tag{2.3.7}$$

Then, given Assumption 2.1.1, there exists a constant K such that for all $M \leqslant N$

$$\pm \pi_M \left(U_N N^{-1} H_N U_N^{-1} - \widetilde{A}_N - \widetilde{B}_N\right) \pi_M \leqslant \frac{C}{N} \sqrt{\frac{M}{N}} \left(b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1} + 1\right). \tag{2.3.8}$$

Proof. According to Eq. (2.3.3), we have

$$U_N N^{-1} H_N U_N^{-1} - \widetilde{A}_N - \widetilde{B}_N = \sum_{r=0}^{6} \mathfrak{Re}\left[B_r \left(f_r(\mathbb{L}) - \sqrt{1-\mathbb{L}}^{\beta_r}\right)\right], \tag{2.3.9}$$

with the functions $f_0, \ldots, f_6$ from Eq. (2.3.2). Note that for all $N \geqslant 2$

$$\pm \pi_M B_0 \left(f_0(\mathbb{L}) - (1-\mathbb{L})^2\right) \pi_M = \pm \frac{1}{2} \hat{v}_{00,00}\, \pi_M \left(f_0(\mathbb{L}) - (1-\mathbb{L})^2\right) \pi_M$$
$$\leqslant \frac{1}{2} |\hat{v}_{00,00}| \sup_{x \leqslant \frac{M}{N}} |f_0(x) - (1-x)^2| \leqslant \frac{1}{2} |\hat{v}_{00,00}| \frac{M}{(N-1)N}.$$

Furthermore, $f_r(x) = \sqrt{1-x}^{\beta_r} + O\left(\frac{1}{N}\right)$ and therefore we obtain with Lemma 2.3.5 and the choice $t = 1$

$$\pm \pi_M B_r \left(f_r(\mathbb{L}) - \sqrt{1-x}^{\,\beta_r}\right) \pi_M \leqslant \frac{C}{N} \sqrt{\frac{M}{N}} \left(b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1} + 1\right),$$

for a constant C and $r \in \{1, \ldots, 6\}$. ■

2.4 Asymptotics of the Ground State Energy

We start by making the formal definition of the Bogoliubov Hamiltonian $\mathbb{H}$ in Eq. (2.1.6) rigorous in Subsection 2.4.1. In the following Subsection 2.4.2, we will verify the upper bound in the energy asymptotics in Eq. (2.1.8). We will then discuss the proof of the lower bound in Subsection 2.4.3, while the verification of the main technical Theorem 2.4.12 for the lower bound will be postponed to Section 2.5.

2.4.1 Construction of the Bogoliubov Operator $\mathbb{H}$

In the following Lemma 2.4.1 we will identify the Hessian $\mathrm{Hess}|_{u_0}\mathcal{E}_\mathrm{H}$, and give a precise definition of the Bogoliubov operator in the subsequent Definition 2.4.3. Furthermore, we shall see that the operator $\mathbb{H}$ is indeed semi-bounded. In the following let us denote with $\mathrm{dom}\,[A] := \mathrm{dom}\big(\sqrt{A}\big)$ the form domain of an operator $A \geqslant 0$.

Lemma 2.4.1. *Given Assumption 2.1.1, the Hessian of the Hartree energy $\mathcal{E}_\mathrm{H}$ at the Hartree minimizer u_0 is given by*

$$\frac{1}{2}\mathrm{Hess}|_{u_0}\mathcal{E}_\mathrm{H}[z] = z^\dagger \cdot Q_\mathrm{H} \cdot z + G_\mathrm{H}^\dagger \cdot z \otimes z + (z \otimes z)^\dagger \cdot G_\mathrm{H}, \tag{2.4.1}$$

where $G_\mathrm{H} := \frac{1}{2}\hat{v} \cdot u_0 \otimes u_0 \in \overline{\mathcal{H}_0 \otimes_\mathrm{s} \mathcal{H}_0}^{\|\cdot\|_*}$ is in the closure of $\mathcal{H}_0 \otimes_\mathrm{s} \mathcal{H}_0$ with respect to the norm $\|G\|_* := \|1_\mathcal{H} \otimes (T+1)^{-\frac{1}{2}} \cdot G\|$, and the operator Q_H is defined by the equation

$$z^\dagger \cdot Q_\mathrm{H} \cdot z : = z^\dagger \cdot T \cdot z + (z \otimes u_0)^\dagger \cdot \hat{v} \cdot z \otimes u_0 - \mu_\mathrm{H}\, z^\dagger \cdot z + (u_0 \otimes z)^\dagger \cdot \hat{v} \cdot z \otimes u_0$$

for all $z \in \mathcal{H}_0 \cap \mathrm{dom}\,[T]$, with $\mu_\mathrm{H} := u_0^\dagger \cdot T \cdot u_0 + (u_0 \otimes u_0)^\dagger \cdot \hat{v} \cdot u_0 \otimes u_0$. Furthermore, Q_H is non-negative and satisfies $\nu^{-1}(T|_{\mathcal{H}_0} + 1) \leqslant Q_\mathrm{H} + 1 \leqslant \nu(T|_{\mathcal{H}_0} + 1)$ for some constant $\nu > 0$.

Remark 2.4.2. By Assumption 2.1.1, we know that $\hat{v} \cdot u_0 \otimes u_0 \in \overline{\mathcal{H}_0 \otimes_\mathrm{s} \mathcal{H}_0}^{\|\cdot\|_*}$, which follows from the fact that $1_\mathcal{H} \otimes (T+1)^{-\frac{1}{2}} \cdot \hat{v} \cdot 1_\mathcal{H} \otimes (T+1)^{-\frac{1}{2}}$ is a bounded operator and that $u_0 \in \mathrm{dom}\,[T]$. For such elements $G \in \overline{\mathcal{H}_0 \otimes_\mathrm{s} \mathcal{H}_0}^{\|\cdot\|_*}$, we have that $G_\mathrm{reg} := 1_\mathcal{H} \otimes (T+1)^{-\frac{1}{2}} \cdot G$ is an element of $\mathcal{H}_0 \otimes_\mathrm{s} \mathcal{H}_0$ and therefore we can define for all $z \in \mathrm{dom}\,[T]$

$$G^\dagger \cdot z \otimes z := G_\mathrm{reg}^\dagger \cdot z \otimes \left((T+1)^{\frac{1}{2}} \cdot z\right).$$

In a similar fashion, we define the operator $G^\dagger \cdot b_{\geqslant 1} \underline{\otimes} b_{\geqslant 1} := G_\mathrm{reg}^\dagger \cdot b_{\geqslant 1} \underline{\otimes} \left((T+1)^{\frac{1}{2}} \cdot b_{\geqslant 1}\right)$.

Proof of Lemma 2.4.1. With the help of the embedding ι defined in Eq. (2.1.10), we can express the Hessian as $\mathrm{Hess}|_{u_0}\mathcal{E}_\mathrm{H}[z] = D^2|_0\,(\mathcal{E}_\mathrm{H} \circ \iota)\,(z)$, where $D^2|_{z_0} f(z)$ denotes the second derivative of a function f in the direction z evaluated at z_0. An explicit computation yields Eq. (2.4.1). Regarding the second part of the Lemma, observe that $Q_\mathrm{H} \geqslant 0$ follows from the fact that we can always find a phase θ_z such that

$$z^\dagger \cdot Q_\mathrm{H} \cdot z = \frac{1}{2}\mathrm{Hess}|_{u_0}\mathcal{E}_\mathrm{H}[e^{i\theta_z} z] \geqslant 0.$$

Furthermore, note that $|v| \leqslant \Lambda(T+1)$ implies $\pm \left(1_{\mathcal{H}_0} \otimes u_0\right)^\dagger \cdot \hat{v} \cdot 1_{\mathcal{H}_0} \otimes u_0 \leqslant c \; 1_{\mathcal{H}_0}$ with $c := u_0^\dagger \cdot \Lambda(T+1) \cdot u_0$ and

$$\pm (u_0 \otimes 1_{\mathcal{H}_0})^\dagger \cdot \hat{v} \cdot 1_{\mathcal{H}_0} \otimes u_0 \leqslant \frac{1}{2} \left(u_0 \otimes 1_{\mathcal{H}_0}\right)^\dagger \cdot |\hat{v}| \cdot u_0 \otimes 1_{\mathcal{H}_0} + \frac{1}{2} \left(1_{\mathcal{H}_0} \otimes u_0\right)^\dagger \cdot |\hat{v}| \cdot 1_{\mathcal{H}_0} \otimes u_0 \leqslant c \; 1_{\mathcal{H}_0}.$$

Hence $Q_{\mathrm{H}} \geqslant 0$ implies $Q_{\mathrm{H}} + 1 \geqslant T|_{\mathcal{H}_0} + 1 - (2c + |\mu| + 1) \geqslant T|_{\mathcal{H}_0} + 1 - (1 + 2c + \mu)(Q_{\mathrm{H}} + 1)$, and therefore $(2 + 2c + \mu)(Q_{\mathrm{H}} + 1) \geqslant T|_{\mathcal{H}_0} + 1$. Furthermore $T \geqslant 0$ implies

$$Q_{\mathrm{H}} + 1 \leqslant T + 2c + |\mu| \leqslant (1 + 2c + |\mu|)(T|_{\mathcal{H}_0} + 1).$$

■

Definition 2.4.3. Let the selfadjoint operator Q_{H} and $G_{\mathrm{H}} \in \overline{\mathcal{H}_0 \otimes_{\mathrm{s}} \mathcal{H}_0}^{\|\cdot\|_*}$ be as in Lemma 2.4.1. Then we define the Bogoliubov operator $\mathbb{H}$ as

$$\mathbb{H} := a_{\geqslant 1}^\dagger \cdot Q_{\mathrm{H}} \cdot a_{\geqslant 1} + G_{\mathrm{H}}^\dagger \cdot a_{\geqslant 1} \underline{\otimes} a_{\geqslant 1} + \left(a_{\geqslant 1} \underline{\otimes} a_{\geqslant 1}\right)^\dagger \cdot G_{\mathrm{H}}. \tag{2.4.2}$$

Theorem 2.4.4. *The quadratic form on the right side of Eq. (2.4.2) is semi-bounded from below and closeable, and consequently defines by Friedrichs extension a selfadjoint operator* $\mathbb{H}$ *with* $\inf \sigma(\mathbb{H}) > -\infty$. *Furthermore there exists a sequence of states* $\Psi_M \in \mathrm{dom}\left[a_{\geqslant 1}^\dagger \cdot (T+1) \cdot a_{\geqslant 1}\right] \cap \mathcal{F}_{\leqslant M}$, $\|\Psi_M\| = 1$, *such that*

$$\langle \mathbb{H} \rangle_{\Psi_M} \underset{M \to \infty}{\longrightarrow} \inf \sigma(\mathbb{H}).$$

Additionally there exists a constant $r_* > 0$ *such that for all* $r < r_*$ *the operator* $\mathbb{H} - r\mathbb{A}$ *satisfies* $\inf \sigma(\mathbb{H} - r\mathbb{A}) > -\infty$ *as well, where*

$$\mathbb{A} := -\frac{1}{4} \sum_{j=1}^{d} \left(a_j - a_j^\dagger\right)^2 + a_{>d}^\dagger \cdot (T+1) \cdot a_{>d}. \tag{2.4.3}$$

The proof of Theorem 2.4.4 is being carried out in Appendix 2.7. We emphasize that $\mathbb{H}$ is degenerate, in the sense that $z^\dagger \cdot Q_{\mathrm{H}} \cdot z + G_{\mathrm{H}}^\dagger \cdot z \otimes z + (z \otimes z)^\dagger \cdot G_{\mathrm{H}} = 0$ for any z in the vector space spanned by $\{u_1, \ldots, u_d\}$, and therefore we cannot directly apply the results in [98]. We also note that the semi-boundedness of Bogoliubov operators with degeneracies has been verified in [59] under the additional assumption that Q_{H} is bounded.

2.4.2 Upper Bound

With the essential definitions at hand, we will derive the upper bound in Theorem 2.4.6 using the representation of $U_N H_N U_N^{-1}$ derived in the previous section. We follow the strategy presented in [72], by sorting the operator $U_N H_N U_N^{-1}$ in terms of different powers in $b_{\geqslant 1}$ and identifying the zero component as the Hartree energy $N e_{\mathrm{H}}$ defined in Eq. (2.1.2) and the second order component as the Bogoliubov operator $\mathbb{H}$ defined in Eq. (2.4.2).

Lemma 2.4.5. *Let Assumption 2.1.1 hold. Then there exists a constant* C *such that*

$$\pm \pi_M \left(U_N N^{-1} H_N U_N^{-1} - e_{\mathrm{H}} - N^{-1} \mathbb{H}\right) \pi_M \leqslant C \left(\frac{M}{N}\right)^{\frac{3}{2}} \left(1 + a_{\geqslant 1}^\dagger \cdot (T+1) \cdot a_{\geqslant 1}\right)$$

for all $M \leqslant N$.

While Lemma 2.4.5 will be useful for proving the upper bound in Theorem 2.4.6, it is insufficient for proving the corresponding lower bound. This is due to the fact that Bose–Einstein condensation only provides the rough a priori information $M = o(N)$, see also the proof of Theorem 2.4.13.

Proof. Observe that u_0 minimizes the Hartree energy, and therefore

$$e_{\mathrm{H}} = \inf_{\|u\|=1} \mathcal{E}_{\mathrm{H}}[u] = u_0^{\dagger} \cdot T \cdot u_0 + \frac{1}{2} (u_0 \otimes u_0)^{\dagger} \cdot \hat{v} \cdot u_0 \otimes u_0 = A_0 + B_0,$$

where A_i and B_i are defined in Definition 2.3.4. Since $\mathcal{E}_{\mathrm{H}}[u_0] \leqslant \mathcal{E}_{\mathrm{H}}[u]$ for $\|u\| = 1$, we obtain by differentiation in any direction $z \perp u_0$

$$0 = D|_{u_0} \mathcal{E}_{\mathrm{H}}(z) = u_0^{\dagger} \cdot T \cdot z + z^{\dagger} \cdot T \cdot u_0 + (z \otimes u_0)^{\dagger} \cdot \hat{v} \cdot u_0 \otimes u_0 + (u_0 \otimes u_0)^{\dagger} \cdot \hat{v} \cdot z \otimes u_0,$$

and consequently $u_j^{\dagger} \cdot T \cdot u_0 + (u_j \otimes u_0)^{\dagger} \cdot \hat{v} \cdot u_0 \otimes u_0 = 0$ for all $j \geqslant 1$. Hence,

$$A_1 + B_1 = 2 \left(b_{\geqslant 1}^{\dagger} \cdot T \cdot u_0 + (b_{\geqslant 1} \underline{\otimes} u_0)^{\dagger} \cdot \hat{v} \cdot u_0 \underline{\otimes} u_0 \right) = 0.$$

By Definition 2.4.3 and Lemma 2.4.1, we have

$$N^{-1} \mathbb{H} = \mathfrak{Re} \left[A_2 + B_2 + B_3 + B_4 - \mu_{\mathrm{H}}\, b_{\geqslant 1}^{\dagger} \cdot b_{\geqslant 1} \right],$$

and consequently we can write for any $M \leqslant N$, using Eq. (2.3.3),

$$\pi_M \left(U_N N^{-1} H_N U_N^{-1} - e_{\mathrm{H}} - N^{-1} \mathbb{H} \right) \pi_M = \pi_M \mathfrak{Re} \left[X \right] \pi_M$$

with

$$X := B_0 \left(f_0 \left(\mathbb{L} \right) - 1 + 2 \mathbb{L} \right) + B_1 \left(f_1 \left(\mathbb{L} \right) - \sqrt{1 - \mathbb{L}} \right) + \sum_{r=2}^{4} B_r \left(f_r \left(\mathbb{L} \right) - 1 \right) + \sum_{r=5}^{6} B_r f_r \left(\mathbb{L} \right),$$

where we used $A_1 \sqrt{1 - \mathbb{L}} = -B_1 \sqrt{1 - \mathbb{L}}$. In order to estimate the first contribution, note that $|f_0(x) - 1 + 2x| \leqslant 2 \frac{M^2}{(N-1)N}$ for all $0 \leqslant x \leqslant \frac{M}{N}$ and therefore

$$\pm \pi_M B_0 \left(f_0 \left(\mathbb{L} \right) - 1 + 2 \mathbb{L} \right) \pi_M = \pm \frac{1}{2} \hat{v}_{00,00} \pi_M \left(f_0 \left(\mathbb{L} \right) - 1 + 2 \mathbb{L} \right) \pi_M \leqslant |\hat{v}_{00,00}| \frac{M^2}{(N-1)N}.$$

Recalling that $b_{\geqslant 1} = \frac{1}{\sqrt{N}} a_{\geqslant 1}$ and Lemma 2.3.5 yields

$$\pm \pi_M B_1 \left(f_1 \left(\mathbb{L} \right) - \sqrt{1 - \mathbb{L}} \right) \pi_M \leqslant c \frac{M}{N-1} \sqrt{\frac{M}{N}}.$$

Furthermore we obtain for $r \in \{2, 3, 4\}$ by Lemma 2.3.5 with the choice $t = \frac{1}{\sqrt{N}}$, together with the bound $\sup_{x \leqslant \frac{M}{N}} |f_r(x) - 1| \leqslant C \frac{M}{N}$ for a constant $C > 0$,

$$\pm \pi_M B_r \left(f_r \left(\mathbb{L} \right) - 1 \right) \pi_M \leqslant c\, C \frac{M^{\frac{3}{2}}}{N^2} \left(1 + a_{\geqslant 1}^{\dagger} \cdot (T + 1) \cdot a_{\geqslant 1} \right).$$

The estimates for $B_5 f_5 \left(\mathbb{L} \right)$ and $B_6 f_6 \left(\mathbb{L} \right)$ can be obtained analogously. ■

Theorem 2.4.6 (Upper Bound). *Let E_N be the ground state energy of H_N, e_{H} the Hartree energy defined in Eq. (2.1.2) and let $\mathbb{H}$ be the Bogoliubov operator defined in Eq. (2.4.2). Given Assumption 2.1.1, we have the upper bound*

$$E_N \leqslant N\, e_{\mathrm{H}} + \inf \sigma\left(\mathbb{H}\right) + o_{N\to\infty}\left(1\right).$$

Proof. Let ν be the constant from Lemma 2.4.1, such that the inequality $Q_{\mathrm{H}} + 1 \leqslant \nu\left(T|_{\mathcal{H}_0} + 1\right)$ holds. For all $\epsilon > 0$, we know by Theorem 2.4.4 that there exists a state $\Psi \in \mathcal{F}_M$ with $M < \infty$ such that $\kappa := \langle a^\dagger_{\geqslant 1} \cdot (T+1) \cdot a_{\geqslant 1}\rangle_\Psi < \infty$ and $\langle \mathbb{H}\rangle_\Psi \leqslant \inf\sigma\left(\mathbb{H}\right) + \epsilon$. Applying Lemma 2.4.5 yields the estimate

$$\begin{aligned} \langle H_N\rangle_{U_N^{-1}\Psi} &\leqslant N\, e_{\mathrm{H}} + \langle \mathbb{H}\rangle_\Psi + C\, M\sqrt{\frac{M}{N}}\, \left(1 + \langle a^\dagger_{\geqslant 1} \cdot (T+1)\cdot a_{\geqslant 1}\rangle_\Psi\right) \\ &\leqslant N\, e_{\mathrm{H}} + \inf\sigma\left(\mathbb{H}\right) + \epsilon + C\, M\sqrt{\frac{M}{N}}\, \left(1+\kappa\right). \end{aligned}$$

■

2.4.3 Lower Bound

In the following, we will give the proof of the lower bound in the energy asymptotics in Eq. (2.1.8). First of all let us define the operators $q, p : \mathrm{dom}\left[\mathcal{N}\right] \longrightarrow \mathcal{F}_0 \otimes \mathcal{H}_0$ as

$$q := \sum_{j=1}^d q_j \otimes u_j := \frac{1}{2}\sum_{j=1}^d \left(b_j + b_j^\dagger\right) \otimes u_j, \tag{2.4.4}$$

$$p := \sum_{j=1}^d p_j \otimes u_j := \frac{1}{2i}\sum_{j=1}^d \left(b_j - b_j^\dagger\right) \otimes u_j, \tag{2.4.5}$$

which satisfy the commutation relations $[p_k, q_\ell] = \frac{1}{2iN}\delta_{k,\ell}$. Recall that due to the translation-invariance of $\mathcal{E}_{\mathrm{H}}$, the Hessian $\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}$ is degenerate on the real subspace $\{\sum_{j=1}^d t_j u_j : t_j \in \mathbb{R}\}$. Therefore the Bogoliubov operator $\mathbb{H}$, which we have defined in Eq. (2.4.2) as the second quantization of the Hessian $\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}$, is degenerate with respect to the operator q, i.e. it can be expressed only in terms of p, $b_{>d}$ and $b^\dagger_{>d}$. Due to this degeneracy, we cannot directly apply the strategy pursued in [72] where the residuum of the Bogoliubov approximation is being estimated by the Bogoliubov operator itself. The problem is that the residuum $U_N H_N U_N^{-1} - N e_{\mathrm{H}} - \mathbb{H}$ includes contributions depending significantly on the modes q_j, like q_j^3, which we cannot compare with the Bogoliubov operator $\mathbb{H}$ due to its degeneracy. Furthermore, it is insufficient to compare the residuum with the (rescaled) particle number operator $\frac{1}{N}\mathcal{N}$, which indeed dominates terms like q_j^3, since we only have the a priori information $\langle \mathcal{N}\rangle_{U_N\Psi_N} = o(N)$ provided by Bose–Einstein condensation. The novel idea of this Subsection and the subsequent Section 2.5 is to apply a further unitary transformation $\mathcal{W}_N$ such that the residuum $\mathcal{W}_N U_N H_N U_N^{-1}\mathcal{W}_N^{-1} - N e_{\mathrm{H}} - \mathbb{H}$ no longer includes this kind of contributions and consequently we can compare the residuum with the Bogoliubov operator $\mathbb{H}$. This leads to the important inequality in Eq. (2.1.13). As a consequence we observe that, in contrast to the particle number operator $\mathcal{N}$, the Bogoliubov operator satisfies $\langle \mathbb{H}\rangle_{U_N\Psi_N} = O(1)$, which, a posteriori, justifies estimating the residuum by the Bogoliubov operator.

Before we are going to construct a unitary map $\mathcal{W}_N$ satisfying Eq. (2.1.13), we are solving the corresponding problem on a classical level, i.e. we are going to construct a map F which satisfies Eq. (2.1.11). We will then define $\mathcal{W}_N$ as the quantum counterpart to F.

Definition 2.4.7. For any $y \in \mathbb{R}^d$, let us recall the functions $u_{0,y}(x) := u_0(x-y)$ defined in Assumption 2.1.1 and let us define the map $\lambda : \mathbb{R}^d \longrightarrow \mathbb{R}^d$

$$\lambda(y) := \left(u_j^\dagger \cdot u_{0,y}\right)_{j=1}^d \in \mathbb{R}^d.$$

Note that u_j and $u_{0,y}$ are real-valued functions, and therefore λ is indeed $\mathbb{R}^d$-valued. Since $y \mapsto u_{0,y}$ is a $C^2\left(\mathbb{R}^d, \mathcal{H}\right)$ function by Assumption 2.1.3, $D_y\lambda(0)$ has full rank and $\lambda(0) = 0$, there exists a local inverse $\lambda^{-1} : B_{2\delta}(0) \longrightarrow \mathbb{R}^d$ for $\delta > 0$ small enough, where $B_r(0) \subset \mathbb{R}^d$ denotes the ball of radius r centered around the origin. Let $0 \leqslant \sigma \leqslant 1$ be a smooth function with $\sigma|_{B_\delta(0)} = 1$ and $\mathrm{supp}(\sigma) \subset B_{2\delta}(0)$. Then we define the function $f : \mathbb{R}^d \longrightarrow \mathcal{H}$

$$f(t) : = \sigma(t)\left[u_{0,\lambda^{-1}(t)} - \left(u_0^\dagger \cdot u_{0,\lambda^{-1}(t)}\right)u_0 - \sum_{j=1}^d t_j\, u_j\right] = \sum_{j=d+1}^\infty f_j(t)u_j, \tag{2.4.6}$$

with $f_j(t) := \sigma(t)u_j^\dagger \cdot u_{0,\lambda^{-1}(t)}$. Note that $t \mapsto f(t)$ is a $C^2\left(\mathbb{R}^d, \mathcal{H}_0\right)$ function, due to the regularity of $y \mapsto u_{0,y}$. Furthermore, $f(0) = 0$. We can now define the map $F : \mathcal{H}_0 \longrightarrow \mathcal{H}_0$ for all $z = \sum_{j=1}^d (t_j + is_j)\, u_j + z_{>d} \in \mathcal{H}_0$ with $t, s \in \mathbb{R}^d$ and $z_{>d} \in \{u_1, \ldots, u_d\}^\perp$ as

$$F(z) := \sum_{j=1}^d \left(t_j + is'_j\right)u_j + z_{>d} + f(t), \tag{2.4.7}$$

where $s'_j := s_j - \mathfrak{Im}\left[\partial_j f(t)^\dagger \cdot z_{>d}\right]$.

The essential property of F is that $\iota \circ F$, where ι is the embedding defined in Eq. (2.1.10), maps the set $\{\sum_{j=1}^d t_j u_j : |t| < \delta\}$ into the set of Hartree minimizers

$$\iota \circ F\left(\sum_{j=1}^d t_j u_j\right) = \iota\left(\sum_{j=1}^d t_j u_j + f(t)\right) = u_{0,\lambda^{-1}(t)},$$

for all $|t| < \delta$. This also implies the central inequality Eq. (2.1.11), as will be demonstrated in the introduction of Section 2.5.

The arguments so far are based only on the fact that F shifts the component $z_{>d}$ by an amount $f(t)$. The identity $(\iota \circ F)\left(\sum_{j=1}^d t_j u_j\right) = u_{0,\lambda^{-1}(t)}$ would still hold if we used s_j instead of s'_j in Eq. (2.4.7). Nevertheless, it is natural that F shifts the s component as well, since this shift makes sure that $\mathrm{d}F$ preserves the symplectic form $\omega(z_1, z_2) := \mathfrak{Re}\left[z_1\right]^\dagger \cdot \mathfrak{Im}\left[z_2\right] - \mathfrak{Im}\left[z_1\right]^\dagger \cdot \mathfrak{Re}\left[z_2\right]$. Therefore it makes sense to look for a quantum counterpart $\mathcal{W}_N$, which we are going to define in the subsequent Definition 2.4.8. In analogy to F preserving the symplectic form ω, the unitary map $\mathcal{W}_N$ is preserving the commutator bracket.

Definition 2.4.8 (Unitary Transformation $\mathcal{W}_N : \mathcal{F}_0 \longrightarrow \mathcal{F}_0$)**.** Based on the fact that the operators $q_1, \ldots, q_d$ defined in Eq. (2.4.4) commute, we can assign to a function $h : \mathbb{R}^d \longrightarrow \mathcal{H}_0$ with components $h_j(t) := u_j^\dagger \cdot h(t)$ an operator $h(q) : \mathcal{F}_0 \longrightarrow \mathcal{F}_0 \otimes \mathcal{H}_0$

$$h(q) := \sum_{j=1}^{\infty} h_j(q_1, \ldots, q_d) \otimes u_j,$$

where the operators $h_j(q_1, \ldots, q_d)$ are well defined via functional calculus. Let f be the function defined in Eq. (2.4.6), then we can define the unitary map $\mathcal{W}_N : \mathcal{F}_0 \longrightarrow \mathcal{F}_0$ as

$$\mathcal{W}_N := \exp\left[N f(q)^\dagger \cdot b_{>d} - N b_{>d}^\dagger \cdot f(q)\right] = \exp\left[N \sum_{j=d+1}^{\infty} f_j(q_1, \ldots, q_d)\left(b_j - b_j^\dagger\right)\right], \tag{2.4.8}$$

where we have used that $u_j^\dagger \cdot f(t) = 0$ for $j \in \{1, \ldots, d\}$. Note that $q_1, \ldots, q_d$ and $b_{>d}$ have an N dependence, which we suppress in our notation. Furthermore, we define the transformed operators

$$\begin{aligned} p_j' &: = \mathcal{W}_N \, p_j \, \mathcal{W}_N^{-1}, \\ p' &: = \mathcal{W}_N \, p \, \mathcal{W}_N^{-1} = \sum_{j=1}^{d} p_j' \otimes u_j, \\ \mathbb{L}' &: = \mathcal{W}_N \, \mathbb{L} \, \mathcal{W}_N^{-1}, \end{aligned}$$

where p is defined in Eq. (2.4.5) and $\mathbb{L}$ is defined in Definition 2.3.1. Note that the domain of $\mathbb{L}'$ is $\mathcal{W}_N \mathcal{F}_{\leqslant N}$, since $\mathbb{L}$ is only defined on $\mathcal{F}_{\leqslant N}$.

That the unitary map $\mathcal{W}_N$ is indeed a quantum counterpart to the classical map F defined in Eq. (2.4.7) can be seen from the transformation laws described in the following Lemma 2.4.9.

Lemma 2.4.9 (Transformation Laws)**.** *We have the following transformation laws*

$$\begin{aligned} &\mathcal{W}_N \, b_j \, \mathcal{W}_N^{-1} = b_j + f_j(q) \ \textit{for } j > d, \\ &\mathcal{W}_N \, q_j \, \mathcal{W}_N^{-1} = q_j \ \textit{for } j \in \{1, \ldots, d\}, \\ &p_j' = p_j - \mathfrak{Im}\left[\partial_{u_j} f(q)^\dagger \cdot b_{>d}\right] \ \textit{for } j \in \{1, \ldots, d\}, \end{aligned}$$

and therefore $\mathcal{W}_N \, b_{\geqslant 1} \, \mathcal{W}_N^{-1} = q + ip' + b_{>d} + f(q)$.

The proof of Lemma 2.4.9 is elementary and is left to the reader. Before we state the main Theorems of this subsection, let us define what it means for a sequence of operators X_N to be asymptotically small compared to another sequence Y_N, in a suitable sense that is specific to our problem.

Definition 2.4.10. We say that sequences of operators X_N, Y_N with $Y_N \geqslant 0$ satisfy

$$X_N = o_*(Y_N),$$

in case for all $\epsilon > 0$ there exists a $\delta > 0$, such that $\left|\langle X_N\rangle_\Psi\right| \leqslant \epsilon\ \langle Y_N\rangle_\Psi$ for all M, N with $\frac{M}{N} \leqslant \delta$ and all elements $\Psi \in \mathcal{W}_N\mathcal{F}_{\leqslant M}$. Furthermore, we say that sequences of operators X_N, Y_N with $Y_N \geqslant 0$ satisfy

$$X_N = O_*(Y_N),$$

in case there exists a constant C and $\delta_0 > 0$, such that $\left|\langle X_N\rangle_\Psi\right| \leqslant C\ \langle Y_N\rangle_\Psi$ for all M, N with $\frac{M}{N} \leqslant \delta_0$ and all $\Psi \in \mathcal{W}_N\mathcal{F}_{\leqslant M}$.

Remark 2.4.11. Let us denote with $\pi_{M,N} := \mathcal{W}_N\,\pi_M\,\mathcal{W}_N^{-1}$ the orthogonal projection onto the subspace $\mathcal{W}_N\mathcal{F}_{\leqslant M} \subset \mathcal{F}_0$. Then the statement $X_N = O_*\left(Y_N\right)$ holds true if and only if there exists a constant C and $\delta_0 > 0$, such that

$$\pi_{M,N}\,\mathfrak{Re}\left[\lambda X_N\right]\pi_{M,N} \leqslant C\ \pi_{M,N}Y_N\pi_{M,N} \tag{2.4.9}$$

for all $\lambda \in \mathbb{C}$ with $|\lambda| = 1$ and $\frac{M}{N} \leqslant \delta_0$. Similarly, $X_N = o_*\left(Y_N\right)$ is equivalent to the existence of a function $\epsilon : \mathbb{R}^+ \longrightarrow \mathbb{R}^+$ with $\lim_{\delta\to 0}\epsilon(\delta) = 0$, such that

$$\pi_{M,N}\,\mathfrak{Re}\left[\lambda X_N\right]\pi_{M,N} \leqslant \epsilon\left(\frac{M}{N}\right)\pi_{M,N}Y_N\pi_{M,N} \tag{2.4.10}$$

for all $\lambda \in \mathbb{C}$ with $|\lambda| = 1$ and $M \leqslant N$.

Theorem 2.4.12. *Recall the $o_*(\cdot)$ notation from Definition 2.4.10, the Hartree energy e_H defined in Eq. (2.1.2) and the Bogoliubov operator $\mathbb{H}$ defined in Eq. (2.4.2), and let us define*

$$\mathbb{T}_N := p^\dagger\cdot p + b^\dagger_{>d}\cdot(T+1)\cdot b_{>d} + \frac{1}{N}. \tag{2.4.11}$$

Then, given Assumptions 2.1.1 and 2.1.3, we have

$$\left(\mathcal{W}_N U_N\right)N^{-1}H_N\left(\mathcal{W}_N U_N\right)^{-1} = e_\mathrm{H} + N^{-1}\mathbb{H} + o_*\left(\mathbb{T}_N\right).$$

The proof of Theorem 2.4.12, which in particular gives rise to a rigorous version of the key inequality Eq. (2.1.13), will be the content of Section 2.5. With Theorem 2.4.12 at hand we can verify the lower bound in the main Theorem 2.1.4.

Theorem 2.4.13 (Lower Bound)**.** *Let E_N be the ground state energy of H_N, e_H the Hartree energy defined in Eq. (2.1.2) and let $\mathbb{H}$ be the Bogoliubov operator defined in Eq. (2.4.2). Given Assumptions 2.1.1 and 2.1.3, we have the lower bound*

$$E_N \geqslant N\,e_\mathrm{H} + \inf\sigma\left(\mathbb{H}\right) + o_{N\to\infty}\left(1\right).$$

Proof. According to Theorem 2.1.2, there exists a sequence of states $\Psi_N \in \bigotimes_\mathrm{s}^N\mathcal{H}$, $\|\Psi_N\| = 1$, such that $\langle H_N\rangle_{\Psi_N} \leqslant E_N + \alpha_N$ with $\alpha_N \underset{N\to\infty}{\longrightarrow} 0$ and

$$\epsilon_N := \langle b^\dagger_{\geqslant 1}\cdot b_{\geqslant 1}\rangle_{U_N\Psi_N} = \langle b^\dagger_{\geqslant 1}\cdot b_{\geqslant 1}\rangle_{\Psi_N} \underset{N\to\infty}{\longrightarrow} 0.$$

Let us abbreviate $\widetilde{H}_N := U_N H_N U_N^{-1}$ and let π_M be the orthogonal projection onto the space $\mathcal{F}_{\leqslant M}$ as before. Furthermore, let $0 \leqslant f, g \leqslant 1$ be smooth functions with $f^2 + g^2 = 1$, $f(x) = 1$

for $x \leqslant \frac{1}{2}$ and $f(x) = 0$ for $x \geqslant 1$, and let us define $f_M(x) := f\left(\frac{x}{M}\right)$ and $g_M(x) := g\left(\frac{x}{M}\right)$. Then the generalized IMS localization formula in [78, Theorem A.1], in the form stated in [72, Proposition 6.1], tells us that

$$\widetilde{H}_N = f_M(\mathcal{N})\, \widetilde{H}_N\, f_M(\mathcal{N}) + g_M(\mathcal{N})\, \widetilde{H}_N\, g_M(\mathcal{N}) - R_{M,N},$$

with $R_{M,N} \leqslant \frac{R}{M^2}\sum_{n=0}^{\infty} P_n\left(\widetilde{H}_N - E_N\right) P_n$, where P_n is the orthogonal projection onto $\mathcal{F}_{\leqslant n} \cap \mathcal{F}_{\leqslant n-1}^{\perp}$, $\mathcal{N} = \sum_{j=1}^{\infty} a_j^{\dagger} a_j$ and $R := 16\left(\|f'\|_{\infty}^2 + \|g'\|_{\infty}^2\right)$. Let us define M_N as the smallest integer larger than $\sqrt{\epsilon_N} N$ and $N^{\frac{2}{3}}$. The exponent $\frac{2}{3}$ is somewhat arbitrary and we could use any sequence ℓ_N with $N^{\frac{1}{2}} \ll \ell_N \ll N$ instead. Using the estimate $1 - f_M(x)^2 \leqslant \frac{2}{M}x$ yields

$$\rho_N := \langle 1 - f_{M_N}(\mathcal{N})^2 \rangle_{U_N\Psi_N} \leqslant \frac{2}{M_N}\langle \mathcal{N} \rangle_{U_N\Psi_N} = \frac{2N}{M_N}\langle b_{\geqslant 1}^{\dagger} \cdot b_{\geqslant 1} \rangle_{U_N\Psi_N} \leqslant \frac{2}{\sqrt{\epsilon_N}}\epsilon_N \underset{N\to\infty}{\longrightarrow} 0.$$

Let us define $\Phi_N := (1-\rho_N)^{-\frac{1}{2}}\, f_{M_N}(\mathcal{N}) U_N \Psi_N$. Using Lemma 2.3.6 and the inequality $\widetilde{H}_N \geqslant E_N$ yields

$$E_N + \alpha_N \geqslant \langle \widetilde{H}_N \rangle_{U_N\Psi_N} \geqslant (1-\rho_N)\langle \widetilde{H}_N \rangle_{\Phi_N} + \rho_N E_N - \frac{R}{M_N^2}\langle k\widetilde{H}_N + k^2 N - E_N \rangle_{U_N\Psi_N}. \tag{2.4.12}$$

Since $\lim_N N^{-1}E_N = e_{\mathrm{H}}$, we obtain that $\beta_N := \frac{R}{M_N^2}\langle k\widetilde{H}_N + k^2N - E_N \rangle_{U_N\Psi_N}$ satisfies

$$\beta_N \leqslant \frac{R}{N^{\frac{4}{3}}}\left((k-1)E_N + k\alpha_N + k^2 N\right) \underset{N\to\infty}{\longrightarrow} 0.$$

We can now rewrite Inequality (2.4.12) as

$$E_N \geqslant \langle \widetilde{H}_N \rangle_{\Phi_N} - \frac{\alpha_N + \beta_N}{1-\rho_N}.$$

Let $r > 0$ be as in the assumption of Theorem 2.4.4 and recall the definition of $\mathbb{A}$ in Eq. (2.4.3). Note that $N\mathbb{T}_N = \mathbb{A} + 1$. By Theorem 2.4.12 and Remark 2.4.11, there exists a function ϵ with $\lim_{\delta\to 0}\epsilon(\delta)$, such that

$$\begin{aligned}
\langle \widetilde{H}_N \rangle_{\Phi_N} &\geqslant N\, e_{\mathrm{H}} + \langle \mathbb{H} \rangle_{\mathcal{W}_N\Phi_N} - \epsilon\left(\frac{M_N}{N}\right)\ \langle \mathbb{A} + 1 \rangle_{\mathcal{W}_N\Phi_N} \\
&= N\, e_{\mathrm{H}} + \left(1 - \frac{1}{r}\epsilon\left(\frac{M_N}{N}\right)\right)\langle \mathbb{H} \rangle_{\mathcal{W}_N\Phi_N} + \frac{1}{r}\epsilon\left(\frac{M_N}{N}\right)\langle \mathbb{H} - r\mathbb{A} \rangle_{\mathcal{W}_N\Phi_N} - \epsilon\left(\frac{M_N}{N}\right) \\
&\geqslant N\, e_{\mathrm{H}} + \inf\sigma(\mathbb{H}) + \frac{1}{r}\epsilon\left(\frac{M_N}{N}\right)\left(\inf\sigma(\mathbb{H} - r\mathbb{A}) - \inf\sigma(\mathbb{H})\right) - \epsilon\left(\frac{M_N}{N}\right)
\end{aligned}$$

for all N large enough such that $1 - \frac{1}{r}\epsilon\left(\frac{M_N}{N}\right) \geqslant 0$. This concludes the proof, since $\inf\sigma(\mathbb{H} - r\mathbb{A}) > -\infty$ by Theorem 2.4.4. ■

2.5 Taylor Expansion of $(\mathcal{W}_N U_N)\, H_N\, (\mathcal{W}_N U_N)^{-1}$

This section is devoted to the verification of the main technical Theorem 2.4.12, which is the rigorous version of inequality Eq. (2.1.13). Before we explain the proof, recall the definition of ι in Eq. (2.1.10) and F in Eq. (2.4.7), and let us verify the classical counterpart Eq. (2.1.11). For this purpose we define the functional

$$\mathcal{E}'(z) := \mathcal{E}_{\mathrm{H}}\left[\iota\left(F(z)\right)\right], \tag{2.5.1}$$

which satisfies according to the definition of F that $\mathcal{E}'(\boldsymbol{t}) = e_{\mathrm{H}}$ for all $t \in \mathbb{R}^d$ with $\boldsymbol{t} := \sum_{j=1}^d t_j u_j$, i.e. F flattens the manifold of minimizers of $\mathcal{E}_{\mathrm{H}} \circ \iota$. We will verify Eq. (2.1.11) by sorting the functional $\mathcal{E}'$ in terms of powers in the variables s and $z_{>d}$ for any $z = \sum_{j=1}^d (t_j + i s_j)\, u_j + z_{>d} \in \mathcal{H}_0$ with $z_{>d} \in \{u_1, \ldots, u_d\}^{\perp}$. In the following, let $\pi(z) := \sum_{j=1}^d i s_j u_j + z_{>d}$ be the projection onto $\mathcal{V} := \pi(\mathcal{H}_0)$. We can now sort $\mathcal{E}'(z)$ in terms of powers in s and $z_{>d}$, i.e. in terms of powers in $\pi(z)$, using a Taylor approximation with expansion point $\boldsymbol{t}$

$$\begin{aligned}\mathcal{E}'(z) = \mathcal{E}'\left(\boldsymbol{t} + \pi(z)\right) &= \mathcal{E}'\left(\boldsymbol{t}\,\right) + D|_{\boldsymbol{t}}\, \mathcal{E}'\big(\pi(z)\big) + \frac{1}{2} D^2|_{\boldsymbol{t}}\, \mathcal{E}'\big(\pi(z)\big) + \{\text{ HigherOrders }\} \\ &= \mathcal{E}'\left(\boldsymbol{t}\,\right) + D_{\mathcal{V}}|_{\boldsymbol{t}}\, \mathcal{E}'(z) + \frac{1}{2} D_{\mathcal{V}}^2|_{\boldsymbol{t}}\, \mathcal{E}'\big(z\big) + \{\text{ HigherOrders }\},\end{aligned} \tag{2.5.2}$$

where $D|_{z_0}\mathcal{E}'(v)$ is the first derivative of $\mathcal{E}'$ in the direction v at z_0, $D^2|_{z_0}\mathcal{E}'(v)$ is the second derivative in the direction v, and $D_{\mathcal{V}}|_{z_0}\mathcal{E}'(v) := D|_{z_0}\mathcal{E}'\left(\pi(v)\right)$ and $D_{\mathcal{V}}^2|_{z_0}\mathcal{E}'\big(v\big) := D^2|_{z_0}\mathcal{E}'\big(\pi(v)\big)$ are the derivatives only with respect to directions in $\mathcal{V}$. Using $\mathcal{E}'\left(\boldsymbol{t}\,\right) = e_{\mathrm{H}}$, $D_{\mathcal{V}}|_{\boldsymbol{t}}\, \mathcal{E}' = 0$ and the fact that $D_{\mathcal{V}}^2|_{\boldsymbol{t}}\, \mathcal{E}'(v) \geqslant \left(1 - \frac{\epsilon}{2}\right) D_{\mathcal{V}}^2|_0\, \mathcal{E}'(v)$ for t small enough by continuity, we formally arrive at Eq. (2.1.11), which is claimed to hold only for small $\|z\|^2 = |t|^2 + \|\pi(z)\|^2$ anyway.

By sorting the expression $(\mathcal{W}_N U_N)\, H_N\, (\mathcal{W}_N U_N)^{-1}$ in terms of powers in the operators p and $b_{>d}$, we will verify that we end up with the same Taylor approximation we obtained by sorting $\mathcal{E}'(z)$ in terms of powers in the variables s and $z_{>d}$. More precisely, our goal is to verify that

$$\begin{aligned}(\mathcal{W}_N U_N) N^{-1} H_N\, (\mathcal{W}_N U_N)^{-1} &= \mathcal{E}(q) + D_{\mathcal{V}}\big|_q \mathcal{E}\Big(b_{\geqslant 1}\Big) + \frac{1}{2} D_{\mathcal{V}}^2\big|_0 \mathcal{E}\Big(b_{\geqslant 1}\Big) + o_*\left(\mathbb{T}_N\right) \\ &= e_{\mathrm{H}} + N^{-1}\mathbb{H} + o_*\left(\mathbb{T}_N\right),\end{aligned} \tag{2.5.3}$$

where $\mathcal{E} : \mathrm{dom}\,[T] \to \mathbb{R}$ is a differentiable extension to all of $\mathrm{dom}\,[T]$ of the functional $\mathcal{E}'\big|_{B_r}$, restricted to the ball $B_r := \{z \in \mathcal{H}_0 \cap \mathrm{dom}\,[T] : \|z\| < r\}$ for a sufficiently small $r > 0$. Note that the spectrum of the operators $q_1, \ldots, q_d$ is the whole real axis $\mathbb{R}$. In order to even define $\mathcal{E}\left(q\right)$ and $D_{\mathcal{V}}\big|_q \mathcal{E}\Big(b_{\geqslant 1}\Big)$ with the help of functional calculus, it is therefore necessary that $\mathcal{E}$, in contrast to $\mathcal{E}'$, is an everywhere defined and differentiable functional. For such a function $\mathcal{E}$ we can define $\mathcal{E}\left(q\right)$ via functional calculus starting from the function $t \mapsto \mathcal{E}\left(\sum_{j=1}^d t_j u_j\right)$ for $t \in \mathbb{R}^d$. The so far formal objects $D_{\mathcal{V}}\big|_q \mathcal{E}\Big(b_{\geqslant 1}\Big)$ and $\frac{1}{2} D_{\mathcal{V}}^2\big|_0 \mathcal{E}\Big(b_{\geqslant 1}\Big)$ are later defined in Definition 2.5.4. Note that it is a necessity to restrict $\mathcal{E}'$ to a sufficiently small ball B_r first, to be precise we require that $\|F(z)\| \leqslant 1 - \delta$ for all $z \in B_r$ where $0 < \delta < 1$, since $\mathcal{E}'$ itself does not have a differentiable extension due to the square root appearing in the definition of ι, see Eq. (2.1.10).

In order to reduce the technical efforts of proving Eq. (2.5.3), we will make use of the fact that

$$(\mathcal{W}_N U_N)\, N^{-1} H_N\, (\mathcal{W}_N U_N)^{-1} = \mathcal{W}_N \widetilde{A}_N \mathcal{W}_N^{-1} + \mathcal{W}_N \widetilde{B}_N \mathcal{W}_N^{-1} + o_*\left(\mathbb{T}_N\right),$$

which, as we will see in the proof of Theorem 2.4.12, is a consequence of Eq. (2.3.8). We can then prove Eq. (2.5.3) separately for the operators $\mathcal{W}_N\, \widetilde{A}_N\, \mathcal{W}_N^{-1}$ and $\mathcal{W}_N\, \widetilde{B}_N\, \mathcal{W}_N^{-1}$. In fact, we are going to verify that

$$\mathcal{W}_N\, \widetilde{A}_N\, \mathcal{W}_N^{-1} = \mathcal{E}_A\left(q\right) + D_{\mathcal{V}}\big|_q \mathcal{E}_A\Big(b_{\geqslant 1}\Big) + \frac{1}{2} D_{\mathcal{V}}^2\big|_0 \mathcal{E}_A\Big(b_{\geqslant 1}\Big) + \frac{c}{N} + o_*\left(\mathbb{T}_N\right), \tag{2.5.4}$$

$$\mathcal{W}_N\, \widetilde{B}_N\, \mathcal{W}_N^{-1} = \mathcal{E}_B\left(q\right) + D_{\mathcal{V}}\big|_q \mathcal{E}_B\Big(b_{\geqslant 1}\Big) + \frac{1}{2} D_{\mathcal{V}}^2\big|_0 \mathcal{E}_B\Big(b_{\geqslant 1}\Big) - \frac{c}{N} + o_*\left(\mathbb{T}_N\right), \tag{2.5.5}$$

where the constant c arises due to the non-commutative nature of the operators q and p, and $\mathcal{E}_A$ and $\mathcal{E}_B$ are differentiable extensions of $\mathcal{E}'_A, \mathcal{E}'_B : B_r \longrightarrow \mathbb{C}$

$$\mathcal{E}'_A(z) := u_z^\dagger \cdot T \cdot u_z, \qquad \mathcal{E}'_B(z) := \frac{1}{2}\left(u_z \otimes u_z\right)^\dagger \cdot \hat{v} \cdot u_z \otimes u_z, \tag{2.5.6}$$

where $u_z := \iota\left(F(z)\right)$. The proofs of Eqs. (2.5.4) and (2.5.5) will be carried out in Subsections 2.5.1 and 2.5.2, respectively. We have to perform a variety of operator estimates, and since $\mathcal{W}_N \widetilde{A}_N \mathcal{W}_N^{-1}$ and $\mathcal{W}_N \widetilde{B}_N \mathcal{W}_N^{-1}$ involve factors of the form $\sqrt{1-\mathbb{L}'}$ with $\mathbb{L}'$ defined in Definition 2.4.8, we need in particular to estimate the Taylor residuum corresponding to approximations of such terms. The operator estimates can be found in Appendix 2.8, respectively Appendix 2.9 for the operator square root specifically.

2.5.1 Taylor Expansion of $\mathcal{W}_N \widetilde{A}_N \mathcal{W}_N^{-1}$

In order to structure the analysis, we split the operator $\mathcal{W}_N \widetilde{A}_N \mathcal{W}_N^{-1}$ into simpler operators H_J, introduced in Definition 2.5.1, and we split the classical counterpart $\mathcal{E}_A$ defined in Eq. (2.5.6) into atoms $\mathcal{E}_J$, defined in Definition 2.5.2. In Lemma 2.5.3, we then explain how $\mathcal{W}_N \widetilde{A}_N \mathcal{W}_N^{-1}$ and $\mathcal{E}_A$ can be written in terms of H_J and $\mathcal{E}_J$, respectively.

Definition 2.5.1. Recall the function $t \mapsto f(t)$ from Definition 2.4.7. For $i \in \{0, \ldots, 4\}$, we define operators $h_i : \mathrm{dom}[\mathcal{N}] \longrightarrow \mathcal{F}_0 \otimes \mathcal{H}$ by $h_0 := 1_{\mathcal{F}_0} \otimes u_0$ and

$$h_1 := q = \sum_{j=1}^d q_j \otimes u_j, \qquad h_3 := ip' = i \sum_{j=1}^d \left(p_j - \mathfrak{Im}\left[\partial_j f(q)^\dagger \cdot b_{>d}\right]\right) \otimes u_j,$$
$$h_2 := f(q), \qquad h_4 := b_{>d},$$

where $f(q)$ and $\partial_j f(q)$ are defined according to Definition 2.4.8. Furthermore, for a multi-index $J = (i,j)$ with $i, j \in \{0, \ldots, 4\}$ we define an operator H_J on $\mathcal{W}_N \mathcal{F}_{\leqslant N}$ as

$$H_J := h_i^\dagger \cdot T \cdot h_j \left(1 - \mathbb{L}'\right)^{\frac{m_J}{2}},$$

where m_J counts how many of the indices in $J = (i,j)$ are zero.

Definition 2.5.2. Let us decompose an arbitrary $z \in \mathcal{H}_0$ as $z = \sum_{j=1}^{d}(t_j + is_j)\, u_j + z_{>d}$, with $t, s \in \mathbb{R}^d$ and $z_{>d} \in \{u_1, \ldots, u_d\}^{\perp}$. For $i \in \{0, \ldots, 4\}$, we define in analogy to Definition 2.5.1 the functions $e_i : \mathcal{H}_0 \longrightarrow \mathcal{H}$ by $e_0(z) := u_0$ and

$$e_1(z) : = \sum_{j=1}^{d} t_j\, u_j, \qquad e_3(z) := i \sum_{j=1}^{d} \left(s_j - \mathfrak{Im}\left[\partial_j f(t_1, \ldots, t_d)^{\dagger} \cdot z\right]\right) u_j,$$
$$e_2(z) : = f\left(t\right), \qquad e_4(z) := z_{>d}.$$

With this at hand, we can write the transformation $F : \mathcal{H}_0 \longrightarrow \mathcal{H}_0$ from Eq. (2.4.7) as

$$F(z) = e_1(z) + e_2(z) + e_3(z) + e_4(z).$$

Furthermore, consider for $m \in \{0, \ldots, 4\}$ the functions

$$\eta_m\left(z\right) := \begin{cases} \left(1 - \|F(z)\|^2\right)^{\frac{m}{2}} & \text{for even } m, \\ \chi\left(\|F(z)\|^2\right)\left(1 - \|F(z)\|^2\right)^{\frac{m}{2}} & \text{for odd } m, \end{cases} \tag{2.5.7}$$

where χ is a smooth function with $0 \leqslant \chi(x) \leqslant 1$, $\operatorname{supp}(\chi) \subset [0, 1)$ and $\chi(x) = 1$ for $|x| < \frac{1}{2}$. Then we can define for a multi-index $J = (i, j)$ with $i, j \in \{0, \ldots, 4\}$ the function $\mathcal{E}_J : \mathcal{H}_0 \cap \operatorname{dom}[T] \longrightarrow \mathbb{C}$ as

$$\mathcal{E}_J(z) := e_i(z)^{\dagger} \cdot T \cdot e_j(z)\ \eta_{m_J}\left(z\right),$$

where m_J counts how many of the two indices i, j are zero.

Lemma 2.5.3. *Let us define for all $i, j \in \{1, \ldots, 4\}$ the coefficients $\lambda_{(0,0)} := 1$, $\lambda_{(i,0)} := 2$, $\lambda_{(i,j)} := 1$ and $\lambda_{(0,j)} := 0$. Then*

$$\mathcal{W}_N\, \widetilde{\mathbb{A}}_N\, \mathcal{W}_N^{-1} = \sum_{J \in \{0, \ldots, 4\}^2} \lambda_J\, \mathfrak{Re}\left[H_J\right], \tag{2.5.8}$$

where $\widetilde{\mathbb{A}}_N$ is defined in Eq. (2.3.6). Furthermore, the functional $\mathcal{E}_A$ defined as

$$\mathcal{E}_A(z) : = \sum_{J \in \{0, \ldots, 4\}^2} \lambda_J\, \mathfrak{Re}\left[\mathcal{E}_J(z)\right], \tag{2.5.9}$$

is an extension of $\mathcal{E}'_A\big|_{B_r}$ defined in Eq. (2.5.6), where $B_r := \{z \in \mathcal{H}_0 \cap \operatorname{dom}[T] : \|z\| < r\}$ and $r > 0$ is a constant such that $\|F(z)\| < \frac{1}{2}$ for all $z \in \mathcal{H}_0$ with $\|z\| < r$.

Note that the operator $\mathcal{W}_N\, \widetilde{\mathbb{A}}_N\, \mathcal{W}_N^{-1}$ involves terms with $\sqrt{1 - \mathbb{L}'}$ on the right side as well as on the left side. In order to reduce the technical effort later, it will be convenient to have all of them on one side, say the right side. This can be achieved by using the real part, e.g. we can write for $j \in \{1, \ldots, 4\}$

$$h_j^{\dagger} \cdot T \cdot u_0 \sqrt{1 - \mathbb{L}'} + \sqrt{1 - \mathbb{L}'} u_0^{\dagger} \cdot T \cdot h_j = \mathfrak{Re}\left[h_j^{\dagger} \cdot T \cdot u_0 \sqrt{1 - \mathbb{L}'}\right] = 2\mathfrak{Re}\left[H_{(j,0)}\right].$$

Therefore we set all the coefficients $\lambda_{(0,j)}$ in Lemma 2.5.3 to zero, since the $(0, j)$-contribution is already included in the real part of the $(j, 0)$-contribution.

Proof. Eq. (2.5.8) follows from the transformation law $\mathcal{W}_N\, b_{\geqslant 1}\, \mathcal{W}_N^{-1} = h_1 + h_2 + h_3 + h_4$, where h_i is defined in Definition 2.5.1, and the definition $\mathbb{L}' = \mathcal{W}_N\, \mathbb{L}\, \mathcal{W}_N^{-1}$. Similarly we obtain $\mathcal{E}_A(z) = \mathcal{E}'_A(z)$ for all z with $\|z\| < r$ for r as above and the fact that

$$\iota\big(F(z)\big) = \iota\left(e_1(z)+e_2(z)+e_3(z)+e_4(z)\right) = \sqrt{1-\|F(z)\|^2}e_0+e_1(z)+e_2(z)+e_3(z)+e_4(z).$$

∎

In order to prove the Taylor approximation in Eq. (2.5.4), we will verify that each of the atoms H_J can be approximated using the quantized Taylor coefficients of $\mathcal{E}_J$. The quantized Taylor coefficients $D_{\mathcal{V}}\big|_q \mathcal{E}_J\Big(b_{\geqslant 1}\Big)$ and $D^2_{\mathcal{V}}\big|_0\, \mathcal{E}_J\Big(b_{\geqslant 1}\Big)$ are rigorously defined by the following Definition.

Definition 2.5.4. Let $L_t : \mathcal{H}_0 \longrightarrow \mathbb{C}$ be a bounded $\mathbb{R}$-linear map for all $t \in \mathbb{R}^d$, and let $w(t), \widetilde{w}(t)$ be the unique elements in $\mathcal{H}_0$ such that $L_t(z) = w(t)^\dagger \cdot z + z^\dagger \cdot \widetilde{w}(t)$. Then we define

$$L_q\left(b_{\geqslant 1}\right) := w(q)^\dagger \cdot b_{\geqslant 1} + b^\dagger_{\geqslant 1} \cdot \widetilde{w}(q). \tag{2.5.10}$$

Let furthermore Λ be an $\mathbb{R}$-quadratic form on $\mathcal{H}_0$ with a unique decomposition $\Lambda(z) = z^\dagger \cdot Q \cdot z + G^\dagger \cdot z \otimes z + (z \otimes z)^\dagger \cdot \widetilde{G}$ where Q is an operator on $\mathcal{H}_0$ and $G, \widetilde{G} \in \mathcal{H} \otimes_{\mathrm{s}} \mathcal{H}_0$ (or, more generally, in $\overline{\mathcal{H}_0 \otimes_{\mathrm{s}} \mathcal{H}_0}^{\|\cdot\|_*}$ as introduced in Lemma 2.4.1). Then we define $\Lambda\left(b_{\geqslant 1}\right)$ as

$$\Lambda\left(b_{\geqslant 1}\right) := b^\dagger_{\geqslant 1} \cdot Q \cdot b_{\geqslant 1} + G^\dagger \cdot b_{\geqslant 1} \underline{\otimes}\, b_{\geqslant 1} + \left(b_{\geqslant 1} \underline{\otimes}\, b_{\geqslant 1}\right)^\dagger \cdot \widetilde{G}.$$

In the following we want to verify that the residuum R_J defined as

$$R_J := H_J - \mathcal{E}_J(q) - D_{\mathcal{V}}\big|_q \mathcal{E}_J\left(b_{\geqslant 1}\right) - \frac{1}{2} D^2_{\mathcal{V}}\big|_0 \mathcal{E}_J\left(b_{\geqslant 1}\right) - \frac{c_J}{N} \tag{2.5.11}$$

is small, where the constant c_J are given by

$$\begin{aligned} c_{(0,0)} &:= \frac{d}{4}\, u_0^\dagger \cdot T \cdot u_0 = -\frac{1}{8} \sum_{j=1}^d \partial^2_{t_j}\big|_{t=0} \mathcal{E}_{(0,0)}\left(\boldsymbol{t}\right), \\ c_{(3,3)} &:= \frac{1}{4} \sum_{j=1}^d u_j^\dagger \cdot T \cdot u_j = \frac{1}{8} \sum_{j=1}^d \partial^2_{t_j}\big|_{t=0} \mathcal{E}_{(1,1)}\left(\boldsymbol{t}\right), \end{aligned} \tag{2.5.12}$$

$c_{(1,3)} := c_{(3,1)} := -c_{(3,3)}$ and $c_J := 0$ for all other $J \in \{0,\ldots,4\}^2$, where $\boldsymbol{t} := \sum_{j=1}^d t_j u_j$. The proof will be spit into two parts. In Lemma 2.5.6 we derive an explicit representation of the residuum R_J by sorting the operator H_J in terms of powers in p and $b_{>d}$, and in Theorem 2.5.7 we will make sure that this residuum is indeed small compared to the operator $\mathbb{T}_N$ defined in Eq. (2.4.11), which is quadratic in the operators p and $b_{>d}$.

In order to illustrate the emergence of the additional constants c_J in the residuum R_J in Eq. (2.5.11), let us first investigate the following toy problem.

Example. Consider the toy Hamiltonian $H_{\mathrm{toy}} := b_1^\dagger b_1$ and the corresponding Hartree functional $\mathcal{E}_{\mathrm{toy}} : \mathbb{C} \longrightarrow \mathbb{C}$ given by $\mathcal{E}_{\mathrm{toy}}[z] := |z|^2$. Using $b_1 = q_1 + ip_1$ and the commutation relation $[ip_1, q_1] = \frac{1}{2N}$, we obtain

$$H_{\mathrm{toy}} = q_1^2 + p_1^2 - \frac{1}{2N} = q_1^2 - \frac{1}{4}\left(b_1 - b_1^\dagger\right)^2 - \frac{1}{2N} = q_1^2 + \frac{1}{2} b_1^\dagger b_1 - \frac{1}{4} b_1^2 - \frac{1}{4}\left(b_1^\dagger\right)^2 - \frac{1}{4N}. \tag{2.5.13}$$

Let $D_\mathcal{V}$ be the derivative with respect to the imaginary part and $z = t + is \in \mathbb{C}$, then

$$\frac{1}{2}D_\mathcal{V}^2|_0\,\mathcal{E}_{\text{toy}}(z) = \frac{1}{2}D^2|_0\,\mathcal{E}_{\text{toy}}(is) = s^2 = \frac{1}{2}|z|^2 - \frac{1}{4}z^2 - \frac{1}{4}\bar{z}^2.$$

With the definition $c_{\text{toy}} := -\frac{1}{8}\partial_t^2\big|_{t=0}\mathcal{E}_{\text{toy}}[t] = -\frac{1}{4}$ we can therefore rewrite Eq. (2.5.13) as

$$H_{\text{toy}} = \mathcal{E}_{\text{toy}}[q_1] + \frac{1}{2}D_\mathcal{V}^2|_0\mathcal{E}_{\text{toy}}(b_1) + \frac{c_{\text{toy}}}{N}.$$

Definition 2.5.5 (Taylor approximation of the square root)**.** Let η_m be the function defined in Eq. (2.5.7) and let us define the constant $c_m := \frac{m}{8}d$. We then define the residuum corresponding to the operator Taylor approximation of $\left(1-\mathbb{L}'\right)^{\frac{m}{2}}$, for different degrees of accuracy, as

$$\begin{aligned}
E_m^0 &:= \left(1-\mathbb{L}'\right)^{\frac{m}{2}} - \eta_m\left(q\right), \\
E_m^1 &:= \left(1-\mathbb{L}'\right)^{\frac{m}{2}} - \eta_m\left(q\right) - D_\mathcal{V}\big|_q\eta_m\left(b_{\geqslant 1}\right), \\
E_m^2 &:= \left(1-\mathbb{L}'\right)^{\frac{m}{2}} - \eta_m\left(q\right) - D_\mathcal{V}\big|_q\eta_m\left(b_{\geqslant 1}\right) - \frac{1}{2}D_\mathcal{V}^2\big|_0\eta_m\left(b_{\geqslant 1}\right) - \frac{c_m}{N}.
\end{aligned}$$

Lemma 2.5.6. *Let $J = (i,j) \in \{0,\dots,4\}^2$ be such that $\lambda_J \neq 0$, where λ_J is defined in Lemma 2.5.3, and let R_J be the residuum defined in Eq. (2.5.11). By distinguishing different cases with the help of the index $e_J := |\{\ell \in J : \ell \in \{3,4\}\}|$ and the index $m_J := |\{\ell \in J : \ell = 0\}|$, we can explicitly express R_J as*

- *In the case $m_J = 2$, i.e. $J = (0,0)$: $R_{(0,0)} = \left(u_0^\dagger \cdot T \cdot u_0\right) E_2^2$.*
- *In the case $e_J = 0$ and $m_J < 2$: $R_J = \left(h_i^\dagger \cdot T \cdot h_j\right) E_{m_J}^1$.*
- *In the case $e_J = 1$, there exists a constant C and functions $F_J : \mathbb{R}^d \longrightarrow \mathbb{R}$ with $|F_J(t)| \leqslant C|t|$, such that*

$$R_J = \left(h_i^\dagger \cdot T \cdot h_j\right) E_{m_J}^0 + \frac{F_J(q)}{N}. \tag{2.5.14}$$

- *For $e_J = 2$ we distinguish further between the individual cases and obtain*

$$\begin{aligned}
R_{(3,3)} &= \left(ip' - ip\right)^\dagger \cdot T \cdot ip' + \left(ip\right)^\dagger \cdot T \cdot \left(ip' - ip\right), \\
R_{(3,4)} &= \left(ip' - ip\right)^\dagger \cdot T \cdot b_{>d} = R_{(4,3)}^\dagger, \\
R_{(4,4)} &= 0.
\end{aligned}$$

Proof. The Lemma can be verified by straightforward computations for the different individual cases. For the purpose of illustration, we will explicitly carry out the computations for the case $J = (3,j)$ with $j \in \{0,1,2\}$, i.e. we are going to verify Eq. (2.5.14) for this special case.

Using the definition of E_m^0 in Definition 2.5.5, the observation $h_j = e_j(q)$ and the fact that $(ip'_\ell)^\dagger = b_{\geqslant 1}^\dagger \cdot \big(u_\ell - \partial_{u_\ell} f(q)\big) - \big(u_\ell - \partial_{u_\ell} f(q)\big)^\dagger \cdot b_{\geqslant 1}$, we obtain

$$\begin{aligned} H_J &= (ip')^\dagger \cdot T \cdot e_j(q)\,(1-\mathbb{L}')^{\frac{m}{2}} = (ip')^\dagger \cdot T \cdot e_j(q)\eta_m(q) + (ip')^\dagger \cdot T \cdot e_j(q) E_m^0 \\ &= \frac{1}{2}\sum_{\ell=1}^d b_{\geqslant 1}^\dagger \cdot \big(u_\ell - \partial_{u_\ell} f(q)\big) u_\ell^\dagger \cdot T \cdot e_j(q)\,\eta_m(q) - \frac{1}{2}\sum_{\ell=1}^d \big(u_\ell - \partial_{u_\ell} f(q)\big)^\dagger \cdot b_{\geqslant 1} u_\ell^\dagger \cdot T \cdot e_j(q)\,\eta_m(q) \\ &\quad + (ip')^\dagger \cdot T \cdot e_j(q) E_m^0, \end{aligned} \tag{2.5.15}$$

where $m := m_J$. Our goal is to commute $b_{\geqslant 1}$ in $\big(u_\ell - \partial_{u_\ell} f(q)\big)^\dagger \cdot b_{\geqslant 1} u_\ell^\dagger \cdot T \cdot e_j(q)\,\eta_m(q)$ to the right side, in order to obtain an expression which is of the same form as (2.5.10). We define the corresponding functions w and $\widetilde{w}$ as

$$w := -\frac{1}{2}\sum_{\ell=1}^d \Big(u_\ell^\dagger \cdot T \cdot e_j(\boldsymbol{t})\eta_m(\boldsymbol{t})\Big)\,\big(u_\ell - \partial_{t_\ell} f(t)\big)$$

and $\widetilde{w}(t) := -w(t)$. The commutation law $\Big[g(q), \big(u_\ell - \partial_{u_\ell} f(q)\big)^\dagger \cdot b_{\geqslant 1}\Big] = [g(q), ip_\ell] = -\frac{1}{2N}\partial_\ell g(q)$, for C^1 functions $g : \mathbb{R}^d \longrightarrow \mathbb{R}$ then yields

$$-\frac{1}{2}\sum_{\ell=1}^d \big(u_\ell - \partial_{u_\ell} f(q)\big)^\dagger \cdot b_{\geqslant 1}\, u_\ell^\dagger \cdot T \cdot e_j(q)\,\eta_m(q) = w(q)^\dagger \cdot b_{\geqslant 1} + \frac{1}{N} y(q),$$

where $y : \mathbb{R}^d \longrightarrow \mathbb{R}$ is defined as $y(t) := -\frac{1}{4}\sum_\ell \partial_\ell\,(u_\ell \cdot T \cdot e_j(\boldsymbol{t})\eta_m(\boldsymbol{t}))$. Furthermore

$$\begin{aligned} D_{\mathcal{V}}\big|_{\boldsymbol{t}}\, \mathcal{E}_J(z) &= e_3(z)^\dagger \cdot T \cdot e_j(\boldsymbol{t})\eta_m(\boldsymbol{t}) = \sum_{\ell=1}^d \Big(i\mathfrak{Im}\Big[\big(u_\ell - \partial_{t_\ell} f(t)\big)^\dagger \cdot z\Big]\, u_\ell\Big)^\dagger \cdot T \cdot e_j(\boldsymbol{t})\eta_m(\boldsymbol{t}) \\ &= w(t)^\dagger \cdot z + z^\dagger \cdot \widetilde{w}(t). \end{aligned}$$

Consequently we can rewrite Eq. (2.5.15) as

$$(ip')^\dagger \cdot T \cdot e_j(q)\,(1-\mathbb{L}')^{\frac{m}{2}} = D_{\mathcal{V}}\big|_q\, \mathcal{E}_J(b_{\geqslant 1}) + \frac{1}{N} y(q) + (ip')^\dagger \cdot T \cdot e_j(q) E_m^0.$$

Note that $\mathcal{E}_J(\boldsymbol{t}) = 0$ and $D_{\mathcal{V}}^2\big|_0 \mathcal{E}_J = 0$. Therefore Eq. (2.5.14) follows from the fact that $F(t) := y(t) - c_J$ is Lipschitz and $F(0) = 0$, which implies that there exists a constant C such that $|F(t)| \leqslant C|t|$. ∎

For the proof of the following Theorem, we will use various operator estimates derived in Appendices 2.8 and 2.9.

Theorem 2.5.7. *Let $J \in \{0, \ldots, 4\}^2$ be such that $\lambda_J \neq 0$ and let R_J be the residuum defined in Eq. (2.5.11). Then,*

$$R_J = o_*(\mathbb{T}_N),$$

with $\mathbb{T}_N$ defined in Eq. (2.4.11) and the $o_*(\cdot)$ notation from Definition 2.4.10.

Proof. Recall the definitions in Lemma 2.5.6 of $e_J := |\{l \in J : l \in \{3,4\}\}|$, which counts how many of the indices in $J = (i,j)$ are equal to 3 or 4, $m_J := |\{l \in J : l = 0\}|$, which counts how many of the indices are zero, and the residuum R_J defined in Eq. (2.5.11). In order to prove the statement of the Theorem, we are going to verify $R_J = o_* (\mathbb{T}_N)$ for all J with $\lambda_J \neq 0$.

The case $J = (0,0)$: In this case we have the identity $R_{(0,0)} = \left(u_0^\dagger \cdot T \cdot u_0\right) E_2^2$, hence we have to verify $E_2^2 = o_* (\mathbb{T}_N)$. In order to do this, recall the function $\eta_2(x) = 1 - \|F(x)\|^2$ from Eq. (2.5.7) and let us compute using Lemma 2.4.9

$$
\begin{aligned}
1 - \mathbb{L}' &= 1 - (q + f(q) + ip' + b_{>d})^\dagger \cdot (q + f(q) + ip' + b_{>d}) \\
&= 1 - q^\dagger \cdot q - f(q)^\dagger \cdot f(q) - f(q)^\dagger \cdot b_{>d} - b_{>d}^\dagger \cdot f(q) \\
&\quad - b_{>d}^\dagger \cdot b_{>d} - \left(p^\dagger \cdot p\right) + \frac{d}{2N} - p^\dagger \cdot (p' - p) - (p' - p)^\dagger \cdot p' \\
&= \eta_2(q) + D_{\mathcal{V}}\big|_q \eta_2(b_{\geqslant 1}) + D^2_{\mathcal{V}}\big|_0 \eta_2(b_{\geqslant 1}) + \frac{d}{4N} - p^\dagger \cdot (p' - p) - (p' - p)^\dagger \cdot p',
\end{aligned}
$$

where we used $\eta_2(q) = 1 - q^\dagger \cdot q - f(q)^\dagger \cdot f(q)$ and $p^\dagger \cdot p = \frac{1}{4}\sum_{j=1}^d \left(2b_j^\dagger b_j - b_j^2 - \left(b_j^\dagger\right)^2\right) + \frac{d}{4N}$. Note that $\frac{c_2}{N} = \frac{d}{4N}$, where c_2 is the constant from Definition 2.5.5. Since $p^2 \leqslant \mathbb{T}_N$, it is clear that $p^2 = O_* (\mathbb{T}_N)$. In Lemmata 2.8.6 and 2.8.5, we will verify that $(p')^2 = O_* (\mathbb{T}_N)$ and $(p' - p)^2 = o_* (\mathbb{T}_N)$. Therefore we obtain by the operator Cauchy–Schwarz inequality in the auxiliary Lemma 2.8.1 that $p^\dagger \cdot (p' - p)$ as well as $(p' - p)^\dagger \cdot p'$ are of order $o_* (\mathbb{T}_N)$. We conclude $E_2^2 = o_* (\mathbb{T}_N)$.

The case $e_J = 0$, with $J \neq (0,0)$: In this case $m_J \in \{0,1\}$ and the error is given by

$$
R_J = h_i^\dagger \cdot T \cdot h_j\, E^1_{m_J} = e_i(q)^\dagger \cdot T \cdot e_j(q)\; E^1_{m_J}.
$$

We clearly have $E_0^1 = 0$. For $m_J = 1$, let us define the function $V(t) := e_i(\boldsymbol{t}\,)^\dagger \cdot T \cdot e_j(\boldsymbol{t}\,)$, which satisfies $V(t) \leqslant C|t|$ for a constant C. In Lemma 2.9.2 we will then verify that $V(q)E_1^1 = o_* (\mathbb{T}_N)$.

The case $e_J = 1$: In this case the error reads $R_J = \left(h_i^\dagger \cdot T \cdot h_j\right) E^0_{m_J} + \frac{F_J(q)}{N}$, where $F_J(t) \leqslant C|t|$ for some constant C. Using Lemma 2.9.2 and Lemma 2.8.4 from the Appendix, we obtain that $(E_1^0)^\dagger E_1^0 = o_* (T_N)$ and $\frac{F_J(q)}{N} = o_* \left(\frac{1}{N}\right)$. Regarding the first term, note that $E_0^0 = 0$. Hence, we assume w.l.o.g. $m_J = 1$. We are done once we can verify

$$
\left(h_i^\dagger \cdot T \cdot h_j\right) \cdot \left(h_i^\dagger \cdot T \cdot h_j\right)^\dagger = O_* (\mathbb{T}_N) \tag{2.5.16}
$$

in case one of the indices i, j is in $\{3,4\}$ and the other is zero. Let us first assume $i \in \{3,4\}$. Then $h_i^\dagger \cdot T \cdot h_j = h_i^\dagger \cdot w$, with $w := T \cdot u_0 \in \mathcal{H}$, and therefore Eq. (2.5.16) follows from Lemma 2.8.6 in the case $i = 3$ and from Lemma 2.8.5 in the case $i = 4$. The proof of the case $j \in \{3,4\}$ follows analogously.

The case $e_J = 2$: In this case, the error is a linear combination of $(ip' - ip)^\dagger \cdot T \cdot h_j$ and $h_i^\dagger \cdot T \cdot (ip' - ip)$ with $h_i, h_j \in \{p', b_{>d}\}$. Note that $A := \sqrt{T}\,(1_{\mathcal{H}} - \pi_{>d})$ is bounded, and therefore

$$\begin{aligned}(ip' - ip)^\dagger \cdot T \cdot (ip' - ip) &= (ip' - ip)^\dagger \cdot A^\dagger A \cdot (ip' - ip) \\ &\leqslant \|A\|^2 \ (ip' - ip)^\dagger \cdot (ip' - ip) = o_* (\mathbb{T}_N)\end{aligned}$$

by Lemma 2.8.5. Similarly, we have $(p')^\dagger \cdot T \cdot p' \leqslant \|A\|^2 (p')^\dagger \cdot p' = O_* (\mathbb{T}_N)$ by Lemma 2.8.6. Hence Lemma 2.8.1 tells us that $(ip' - ip)^\dagger \cdot T \cdot h_j$ and $h_i^\dagger \cdot T \cdot (ip' - ip)$ are of order $o_* (\mathbb{T}_N)$. ■

Corollary 2.5.8. *Recall the functional $\mathcal{E}_A$ defined in Eq. (2.5.9) and let us define the constant $c := \sum_{J \in \{0,\dots,4\}^2} \lambda_J c_J$. Then*

$$\mathcal{W}_N \widetilde{A}_N \mathcal{W}_N^{-1} = \mathcal{E}_A(q) + D_{\mathcal{V}}\big|_q \mathcal{E}_A (b_{\geqslant 1}) + \frac{1}{2} D_{\mathcal{V}}^2\big|_0 \mathcal{E}_A (b_{\geqslant 1}) + \frac{c}{N} + o_* (\mathbb{T}_N) .$$

Proof. The statement follows from combining Lemma 2.5.3 and Theorem 2.5.7. ■

2.5.2 Taylor Expansion of $\mathcal{W}_N \widetilde{B}_N \mathcal{W}_N^{-1}$

Similar to the previous subsection, we introduce atoms H_J in Definition 2.5.9 as well as their classical counterparts $\mathcal{E}_J$ in Definition 2.5.10. In Lemma 2.5.11 we explain how $\mathcal{W}_N \widetilde{B}_N \mathcal{W}_N^{-1}$ and $\mathcal{E}_B$ can be written in terms of H_J and $\mathcal{E}_J$, respectively.

Definition 2.5.9. Recall the definition of $h_i : \mathrm{dom}[\mathcal{N}] \longrightarrow \mathcal{F}_0 \otimes \mathcal{H}$ from Definition 2.5.1. For a multi-index $J = (i, j, k, \ell)$ with $i, j, k, \ell \in \{0, \dots, 4\}$, we define an operator H_J on $\mathcal{W}_N \mathcal{F}_{\leqslant N}$ as

$$H_J := (h_i \underline{\otimes} h_j)^\dagger \cdot \hat{v} \cdot h_k \underline{\otimes} h_\ell (1 - \mathbb{L}')^{\frac{m_J}{2}} ,$$

where m_J counts how many of the indices i, j, k, ℓ are zero.

Definition 2.5.10. Recall the definition of $e_i : \mathcal{H}_0 \longrightarrow \mathcal{H}$ and η_m from Definition 2.5.2. For a multi-index $J = (i, j, k, \ell)$ with $i, j, k, \ell \in \{0, \dots, 4\}$, we define $\mathcal{E}_J : \mathcal{H}_0 \cap \mathrm{dom}[T] \longrightarrow \mathbb{C}$

$$\mathcal{E}_J(z) := \Big[e_i(z) \otimes e_j(z)\Big]^\dagger \cdot \hat{v} \cdot e_k(z) \otimes e_\ell(z) \ \eta_{m_J}(z),$$

where m_J counts how many of the indices i, j, k, ℓ are zero and η_m are the functions defined in Eq. (2.5.7).

Lemma 2.5.11. *Let us define for all $i, j, k, \ell \in \{1, \dots, 4\}$ the coefficients $\lambda_{(0,0,0,0)} := \frac{1}{2}$, $\lambda_{(i,0,0,0)} := 2$, $\lambda_{(i,j,0,0)} := \lambda_{(i,0,k,0)} := \lambda_{(0,j,k,0)} := 1$, $\lambda_{(i,j,k,0)} := 2$, $\lambda_{(i,j,k,\ell)} := \frac{1}{2}$ and all other coefficients are defined as $\lambda_J := 0$. Then*

$$\mathcal{W}_N\, \widetilde{B}_N\, \mathcal{W}_N^{-1} = \sum_{J \in \{0,\dots,4\}^4} \lambda_J\, \mathfrak{Re}\, [H_J] .$$

Furthermore, the functional $\mathcal{E}_B$ defined as

$$\mathcal{E}_B(z) := \sum_{J \in \{0,\dots,4\}^4} \lambda_J\, \mathfrak{Re}\, [\mathcal{E}_J(z)] , \tag{2.5.17}$$

is an extension of $\mathcal{E}_B'\big|_{B_r}$ defined in Eq. (2.5.6), where $B_r := \{z \in \mathcal{H}_0 \cap \mathrm{dom}\, [T] : \|z\| < r\}$ and $r > 0$ is a constant such that $\|F(z)\| < \frac{1}{2}$ for all $z \in \mathcal{H}_0$ with $\|z\| < r$.

The proof of Lemma 2.5.11 works analogously to the proof of Lemma 2.5.3. Following the strategy from Subsection 2.5.1 we are going to verify that the residuum R_J

$$R_J := H_J - \mathcal{E}_J(q) - D_{\mathcal{V}}\big|_q \mathcal{E}_J\left(b_{\geqslant 1}\right) - \frac{1}{2} D_{\mathcal{V}}^2\big|_0 \mathcal{E}_J\left(b_{\geqslant 1}\right) - \frac{c_J}{N} \tag{2.5.18}$$

is small, where the constant c_J are given by $c_{(0,0,0,0)} := -\frac{1}{8}\sum_{j=1}^d \partial_{t_j}^2\big|_{t=0}\mathcal{E}_{(0,0,0,0)}\left(\boldsymbol{t}\right)$ and

$$\begin{aligned}
c_{(3,3,0,0)} &:= -\frac{1}{8}\sum_{j=1}^d \partial_{t_j}^2\big|_{t=0}\mathcal{E}_{(1,1,0,0)}\left(\boldsymbol{t}\right), \quad c_{(3,1,0,0)} := -c_{(3,3,0,0)}, \quad c_{(1,3,0,0)} := c_{(3,3,0,0)},\\
c_{(3,0,3,0)} &:= \frac{1}{8}\sum_{j=1}^d \partial_{t_j}^2\big|_{t=0}\mathcal{E}_{(1,0,1,0)}\left(\boldsymbol{t}\right), \quad c_{(1,0,3,0)} := -c_{(3,0,3,0)}, \quad c_{(3,0,1,0)} := -c_{(3,0,3,0)},\\
c_{(0,3,3,0)} &:= \frac{1}{8}\sum_{j=1}^d \partial_{t_j}^2\big|_{t=0}\mathcal{E}_{(0,1,1,0)}\left(\boldsymbol{t}\right), \quad c_{(0,1,3,0)} := -c_{(0,3,3,0)}, \quad c_{(0,3,1,0)} := -c_{(0,3,3,0)},
\end{aligned} \tag{2.5.19}$$

and all other constants are defined as $c_J := 0$. The proof will be split into two parts. In Lemma 2.5.12 we derive an explicit representation of the residuum R_J by sorting the operator H_J in terms of powers in p and $b_{>d}$, and in Theorem 2.5.16 we will make sure that this residuum is indeed small compared to the operator $\mathbb{T}_N$.

Lemma 2.5.12. *Let $J = (i,j,k,\ell) \in \{0,\ldots,4\}^4$ be such that $\lambda_J \neq 0$, where λ_J is defined in Lemma 2.5.11, and let R_J be the residuum defined in Eq. (2.5.18). By distinguishing different cases with the help of the indices $e_J := |\{\ell \in J : \ell \in \{3,4\}\}|$ and $m_J := |\{\ell \in J : \ell = 0\}|$, we can explicitly express R_J as:*

- *In the case $m_J = 4$, i.e. $J = (0,0,0,0)$: $R_J = (h_i \otimes h_j)^\dagger \cdot \hat{v} \cdot h_k \otimes h_\ell\, E_4^2$.*
- *In the case $e_J = 0$ and $m_J < 4$: $R_J = (h_i \otimes h_j)^\dagger \cdot \hat{v} \cdot h_k \otimes h_\ell\, E_{m_J}^1$.*
- *In the case $e_J = 1$, there exists a constant C and functions $F_J : \mathbb{R}^d \longrightarrow \mathbb{R}$ with $|F_J(t)| \leqslant C|t|$, such that $R_J = (h_i \otimes h_j)^\dagger \cdot \hat{v} \cdot h_k \otimes h_\ell\, E_{m_J}^0 + \frac{F_J(q)}{N}$.*
- *In the case $e_J = 2$ and $m_J = 2$ when two of the indices are 4:*

$$R_J = -\left(h_i \otimes h_j\right)^\dagger \cdot \hat{v} \cdot h_k \otimes h_\ell\, \mathbb{L}'.$$

- *In the case $e_J = 2$ and $m_J = 2$ when one of the indices is 3 and another one is 4, let us define $\widetilde{h}_3 := p' - p$ and $\widetilde{h}_r := h_r$ for $r \in \{0,1,2,4\}$. Then,*

$$R_J = -\left(h_i \otimes h_j\right)^\dagger \cdot \hat{v} \cdot h_k \otimes h_\ell\, \mathbb{L}' + \left(\widetilde{h}_i \otimes \widetilde{h}_j\right)^\dagger \cdot \hat{v} \cdot \widetilde{h}_k \otimes \widetilde{h}_\ell.$$

- *In the case $e_J = 2$ and $m_J = 2$ when two of the indices are 3, let us define the coefficients $\Lambda_{(3,3,0,0)}^{r,r'} := -\left(u_r \otimes u_{r'}\right)^\dagger \cdot \hat{v} \cdot u_0 \otimes u_0$, $\Lambda_{(3,0,3,0)}^{r,r'} := \left(u_r \otimes u_0\right)^\dagger \cdot \hat{v} \cdot u_{r'} \otimes u_0$ and $\Lambda_{(0,3,3,0)}^{r,r'} := \left(u_0 \otimes u_r\right)^\dagger \cdot \hat{v} \cdot u_{r'} \otimes u_0$. Then,*

$$R_J = -\left(h_i \otimes h_j\right)^\dagger \cdot \hat{v} \cdot h_k \otimes h_\ell\, \mathbb{L}' + \sum_{r,r'=1}^d \Lambda_J^{r,r'}\left[\left(p_r' - p_r\right)\cdot p_{r'}' + p_r \cdot \left(p_{r'}' - p_{r'}\right)\right]. \tag{2.5.20}$$

- *In the cases* $e_J = 2$ *and* $m_J < 2$*, respectively* $e_J > 2$*:* $R_J = H_J$.

Proof. Similar to the proof of Lemma 2.5.6, the proof of Lemma 2.5.12 follows from a straightforward computation for the individual cases. For the purpose of illustration, we will explicitly carry out the computations for the case $J = (3, 0, 3, 0)$, i.e. we are going to verify Eq. (2.5.20). Since $\mathcal{E}_{(3,0,3,0)}(z)$ is quadratic in $\pi(z)$, we immediately obtain $\mathcal{E}_{(3,0,3,0)}(\boldsymbol{t}\,) = 0$ and $D_{\mathcal{V}}\big|_{\boldsymbol{t}}\, \mathcal{E}_{(3,0,3,0)} = 0$. Let us define the coefficients $\lambda_{\alpha,\gamma} := (u_\alpha \otimes u_0)^\dagger \cdot \hat{v} \cdot u_\gamma \otimes u_0$, the operator $Q = \frac{1}{2} \sum_{\alpha,\gamma=1}^{d} \hat{v}_{\alpha 0,\gamma 0}\, u_\alpha \cdot u_\gamma^\dagger$ and $G \in \mathcal{H}_0 \otimes \mathcal{H}_0$ by $G = -\frac{1}{4} \sum_{\alpha,\gamma=1}^{d} \hat{v}_{\alpha 0,\gamma 0}\, u_\alpha \otimes u_\gamma$. Then

$$D_{\mathcal{V}}^2\big|_0\, \mathcal{E}_{(3,0,3,0)}(z) = z^\dagger \cdot Q \cdot z + G^\dagger \cdot z \otimes z + (z \otimes z) \cdot G$$

and therefore $D_{\mathcal{V}}^2\big|_0\, \mathcal{E}_{(3,0,3,0)}(b_{\geqslant 1}) = b_{\geqslant 1}^\dagger \cdot Q \cdot b_{\geqslant 1} + G^\dagger \cdot b_{\geqslant 1} \otimes b_{\geqslant 1} + (b_{\geqslant 1} \otimes b_{\geqslant 1}) \cdot G$. This concludes the proof of Eq. (2.5.20), since

$$\begin{aligned} & H_J - (ip' \underline{\otimes} u_0)^\dagger \cdot \hat{v} \cdot ip' \underline{\otimes} u_0 \, (-\mathbb{L}') - \sum_{r,r'=1}^{d} \Lambda_J^{r,r'} \left[(p'_r - p_r) \cdot p'_{r'} + p_r \cdot (p'_{r'} - p_{r'}) \right] \\ & = (ip \underline{\otimes} u_0)^\dagger \cdot \hat{v} \cdot ip \underline{\otimes} u_0 = \sum_{\alpha,\gamma=1}^{d} (u_\alpha \otimes u_0)^\dagger \cdot \hat{v} \cdot u_\gamma \otimes u_0 \, \frac{1}{2} \left(b_\alpha - b_\alpha^\dagger \right)^\dagger \cdot \frac{1}{2} \left(b_\gamma - b_\gamma^\dagger \right) \\ & = b_{\geqslant 1}^\dagger \cdot Q \cdot b_{\geqslant 1} + (b_{\geqslant 1} \underline{\otimes} b_{\geqslant 1})^\dagger \cdot G + G^\dagger \cdot b_{\geqslant 1} \underline{\otimes} b_{\geqslant 1} + \frac{C_{(3,0,3,0)}}{N}. \end{aligned}$$

■

In the remainder of this subsection, we are going to verify that the residuum R_J is small compared to the quadratic operator $\mathbb{T}_N$. Note that the error term in the last case of Lemma 2.5.12 is quite different from the other cases, since it simply corresponds to the whole operator H_J. This is not surprising, however, since the second order Taylor approximation of an object that is already of an higher order than two is zero, i.e. the residuum coincides with the object itself. With the help of the following three results in Lemma 2.5.13, Lemma 2.5.14 and Theorem 2.5.15, we will systematically verify that H_J is small compared to the quadratic operator $\mathbb{T}_N$ in the cases $e_J = 2$ and $m_J < 2$, respectively $e_J > 2$. Regarding all other cases, we will verify the smallness of the residuum in Theorem 2.5.16. In order to do this, we will repeatedly use results derived in Appendices 2.8 and 2.9.

Lemma 2.5.13. *For indices* $i, j \in \{0, \ldots, 4\}$*, we have the following estimates:*

- *In case one of the indices is contained in* $\{3, 4\}$*, we have*

$$(h_i \underline{\otimes} h_j)^\dagger \cdot |\hat{v}| \cdot h_i \underline{\otimes} h_j = O_* (\mathbb{T}_N) .$$

- *In case one of the indices is contained in* $\{3, 4\}$ *and the other one is contained in* $\{1, \ldots, 4\}$*, we have*

$$(h_i \underline{\otimes} h_j)^\dagger \cdot |\hat{v}| \cdot h_i \underline{\otimes} h_j = o_* (\mathbb{T}_N) .$$

Proof. We will repeatedly use the inequality $|v| \leqslant \Lambda(T+1) =: S$ from Assumption 2.1.1, which implies together with the translation-invariance of T the inequalities $|\hat{v}| \leqslant S \otimes 1_{\mathcal{H}}$ and $|\hat{v}| \leqslant 1_{\mathcal{H}} \otimes S$.

The case $i \in \{1,2\}$ and $j \in \{3,4\}$: Recall that $h_k = e_k(q)$ for $k \in \{0,1,2\}$ and let us define the function $\varphi(t) := e_i(\boldsymbol{t})^\dagger \cdot S \cdot e_i(\boldsymbol{t})$. Using the inequality $|\hat{v}| \leqslant S \otimes 1_{\mathcal{H}}$ we obtain

$$(e_i(q) \underline{\otimes} h_j)^\dagger \cdot |\hat{v}| \cdot e_i(q) \underline{\otimes} h_j \leqslant h_j^\dagger \cdot \varphi(q) \cdot h_j.$$

Since $|\varphi(t)| \leqslant C(|t| + |t|^2)$ for a constant C, we obtain $h_3^\dagger \cdot \varphi(q) \cdot h_3 = o_*(\mathbb{T}_N)$ and $h_4^\dagger \cdot \varphi(q) \cdot h_4 = o_*(\mathbb{T}_N)$ by Lemmata 2.8.4 and 2.8.6.

The case $i \in \{3,4\}$ and $j \in \{1,2\}$: Making use of the commutation laws $[b_\alpha, q_\beta] = 0$ and $[ip_\alpha, q_\beta] = \frac{1}{2N}\delta_{\alpha,\beta}$, this case follows from the previous one.

The case $i = 3, j = 3$: Let $\pi_{\leqslant d} := \sum_{r=1}^d u_r \cdot u_r^\dagger$. Since $\left((p')^\dagger \cdot p'\right)^2 = o_*(\mathbb{T}_N)$, we obtain

$$(p' \underline{\otimes} p')^\dagger \cdot |\hat{v}| \cdot p' \underline{\otimes} p' \leqslant (p')^\dagger \cdot \left((p')^\dagger \cdot p'\right) \otimes S \cdot p' \leqslant \left\|\pi_{\leqslant d}\, S\, \pi_{\leqslant d}\right\| \left((p')^\dagger \cdot p'\right)^2 = o_*(\mathbb{T}_N).$$

The case $i = 4$ and $j \in \{3,4\}$: Note that

$$\begin{aligned}(b_{>d} \underline{\otimes} h_j)^\dagger \cdot |\hat{v}| \cdot b_{>d} \underline{\otimes} h_j \leqslant\, & 2\,(f(q) \underline{\otimes} h_j)^\dagger \cdot |\hat{v}| \cdot f(q) \underline{\otimes} h_j \\ & + 2\,((b_{>d} + f(q)) \underline{\otimes} h_j)^\dagger \cdot |\hat{v}| \cdot (b_{>d} + f(q)) \underline{\otimes} h_j\end{aligned}$$

By the previous case $i \in \{1,2\}$ and $j \in \{3,4\}$, we know that $(f(q) \underline{\otimes} h_j)^\dagger \cdot |\hat{v}| \cdot f(q) \underline{\otimes} h_j = o_*(\mathbb{T}_N)$. For the second contribution, recall the definition of $\pi_{M,N}$ from Remark 2.4.11 and let $\tilde{\pi}_{M,N}$ be the orthogonal projection onto the subspace $\mathcal{W}_N \mathcal{F}^+_{\leqslant M} \subset \mathcal{F}_0$, where

$$\mathcal{F}^+_{\leqslant M} := \mathbb{1}_{[0,M]}\left(\sum_{j>d}^{\infty} a_j^\dagger \cdot a_j\right). \tag{2.5.21}$$

Since we have $b_k\, \tilde{\pi}_{M,N} = \tilde{\pi}_{M,N}\, b_k\, \tilde{\pi}_{M,N}$ for $k > d$ and $[p_j', \tilde{\pi}_{M,N}] = 0$ by Lemma 2.8.3, we obtain using $\pi_{M,N} = \tilde{\pi}_{M,N}\, \pi_{M,N}$ (which follows from $\mathcal{W}_N \mathcal{F}_{\leqslant M} \subset \mathcal{W}_N \mathcal{F}^+_{\leqslant M}$)

$$\begin{aligned}&\pi_{M,N}\left((b_{>d} + f(q)) \underline{\otimes} h_j\right)^\dagger \cdot |\hat{v}| \cdot (b_{>d} + f(q)) \underline{\otimes} h_j\, \pi_{M,N} \\ &\quad\leqslant \pi_{M,N}\, h_j^\dagger \cdot \left(\tilde{\pi}_{M,N}\,(b_{>d} + f(q))^\dagger \cdot (b_{>d} + f(q))\, \tilde{\pi}_{M,N}\right) \otimes S \cdot h_j\, \pi_{M,N} \\ &\quad\leqslant \frac{M}{N}\, \pi_{M,N}\, h_j^\dagger \cdot S \cdot h_j\, \pi_{M,N} \leqslant C\, \frac{M}{N}\, \pi_{M,N}\, \mathbb{T}_N\, \pi_{M,N}\end{aligned}$$

for a constant $0 < C < \infty$, where we used $h_j^\dagger \cdot S \cdot h_j = O_*(\mathbb{T}_N)$ and and the characterization of the $O_*(\cdot)$ notation in Remark 2.4.11 for the last inequality. Using this characterization for the inequality above yields $((b_{>d} + f(q)) \underline{\otimes} h_j)^\dagger \cdot |\hat{v}| \cdot (b_{>d} + f(q)) \underline{\otimes} h_j = o_*(\mathbb{T}_N)$.

The case $i = 3$ and $j = 4$: Making use of the commutation laws $[ip_\alpha', b] = -\frac{1}{2N}\partial_\alpha f(q)$, this case follows from the previous one.

The case $i = 0$ and $j \in \{3,4\}$, respectively $i \in \{3,4\}$ and $j = 0$: Since $h_0 = 1_{\mathcal{F}_0} \otimes u_0$ commutes with $h_3 = ip'$ and $h_4 = b_{>d}$, we assume w.l.o.g. $i = 0$ and $j \in \{3,4\}$. With $\lambda := u_0^\dagger \cdot S \cdot u_0$, we obtain

$$(u_0 \underline{\otimes} h_j)^\dagger \cdot |\hat{v}| \cdot u_0 \underline{\otimes} h_j \leqslant \lambda\, h_j^\dagger \cdot h_j = O_*\left(\mathbb{T}_N\right).$$

■

Lemma 2.5.14. *In the following, let $G : \mathbb{R}^d \longrightarrow \mathcal{H} \otimes \mathcal{H}$ be a differentiable function and let us define the operators $X, Y : \mathrm{dom}[\mathcal{N}] \longrightarrow \mathcal{F}_0 \otimes \mathcal{H}$ as*

$$X := (ip')^\dagger \otimes 1_{\mathcal{H}} \cdot G(q) = -\sum_{k=1}^{\infty} \left(\sum_{j=1}^{d} iG_{j,k} p'_j \right) \otimes u_k,$$
$$Y := b_{>d}^\dagger \otimes 1_{\mathcal{H}} \cdot G(q) = \sum_{k=1}^{\infty} \left(\sum_{j>d} iG_{j,k} b_j^\dagger \right) \otimes u_k.$$

Then we have the estimates

$$X^\dagger \cdot X \leqslant 2 \left[(p')^\dagger \cdot \|G\|^2(q) \cdot p' + \frac{d}{N^2} \sum_{\alpha=1}^{d} \|\partial_\alpha G\|^2(q) \right],$$
$$Y^\dagger \cdot Y \leqslant b_{>d}^\dagger \cdot \|G\|^2(q) \cdot b_{>d} + \frac{1}{N} \|G\|^2(q).$$

The proof of Lemma 2.5.14 is based on the commutation relations $[b_\alpha, b_\beta^\dagger] = \frac{1}{N}\delta_{\alpha,\beta}$ and $[p_\alpha, q_\beta] = \frac{1}{2iN}\delta_{\alpha,\beta}$, and is left to the reader.

Theorem 2.5.15. *Let $\mathbb{L}'$ be the operator from Definition 2.4.8. Then we have the following estimates:*

- *In case at least two of the indices $i, j, k, \ell \in \{1, \dots, 4\}$ are contained in $\{3,4\}$, we have*

$$(h_i \underline{\otimes} h_j)^\dagger \cdot \hat{v} \cdot h_k \underline{\otimes} h_\ell = o_*\left(\mathbb{T}_N\right),$$

- *In case at least two of the indices $i, j, k \in \{0, \dots, 4\}$ are contained in $\{3,4\}$, we have*

$$(h_i \underline{\otimes} h_j)^\dagger \cdot \hat{v} \cdot h_k \underline{\otimes} u_0\, \mathbb{L}' = o_*\left(\mathbb{T}_N\right),$$

- *In case at least two of the indices $i, j, k \in \{1, \dots, 4\}$ are contained in $\{3,4\}$, we have*

$$(h_i \underline{\otimes} h_j)^\dagger \cdot \hat{v} \cdot h_k \underline{\otimes} u_0 \sqrt{1 - \mathbb{L}'} = o_*\left(\mathbb{T}_N\right).$$

Proof. Let us denote with $e_{(a,b)}$ the number of indices in (a,b) that are elements of $\{3,4\}$. In the following, we will verify the theorem separately for the case $e_{(i,j)} \geqslant 1$ and $e_{(k,\ell)} \geqslant 1$, and the case $e_{(k,\ell)} = 0$. Note that the case $e_{(i,j)} = 0$ is only possible for the first bullet point, and the proof of the statement follows from the case $e_{(k,\ell)} = 0$, since

$$\left[(h_i \underline{\otimes} h_j)^\dagger \cdot \hat{v} \cdot h_k \underline{\otimes} h_\ell \right]^\dagger = (h_k \underline{\otimes} h_\ell)^\dagger \cdot \hat{v} \cdot h_i \underline{\otimes} h_j.$$

The case $e_{(i,j)} \geqslant 1$ and $e_{(k,\ell)} \geqslant 1$: Let us define the operators $A := h_i \underline{\otimes} h_j$ and $Q := \hat{v}$, and depending on the concrete bullet point let us define B as $h_k \underline{\otimes} h_\ell$, $h_k \underline{\otimes} u_0 \mathbb{L}'$ or $h_k \underline{\otimes} u_0 \sqrt{1-\mathbb{L}'}$. In any case we have to verify

$$A^\dagger \cdot Q \cdot B = o_* \left(\mathbb{T}_N\right).$$

By Lemma 2.8.1, it is enough to verify that one of the operators $A^\dagger \cdot |Q| \cdot A$ and $B^\dagger \cdot |Q| \cdot B$ is of order $o_* \left(\mathbb{T}_N\right)$, and the other one is of order $O_* \left(\mathbb{T}_N\right)$, which follows from Lemma 2.5.13 and the auxiliary Corollary 2.9.4.

The case $e_{(k,\ell)} = 0$: In this case we have $i, j \in \{3,4\}$ for any of the bullet points. Let us define the function $G : \mathbb{R}^d \longrightarrow \mathcal{H} \otimes \mathcal{H}$ by $G(t) := 1_{\mathcal{H}} \otimes (T+1)^{-\frac{1}{2}} \cdot \hat{v} \cdot e_k(\boldsymbol{t}) \otimes e_\ell(\boldsymbol{t})$. Note that $G(t) \in \mathcal{H} \otimes \mathcal{H}$ follows from Assumption 2.1.1. We define the operator $X := (T+1)^{\frac{1}{2}} \cdot h_i$ and depending on the concrete bullet point let us define $Y := h_j^\dagger \otimes 1_{\mathcal{H}} \cdot G(q)\, Z$ with $Z := 1_{\mathcal{F}_0}$, $Z := \mathbb{L}'$ or $Z := \sqrt{1-\mathbb{L}'}$. In the following, we have to verify $X^\dagger \cdot Y = o_* \left(\mathbb{T}_N\right)$. Since $i \in \{3,4\}$, we know that $X^\dagger \cdot X = O_* \left(\mathbb{T}_N\right)$. By the Cauchy–Schwarz like result in Lemma 2.8.1, it is therefore enough to verify $Y^\dagger \cdot Y = o_* \left(\mathbb{T}_N\right)$. Applying Lemma 2.5.14 yields in any case

$$\begin{aligned} Y^\dagger \cdot Y &= Z^\dagger \left(h_j^\dagger \otimes 1_{\mathcal{H}} \cdot G(q)\right)^\dagger \cdot \left(h_j^\dagger \otimes 1_{\mathcal{H}} \cdot G(q)\right) Z \\ &\leqslant 2\, Z^\dagger \left[h_j^\dagger \cdot \|G(q)\|^2 \cdot h_j + \frac{1}{N}\|G(q)\|^2 + \frac{d}{N^2} \sum_{r=1}^d \|\partial_r G(q)\|^2 \right] Z, \end{aligned}$$

and Corollary 2.9.4 then yields that $Z^\dagger \|G(q)\|^2 Z$ and $Z^\dagger \frac{1}{N}\left(\sum_{r=1}^d \|\partial_r G(q)\|^2\right) Z$ are of order $o_*(1)$. Therefore, $Z^\dagger \frac{1}{N}\|G(q)\|^2 Z$ and $Z^\dagger \frac{d}{N^2}\left(\sum_{r=1}^d \|\partial_r G(q)\|^2\right) Z$ are both of order $o_* \left(\mathbb{T}_N\right)$. Finally, $Z^\dagger h_j^\dagger \cdot \|G(q)\|^2 \cdot h_j\, Z = o_* \left(\mathbb{T}_N\right)$ follows from the auxiliary Lemmata 2.8.4 and 2.8.6, and the auxiliary Corollary 2.9.4. ■

Theorem 2.5.16. *Let $J \in \{0, \dots, 4\}^4$ be such that $\lambda_J \neq 0$ and let R_J be the residuum defined in Eq. (2.5.18). Then,*

$$R_J = o_* \left(\mathbb{T}_N\right).$$

Proof. Let $J = (i,j,k,\ell)$ be a multi index with $\lambda_J \neq 0$, and recall the index $e_J := |\{l \in J : l \in \{3,4\}\}|$ and the index $m_J := |\{l \in J : l = 0\}|$ from Lemma 2.5.12 as well as the residuum defined in Eq. (2.5.18). In order to prove the statement of the Theorem, we have to verify $R_J = o_* \left(\mathbb{T}_N\right)$ for all $J \in \{0, \dots, 4\}^4$.

The case $e_J = 0$ and $m_J = 0$: In this case we have a trivial residuum $R_J = 0$.

The case $e_J = 0$ and $m_J = 1$: In this case, $R_J = V(q)E_1^1$, with $V(t) := \left(e_i(\boldsymbol{t}) \otimes e_j(\boldsymbol{t})\right)^\dagger \cdot \hat{v} \cdot e_k(\boldsymbol{t}) \otimes e_\ell(\boldsymbol{t})$. Since the C^1 function V satisfies $F(0) = 0$, we obtain $V(q)E_1^1 = o_* \left(\mathbb{T}_N\right)$ by Lemma 2.9.2.

The case $e_J = 0$ and $m_J = 2$: In this case $R_J = V(q)E_2^1$, with $V(t) := \left(e_i(\boldsymbol{t}) \otimes e_j(\boldsymbol{t})\right)^\dagger \cdot \hat{v} \cdot e_k(\boldsymbol{t}) \otimes e_\ell(\boldsymbol{t})$. We compute

$$E_2^1 = (1 - \mathbb{L}') - \eta_2(q) - D_{\mathcal{V}}\big|_q \eta_2(b_{\geqslant 1}) = -\left(b_{>d}^\dagger \cdot b_{>d} + (p')^\dagger \cdot p' - \frac{d}{2N}\right).$$

By Lemmata 2.8.4 and 2.8.6 we know that $V(q)\, b_{>d}^\dagger \cdot b_{>d} = V(q)\, b_{>d}^\dagger \cdot b_{>d}$ and $V(q)\,(p')^\dagger \cdot p'$ are of order $o_*(\mathbb{T}_N)$, and consequently $V(q)E_2^1 = o_*(\mathbb{T}_N)$.

The case $e_J = 0$ and $m_J = 3$: In this case $R_J = V(q)E_3^1$, with $V(t) := \left(e_i(\boldsymbol{t}) \otimes e_j(\boldsymbol{t})\right)^\dagger \cdot \hat{v} \cdot e_k(\boldsymbol{t}) \otimes e_\ell(\boldsymbol{t})$. We compute

$$\begin{aligned}E_3^1 :&= (1 - \mathbb{L}')\sqrt{1 - \mathbb{L}'} - \eta_3(q) - D_{\mathcal{V}}\big|_q \eta_3(b_{\geqslant q})\\ &= (1 - \eta_2(q))E_1^1 - \left(f(q)^\dagger \cdot b_{>d} + b_{>d} \cdot f(q)\right) E_1^0 - \left(b_{>d}^\dagger \cdot b_{>d} + (p')^\dagger \cdot p' - \frac{d}{2N}\right)\sqrt{1 - \mathbb{L}'}.\end{aligned}$$

By Lemma 2.9.2, we know that $V(q)(1 - \eta_2(q))E_1^1 = o_*(\mathbb{T}_N)$ and $(E_1^0)^2 = o_*(\mathbb{T}_N)$. Note that we further have $\left[V(q)\left(f(q)^\dagger \cdot b_{>d} + b_{>d} \cdot f(q)\right)\right]^2 = o_*(\mathbb{T}_N)$, and therefore the product $V(q)\left(f(q)^\dagger \cdot b_{>d} + b_{>d} \cdot f(q)\right) E_1^0$ is of order $o_*(\mathbb{T}_N)$ as well. By making use of Lemmata 2.8.4 and 2.8.6, and Corollary 2.9.4, we obtain

$$V(q)\left(b_{>d}^\dagger \cdot b_{>d} + (p')^\dagger \cdot p' - \frac{d}{2N}\right)\sqrt{1 - \mathbb{L}'} = o_*(\mathbb{T}_N).$$

The case $e_J = 0$ and $m_J = 4$: In this case $R_J = (u_0 \otimes u_0) \cdot \hat{v} \cdot u_0 \otimes u_0\, E_4^2$. We compute

$$\begin{aligned}E_4^2 :&= (1 - \mathbb{L}')^2 - \eta_4(q) - D_{\mathcal{V}}\big|_q \eta_4(b_{\geqslant 1}) - D_{\mathcal{V}}^2\big|_0 \eta_4(b_{\geqslant 1}) - \frac{c_4}{N}\\ &= \left(f(q)^\dagger \cdot b_{>d} + b_{>d} \cdot f(q)\right)^2 + \left\{f(q)^\dagger \cdot b_{>d} + b_{>d} \cdot f(q),\ (p')^\dagger \cdot p' + b_{>d}^\dagger \cdot b_{>d}\right\}\\ &\quad + \left((p')^\dagger \cdot p' + b_{>d}^\dagger \cdot b_{>d}\right)^2 + \left\{\eta_2(q),\ (p')^\dagger \cdot p' + b_{>d}^\dagger \cdot b_{>d}\right\}\\ &\quad + 2p^\dagger \cdot (p' - p) + 2\,(p' - p)^\dagger \cdot p' - \frac{d}{N}\mathbb{L}' + \frac{d^2}{4N^2},\end{aligned}$$

with the notation $\{A, B\} := AB + BA$. Clearly $\frac{d}{N}\mathbb{L}' = o_*(\mathbb{T}_N)$. From Lemmata 2.8.4, 2.8.5 and 2.8.6, we know that all the operators $p^\dagger \cdot (p' - p)$, $(p' - p)^\dagger \cdot p'$, $\left((p')^\dagger \cdot p'\right)^2$, $\left(b_{>d}^\dagger \cdot b_{>d}\right)^2$, $\left(b_{>d}^\dagger \cdot f(q) + f(q)^\dagger \cdot b_{>d}\right)^2$, $\eta_2(q)\, b_{>d}^\dagger \cdot b_{>d}$ and $\eta_2(q)\ (p')^\dagger \cdot p'\, \eta_2(q)$ are of order $o_*(\mathbb{T}_N)$. Consequently, $\{\eta_2(q), (p')^\dagger \cdot p' + b_{>d}^\dagger \cdot b_{>d}\}$ and $\left\{f(q)^\dagger \cdot b_{>d} + b_{>d} \cdot f(q),\ (p')^\dagger \cdot p' + b_{>d}^\dagger \cdot b_{>d}\right\}$ are of order $o_*(\mathbb{T}_N)$ as well.

The case $e_J = 1$: In this case, we have $R_J = (h_i \otimes h_j)^\dagger \cdot \hat{v} \cdot h_k \otimes h_\ell\, E_{m_J}^0 + \frac{F_J(q)}{N}$. By Lemma Lemma 2.8.4, we know that $\frac{F_J(q)}{N} = o_*(\mathbb{T}_N)$. Since we know that $\left(E_{m_J}^0\right)^2 = o_*(\mathbb{T}_N)$ by Corollary 2.9.5, we are done once we can verify that $X_J \cdot X_J^\dagger = O_*(\mathbb{T}_N)$, where $X_J := (h_i \otimes h_j)^\dagger \cdot \hat{v} \cdot h_k \otimes h_\ell$.

With $3 \in \{i,j,k,\ell\}$: Let us first assume $j = 3$, and define $w(t) := e_i(\boldsymbol{t})^\dagger \otimes 1_{\mathcal{H}} \cdot \hat{v} \cdot e_k(\boldsymbol{t}) \otimes e_\ell(\boldsymbol{t})$. Clearly, $X_J = (ip')^\dagger \cdot w(q)$ and therefore $X_J X_J^\dagger = O_*(\mathbb{T}_N)$ follows from 2.8.6. The other cases $i = 3, k = 3$ and $\ell = 3$ follows from the commutation relation $[ip'_\alpha, q_\beta] = \frac{1}{2N}\delta_{\alpha,\beta}$.

With $4 \in \{i,j,k,\ell\}$: In any case, X_J is either equal to $w(q)^\dagger \cdot b_{>d}$ or $b_{>d}^\dagger \cdot w(q)$, where $w : \mathbb{R}^d \longrightarrow \mathcal{H}$ with $\|w(t)\| \leqslant c|t|^j$ and $j \geqslant 0$. Note that we use the commutativity of q_j and $b_{>d}$ here. Therefore, Lemma 2.8.5 implies $X_J \cdot X_J^\dagger = O_*(\mathbb{T}_N)$.

The case $e_J = 2$ *and* $m_J = 2$: In any case, we know by the second bullet point of Theorem 2.5.15, that $(h_i \underline{\otimes} h_j)^\dagger \cdot \hat{v} \cdot h_k \underline{\otimes} h_\ell(-\mathbb{L}') = o_*(\mathbb{T}_N)$. In case $\{i,j,k,\ell\} = \{0,4\}$, this is the whole residuum R_J. In case $\{i,j,k,\ell\} = \{0,3\}$, the residuum reads

$$R_J = (h_i \underline{\otimes} h_j)^\dagger \cdot \hat{v} \cdot h_k \underline{\otimes} h_\ell(-\mathbb{L}') + \sum_{r,r'=1}^{d} \Lambda_J^{r,r'}\left[(p'_r - p_r)\cdot p'_{r'} + p_r \cdot (p'_{r'} - p_{r'})\right].$$

Since any of the products $(p'_r - p_r)\cdot p'_{r'}$ and $p_r \cdot (p'_{r'} - p_{r'})$ are of order $o_*(\mathbb{T}_N)$, we conclude $R_J = o_*(\mathbb{T}_N)$. The case $\{i,j,k,\ell\} = \{0,3,4\}$ works similarly, and is left to the reader.

The cases $e_J = 2$ *and* $m_J < 2$*, respectively* $e_J > 2$: We obtain for $m_J = 0$ by the first bullet point of Theorem 2.5.15, and for $m_J = 1$ by the third bullet point, that

$$R_J = H_J = o_*(\mathbb{T}_N).$$

∎

Corollary 2.5.17. *Recall the functional* $\mathcal{E}_B$ *defined in Eq. (2.5.17) and the constant* c *from Corollary 2.5.8. Then,*

$$\mathcal{W}_N \widetilde{B}_N \mathcal{W}_N^{-1} = \mathcal{E}_B(q) + D_{\mathcal{V}}\big|_q \mathcal{E}_B(b_{\geqslant 1}) + \frac{1}{2} D_{\mathcal{V}}^2\big|_0 \mathcal{E}_B(b_{\geqslant 1}) - \frac{c}{N} + o_*(\mathbb{T}_N).$$

Proof. Let us define $\widetilde{c} := \sum_{J \in \{0,\ldots,4\}^4} \lambda_J c_J$. Combining Lemma 2.5.11 and Theorem 2.5.16 immediately yields

$$\mathcal{W}_N \widetilde{B}_N \mathcal{W}_N^{-1} = \mathcal{E}_B(q) + D_{\mathcal{V}}\big|_q \mathcal{E}_B(b_{\geqslant 1}) + \frac{1}{2} D_{\mathcal{V}}^2\big|_0 \mathcal{E}_B(b_{\geqslant 1}) + \frac{\widetilde{c}}{N} + o_*(\mathbb{T}_N).$$

Recall the definition of c_J in Eq. (2.5.12) for $J \in \{0,\ldots,4\}^2$, respectively Eq. (2.5.19) for

$J \in \{0,\dots,4\}^4$. Making use of the observation that most of the c_J are zero, we obtain

$$\begin{aligned}
c + \widetilde{c} = & \sum_{J\in\{0,\dots,4\}^2} \lambda_J c_J + \sum_{J\in\{0,\dots,4\}^4} \lambda_J c_J = \lambda_{(0,0)} c_{(0,0)} + \lambda_{(1,1)}\Big[c_{(1,3)} + c_{(3,1)} + c_{(3,3)}\Big] \\
& + \lambda_{(0,0,0,0)} c_{(0,0,0,0)} + \lambda_{(1,1,0,0)}\Big[c_{(3,3,0,0)} + c_{(3,1,0,0)} + c_{(1,3,0,0)}\Big] \\
& + \lambda_{(1,0,1,0)}\Big[c_{(3,0,3,0)} + c_{(3,0,1,0)} + c_{(1,0,3,0)}\Big] + \lambda_{(0,1,1,0)}\Big[c_{(0,3,3,0)} + c_{(0,1,3,0)} + c_{(0,3,1,0)}\Big] \\
& = -\frac{1}{8}\partial_{t_j}^2\big|_{t=0} \sum_{j=1}^d \Big(\lambda_{(0,0)}\mathcal{E}_{(0,0)}(\boldsymbol{t}) + \lambda_{(1,1)}\mathcal{E}_{(1,1)}(\boldsymbol{t}) + \lambda_{(0,0,0,0)}\mathcal{E}_{(0,0,0,0)}(\boldsymbol{t}) \\
& + \lambda_{(1,1,0,0)}\mathcal{E}_{(1,1,0,0)}(\boldsymbol{t}) + \lambda_{(1,0,1,0)}\mathcal{E}_{(1,0,1,0)}(\boldsymbol{t}) + \lambda_{(0,1,1,0)}\mathcal{E}_{(0,1,1,0)}(\boldsymbol{t})\Big) \\
& = -\frac{1}{8}\sum_{j=1}^d \partial_{t_j}^2\big|_{t=0}\Big(\mathcal{E}_A(\boldsymbol{t}) + \mathcal{E}_B(\boldsymbol{t})\Big) = 0,
\end{aligned}$$

where we have used in the first equality of the last line that $\partial_{t_j}^2\big|_{t=0}\lambda_J \mathcal{E}_J(\boldsymbol{t}) = 0$ for

$$J \notin \{(0,0),(1,1),(1,1,0,0),(1,0,1,0),(0,1,1,0)\}$$

and in the second equality of the last line that $\mathcal{E}_A(\boldsymbol{t}) + \mathcal{E}_B(\boldsymbol{t}) = \mathcal{E}'(\boldsymbol{t}) = e_{\mathrm{H}}$ for t small enough, where $\mathcal{E}'$ is defined in Eq. (2.5.1). ■

Proof of Theorem 2.4.12. Making use of Eq. (2.3.8), we obtain

$$(\mathcal{W}_N U_N) N^{-1} H_N (\mathcal{W}_N U_N)^{-1} = \mathcal{W}_N \widetilde{A}_N \mathcal{W}_N^{-1} + \mathcal{W}_N \widetilde{B}_N \mathcal{W}_N^{-1} + o_*(\mathbb{T}_N), \tag{2.5.22}$$

where we have used that $\mathcal{W}_N\, b_{\geqslant 1}^\dagger \cdot T \cdot b_{\geqslant 1}\, \mathcal{W}_N^{-1} \leqslant 2(X_1 + X_2)$ with

$$\begin{aligned}
X_1 &:= (q + f(q))^\dagger \cdot T \cdot (q + f(q)) = o_*(1), \\
X_2 &:= (ip' + b_{>d})^\dagger \cdot T \cdot (ip' + b_{>d}) = O_*(\mathbb{T}_N),
\end{aligned}$$

see Lemmata 2.8.4 and 2.8.6. Combining Corollaries 2.5.8 and 2.5.17 yields

$$\mathcal{W}_N \widetilde{A}_N \mathcal{W}_N^{-1} + \mathcal{W}_N \widetilde{B}_N \mathcal{W}_N^{-1} = \mathcal{E}(q) + D_{\mathcal{V}}\big|_q \mathcal{E}\Big(b_{\geqslant 1}\Big) + \frac{1}{2} D_{\mathcal{V}}^2\big|_0 \mathcal{E}\Big(b_{\geqslant 1}\Big) + o_*(\mathbb{T}_N),$$

with $\mathcal{E} := \mathcal{E}_A + \mathcal{E}_B$. Furthermore, note that $\mathcal{E}(z) = \mathcal{E}'(z)$ for $\|z\| < r$ where $\mathcal{E}'$ is defined in Eq. (2.5.1), see Lemmata 2.5.3 and 2.5.11. Therefore, $\mathcal{E}(\boldsymbol{t}) = e_{\mathrm{H}}$ and $D_{\mathcal{V}}\big|_t \mathcal{E} = 0$ for t small enough. As we will show in Lemma 2.8.2, this implies $\mathcal{E}(q) = e_{\mathrm{H}} + o_*(\mathbb{T}_N)$ and $D_{\mathcal{V}}\big|_q \mathcal{E}\Big(b_{\geqslant 1}\Big) = o_*(\mathbb{T}_N)$. Furthermore, we have $\frac{1}{2} D_{\mathcal{V}}^2\big|_0\, \mathcal{E} = \mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}$ and therefore

$$\frac{1}{2} D_{\mathcal{V}}^2\big|_0\, \mathcal{E}\Big(b_{\geqslant 1}\Big) = N^{-1}\mathbb{H}.$$

In combination with Eq. (2.5.22) this concludes the proof. ■

2.6 Coercivity of the Hessian in Example (II)

In the following we are going to verify that the Hartree energy of a system of pseudo-relativistic bosons in $\mathbb{R}^3$ interacting via a Newtonian potential, given by

$$\mathcal{E}_g\left[u\right] := \left\langle \sqrt{m^2-\Delta} - m\right\rangle_u - (u\otimes u)^\dagger \cdot \frac{g}{2|x-y|}\cdot u\otimes u,$$

satisfies the coercivity assumption in Eq. (2.1.7) for g small enough, see Example (II) in the introduction. Note that we are using the notation introduced in Section 2.3. Let us denote with $u_{g,\beta}$ the unique radial minimizer of the functional $\mathcal{E}_g$ subject to the rescaled condition $\|u\| = 1+\beta$, i.e. $u_{g,\beta}$ is radial, and satisfies $\|u_{g,\beta}\| = 1+\beta$ and $\mathcal{E}_g[u_{g,\beta}] = \inf_{\|u\|=1+\beta} \mathcal{E}_g[u]$. Let us further denote the normed minimizers by $u_g := u_{g,0}$. By a scaling argument it is easy to see that $u_{g,\beta} = (1+\beta)u_{g(1+\beta)^2}$. For real-valued functions f and h in $\{u_{g,\beta}\}^\perp$ we can express the Hessian as $\frac{1}{2}\mathrm{Hess}|_{u_{g,\beta}}\mathcal{E}_g[f+ih] = \langle L^+_{g,\beta}\rangle_f + \langle L^-_{g,\beta}\rangle_h$, where $L^+_{g,\beta}$ and $L^-_{g,\beta}$ are selfadjoint operators given by

$$L^-_{g,\beta} := \sqrt{m^2-\Delta} - m - \mu_{g,\beta} - (1\otimes u_{g,\beta})^\dagger \cdot \frac{g}{|x-y|}\cdot 1\otimes u_{g,\beta},$$
$$L^+_{g,\beta} := L^-_{g,\beta} - (1\otimes u_{g,\beta})^\dagger \cdot \frac{2g}{|x-y|}\cdot u_{g,\beta}\otimes 1,$$

with $\mu_{g,\beta} := \left\langle \sqrt{m^2-\Delta} - m\right\rangle_{u_{g,\beta}} - (u_{g,\beta}\otimes u_{g,\beta})^\dagger \cdot \frac{g}{|x-y|}\cdot u_{g,\beta}\otimes u_{g,\beta}$. Furthermore we denote the operators associated to the normed minimizers u_g by $L^\pm_g := L^\pm_{g,0}$. Note that

$$\langle L^-_g - L^+_g\rangle_f = (f\otimes u_g)^\dagger \cdot \frac{2g}{|x-y|}\cdot u_g\otimes f > 0$$

for all $f\neq 0$, and consequently it is enough to verify the following Theorem 2.6.1 in order to prove Eq. (2.1.7).

Theorem 2.6.1. *There exist constants g_0 and $\eta > 0$ such that for all $0 < g < g_0$ and $f \in L^2\left(\mathbb{R}^d\right)$ with $f \perp \{u_g, \partial_{x_1}u_g, \partial_{x_2}u_g, \partial_{x_3}u_g\}$*

$$\langle L^+_g\rangle_f \geqslant \eta\|f\|^2.$$

In order to prove Theorem 2.6.1, we first need some auxiliary results regarding the minimizers $u_{g,\beta}$ subject to the rescaled condition $\|u_{g,\beta}\| = 1+\beta$.

Lemma 2.6.2. *Let us define $R_{g,\beta} := u_{g,\beta} - u_g$ for $\beta \in [0,1)$ (where 1 can be replaced by any other positive number). Then there exist constants $g_0, C > 0$ such that*

$$L^+_g R_{g,\beta} = \delta_{g,\beta}u_g + \epsilon_{g,\beta},$$

with $|\delta_{g,\beta}| \leqslant C\beta$ and $\|\epsilon_{g,\beta}\| \leqslant C\|R_{g,\beta}\|^2$ for $g \in (0,g_0)$ and $\beta \in [0,1)$.

Proof. Since the elements $u_{g,\beta}$ are minimizers of $\mathcal{E}_g$, they satisfy the corresponding Euler-Lagrange equations $L^-_{g,\beta}u_{g,\beta} = 0$. A straightforward computation yields

$$0 = L^-_{g,\beta}u_{g,\beta} - L^-_g u_g = L^+_g R_{g,\beta} - \delta_{g,\beta}u_g - \epsilon_{g,\beta}$$

with

$$\begin{aligned}
\delta_{g,\beta} &:= \mu_{g,\beta} - \mu_g, \\
\epsilon_{g,\beta} &:= \left(\mu_{g,\beta} - \mu_g\right) R_{g,\beta} + \left(1 \otimes u_{g,\beta}\right)^\dagger \cdot \frac{g}{|x-y|} \cdot R_{g,\beta} \otimes R_{g,\beta} \\
&\quad + \left(1 \otimes R_{g,\beta}\right)^\dagger \cdot \frac{g}{|x-y|} \cdot R_{g,\beta} \otimes u_g + \left(1 \otimes R_{g,\beta}\right)^\dagger \cdot \frac{g}{|x-y|} \cdot u_g \otimes R_{g,\beta}. \qquad (2.6.1)
\end{aligned}$$

Let us first investigate the contributions involving $\frac{g}{|x-y|}$. From [69, Proposition 1] it is clear that there exists a constant C such that $\|u_{g,\beta}\|_{H^1(\mathbb{R}^3)} \leqslant C < \infty$ for all g small enough and $\beta \in [0,1)$. With the notation $S := \sqrt{1-\Delta}$ we obtain

$$\begin{aligned}
&\left\| \left(1 \otimes u_{g,\beta}\right)^\dagger \cdot \frac{g}{|x-y|} \cdot R_{g,\beta} \otimes R_{g,\beta} \right\| = \left\| \left(1 \otimes S u_{g,\beta}\right)^\dagger \cdot 1 \otimes S^{-1} \frac{g}{|x-y|} \cdot R_{g,\beta} \otimes R_{g,\beta} \right\| \\
&\leqslant g \|S u_{g,\beta}\| \left\| 1 \otimes S^{-1} \frac{1}{|x-y|} \right\| \|R_{g,\beta}\|^2 \leqslant Cg \left\| S^{-1} \frac{1}{|x|} \right\| \|R_{g,\beta}\|^2,
\end{aligned}$$

where $\left\| S^{-1} \frac{1}{|x|} \right\|$ is the operator norm of the bounded one-particle operator $S^{-1}\frac{1}{|x|}$. Similarly, the other contributions involving $\frac{g}{|x-y|}$ in Eq. (2.6.1) can be estimated by $Cg \left\| S^{-1}\frac{1}{|x|}\right\| \|R_{g,\beta}\|^2$ as well. The uniform control of the norm $\|u_{g,\beta}\|_{H^1(\mathbb{R}^3)} \leqslant C < \infty$ furthermore implies $|\delta_{g,\beta}| = |\mu_{g,\beta} - \mu_g| \leqslant \widetilde{C}\beta$ for some constant $\widetilde{C}$. Note that $\|R_{g,\beta}\| \geqslant \|u_{g,\beta}\| - \|u_g\| = \beta$, and consequently $\|\left(\mu_{g,\beta} - \mu_g\right) R_{g,\beta}\| \leqslant \widetilde{C}\beta \|R_{g,\beta}\| \leqslant \widetilde{C}\|R_{g,\beta}\|^2$. We conclude that

$$\|\epsilon_{g,\beta}\| \leqslant \left(\widetilde{C} + 3Cg \left\| S^{-1} \frac{1}{|x|} \right\| \right) \|R_{g,\beta}\|^2.$$

■

Lemma 2.6.3. *Let $R_{g,\beta}$ and $\epsilon_{g,\beta}$ be as in Lemma 2.6.2. Then there exists a constant $g_0 > 0$ such that $\lim_{\beta \to 0} \frac{\|\epsilon_{g,\beta}\|}{\langle u_g, R_{g,\beta}\rangle} = 0$ and $\limsup_{\beta \to 0} \frac{|\delta_{g,\beta}|}{\langle u_g, R_{g,\beta}\rangle} \leqslant C$ for a suitable constant $C > 0$ and $g \in (0, g_0)$.*

Proof. By the results in [69] we know that 0 is an isolated eigenvalue of L_g^+, i.e. there exists a constant $\delta > 0$ such that $\sigma\left(L_g^+\right) \cap (-\delta, \delta) = \{0\}$, with corresponding eigenvectors $\partial_{x_1} u_g, \partial_{x_2} u_g, \partial_{x_3} u_g$. Since $u_{g,\beta}$ is radial, we know that $R_{g,\beta} \perp \partial_{x_j} u_g$, and therefore we obtain by Lemma 2.6.2

$$\delta \|R_{g,\beta}\| \leqslant \|L_g^+ R_{g,\beta}\| \leqslant C\left(\beta + \|R_{g,\beta}\|^2\right). \qquad (2.6.2)$$

Using [69, Proposition 1] again, it is clear that $\lim_{g \to 0, \beta \to 0} \|R_{g,\beta}\| = 0$ and therefore there exists a constant g_0 such that $\|R_{g,\beta}\| \leqslant \frac{\delta}{2C}$ for all $g \in (0, g_0)$ and β small enough. Consequently Eq. (2.6.2) yields $\|R_{g,\beta}\| \leqslant \frac{2C}{\delta}\beta$. Using the fact that $\|u_{g,\beta}\| = 1 + \beta$, we further obtain

$$1 + 2\beta \leqslant (1+\beta)^2 = 1 + 2\langle u_g, R_{g,\beta}\rangle + \|R_{g,\beta}\|^2 \leqslant 1 + 2\langle u_g, R_{g,\beta}\rangle + \left(\frac{2C}{\delta}\right)^2 \beta^2,$$

and therefore

$$\frac{\|\epsilon_{g,\beta}\|}{\langle u_g, R_{g,\beta}\rangle} \leqslant \frac{C\left(\frac{2C}{\delta}\right)^2 \beta^2}{\beta - 2\left(\frac{C}{\delta}\right)^2 \beta^2} \underset{\beta\to 0}{\longrightarrow} 0,$$
$$\frac{|\delta_{g,\beta}|}{\langle u_g, R_{g,\beta}\rangle} \leqslant \frac{C\beta}{\beta - 2\left(\frac{C}{\delta}\right)^2 \beta^2} \underset{\beta\to 0}{\longrightarrow} C.$$

■

Proof of Theorem 2.6.1. Let Q denote the projection onto the space $\{u_g\}^\perp$. Clearly there exists a $w \in L^2(\mathbb{R}^3)$ such that

$$L_g^+ f = QL_g^+ f + \langle w, f\rangle u_g$$

for all $f \in L^2(\mathbb{R}^3)$. With $R_{g,\beta}, \delta_{g,\beta}$ and $\epsilon_{g,\beta}$ from Lemma 2.6.2 at hand, we obtain

$$L_g^+\left(\delta_{g,\beta} f - \langle w, f\rangle R_{g,\beta}\right) = \delta_{g,\beta} QL_g^+ f - \langle w, f\rangle \epsilon_{g,\beta},$$

and therefore $\|L_g^+\left(\delta_{g,\beta} f - \langle w, f\rangle R_{g,\beta}\right)\| \leqslant |\delta_{g,\beta}|\,\|QL_g^+ f\| + \|w\|\,\|\epsilon_{g,\beta}\|\,\|f\|$. Using again that there exists a constant $\delta > 0$ such that $\sigma\left(L_g^+\right) \cap (-\delta,\delta) = \{0\}$ with corresponding eigenvectors $\partial_{x_1} u_g, \partial_{x_2} u_g, \partial_{x_3} u_g$, see [69], and that $R_{g,\beta}$ as a radial function is orthogonal to them, we obtain for all $f \in \{u_g, \partial_{x_1} u_g, \partial_{x_2} u_g, \partial_{x_3} u_g\}^\perp$

$$\|L_g^+\left(\delta_{g,\beta} f - \langle w, f\rangle R_{g,\beta}\right)\| \geqslant \delta \|\delta_{g,\beta} f - \langle w, f\rangle R_{g,\beta}\| \geqslant \delta |\langle u_g, R_{g,\beta}\rangle|\,|\langle w, f\rangle|.$$

Combining the estimates we have so far yields

$$|\langle w, f\rangle| \leqslant \frac{|\delta_{g,\beta}|}{\delta|\langle u_g, R_{g,\beta}\rangle|}\|QL_g^+ f\| + \frac{\|w\|\,\|\epsilon_{g,\beta}\|}{\delta|\langle u_g, R_{g,\beta}\rangle|}\|f\| =: x_\beta \|QL_g^+ f\| + y_\beta \|f\|.$$

By Lemma 2.6.3 we know that $\limsup_{\beta\to 0}|x_\beta| \leqslant C$ for some constant $C > 0$ and $y_\beta \underset{\beta\to 0}{\longrightarrow} 0$. Using again that $\sigma\left(L_g^+\right) \cap (-\delta,\delta) = \{0\}$, we obtain

$$\delta\|f\| \leqslant \|L_g^+ f\| \leqslant \|QL_g^+ f\| + |\langle w, f\rangle| \leqslant (1 + x_\beta)\|QL_g^+ f\| + y_\beta \|f\|$$

and consequently $\|QL_g^+ f\| \geqslant \frac{\delta - y_\beta}{1 + x_\beta}\|f\|$. This holds for all (small) β, hence $\beta \to 0$ gives $\|QL_g^+ f\| \geqslant \frac{\delta}{1+C}\|f\|$. Finally note that $QL_g^+ Q \geqslant 0$ since $\langle L_g^+\rangle_f = \frac{1}{2}\mathrm{Hess}|_{u_g}\mathcal{E}_g[f] \geqslant 0$ for real-valued $f \perp u_g$, which concludes the proof. ■

2.7 The Bogoliubov Operator

In the following we will prove Theorem 2.4.4, i.e. we are going to verify that the Bogoliubov operator $\mathbb{H}$ constructed in Definition 2.4.3 is bounded from below and that its ground state energy can be approximated by $\Psi \in \bigcup_{M\in\mathbb{N}} \mathrm{dom}[a_{\geqslant 1}^\dagger \cdot (T+1) \cdot a_{\geqslant 1}] \cap \mathcal{F}_{\leqslant M}$ with $\|\Psi\| = 1$. Our strategy is to decouple the degenerate modes from the non-degenerate ones and to apply the general framework for non-degenerate Bogoliubov operators in [98].

Definition 2.7.1. Let $Q_{\rm H} = \sum_{i,j\geqslant 1} Q_{i,j}\ u_i \cdot u_j^\dagger$ and $G_{\rm H} = \sum_{i,j\geqslant 1} G_{ij}\ u_i \otimes u_j$ be as in Lemma 2.4.1, and let us denote the operator $Q_\perp := \sum_{i,j>d} Q_{i,j}\ u_i \cdot u_j^\dagger$ on $\mathcal{H}_\perp := \langle u_0, u_1, \ldots, u_d\rangle^\perp$ as well as $G_\perp := \sum_{i,j>d} G_{ij} u_i \otimes u_j$. Then we define the operator $\mathbb{H}_\perp$ as

$$\mathbb{H}_\perp := a_{>d}^\dagger \cdot Q_\perp \cdot a_{>d} + 2\mathfrak{Re}\left[G_\perp^\dagger \cdot a_{>d} \underline{\otimes}\, a_{>d}\right].$$

Lemma 2.7.2. *The operator $\mathbb{H}_\perp$ is semi-bounded from below, i.e. $\inf \sigma(\mathbb{H}_\perp) > -\infty$. Furthermore, there exists a constant $R > 0$ such that*

$$\mathbb{H}_\perp \leqslant R\left(a_{>d}^\dagger \cdot Q_\perp \cdot a_{>d} + 1\right). \tag{2.7.1}$$

Proof. Let us define the operator $G_{\rm op}$ on $\mathcal{H}_\perp$ by the condition $z^\dagger \cdot G_{\rm op} \cdot z = 2G_\perp^\dagger \cdot \overline{z} \otimes z$, with $\overline{z}$ being the usual complex conjugation in $L^2\left(\mathbb{R}^d\right)$. Then, $z^\dagger \cdot Q_\perp \cdot z + 2\mathfrak{Re}\left[\overline{z}^\dagger \cdot G_{\rm op} \cdot z\right] = \mathrm{Hess}|_{u_0}\mathcal{E}_{\rm H}[z] \geqslant \eta\|z\|^2$ for all $z \in \mathcal{H}_\perp$ with $\eta > 0$ by Assumption 2.1.3. As pointed out in Section 2.1 in [72], this implies $Q_\perp \geqslant r > 0$ as well as

$$\begin{pmatrix} Q_\perp & G_{\rm op}^\dagger \\ G_{\rm op} & Q_\perp \end{pmatrix} \geqslant 0,$$

where we have used that $Q_\perp$ is a real operator. Since $Q_\perp > 0$, this is further equivalent to $G_{\rm op}\, Q_\perp^{-1}\, G_{\rm op}^\dagger \leqslant Q_\perp$. Since $G_{\rm H} \in \overline{\mathcal{H}_0 \otimes \mathcal{H}_0}^{\|\cdot\|_*}$, where the $\|.\|_*$ norm is defined in Lemma 2.4.1, and since $z^\dagger \cdot Q_\perp^{-\frac{1}{2}} \cdot z \leqslant c\, z^\dagger \cdot (T+1)^{-\frac{1}{2}} \cdot z$ for a suitable constant c and $z \in \mathcal{H}_\perp$, which is an easy consequence of the operator inequality in Lemma 2.4.1 and the fact that $Q_\perp \geqslant r > 0$, we obtain

$$\mathrm{Tr}\left[G_{\rm op}\, Q_\perp^{-1}\, G_{\rm op}^\dagger\right] = \|1_{\mathcal{H}_\perp} \otimes Q_\perp^{-\frac{1}{2}} \cdot G_\perp\|^2_{\mathcal{H}\otimes\mathcal{H}} \leqslant c^2\, \|G_{\rm H}\|_*^2 < \infty, \tag{2.7.2}$$

i.e. $G_{\rm op}\, Q_\perp^{-\frac{1}{2}}$ is a Hilbert-Schmidt operator. By the general results in [98], this implies that $\mathbb{H}_\perp$ is semi-bounded as well as the existence of a constant $R > 0$ such that Eq. (2.7.1) holds. ■

Lemma 2.7.3. *Let us define $P_j := \frac{1}{2i}\left(a_j - a_j^\dagger\right) = \sqrt{N} p_j$ for $j \in \{1, \ldots, d\}$, the constant $c_0 := \sum_{j=1}^d G_{j,j}$, the quadratic function $\nu(y) := -4\sum_{j,k=1}^d G_{j,k} y_j y_k$ for $y \in \mathbb{R}^d$ and the linear $\mathcal{H}_\perp$ valued function*

$$u(y_1, \ldots, y_d) := 4i \sum_{j=1}^d y_j \sum_{k>d} G_{j,k} u_k \in \mathcal{H}_\perp.$$

Then we can rewrite the Bogoliubov operator $\mathbb{H}$ from Definition (2.4.3) as

$$\mathbb{H} = c_0 + \nu\left(P_1, \ldots, P_d\right) + u\left(P_1, \ldots, P_d\right)^\dagger \cdot a_{>d} + a_{>d}^\dagger \cdot u\left(P_1, \ldots, P_d\right) + \mathbb{H}_\perp. \tag{2.7.3}$$

Proof. Since $\mathrm{Hess}|_{u_0}\mathcal{E}_{\rm H}[z] = z^\dagger \cdot Q_{\rm H} \cdot z + 2\mathfrak{Re}\left[G_{\rm H}^\dagger \cdot z \otimes z\right]$ is degenerate in the directions $u_1, \ldots, u_d$, we obtain $Q_{j,k} = -2G_{j,k}$ in case j or k is in $\{1, \ldots, d\}$. Writing $\mathbb{H}$ in coordinates therefore yields

$$\begin{aligned}
\mathbb{H} =& \sum_{j,k=1}^d G_{j,k}\left(-2a_j^\dagger a_k + a_j a_k + a_j^\dagger a_k^\dagger\right) + 2\sum_{j=1}^d \sum_{k>d} G_{j,k}\left(a_j - a_j^\dagger\right) a_k - 2\sum_{j=1}^d \sum_{k>d} G_{j,k}\left(a_j - a_j^\dagger\right) a_k^\dagger \\
&+ \sum_{j,k>d}\left(Q_{j,k} a_j^\dagger a_k + G_{j,k} a_j a_k + G_{j,k} a_j^\dagger a_k^\dagger\right) \\
=& \left\{c_0 + \nu\left(P_1, \ldots, P_d\right)\right\} + u\left(P_1, \ldots, P_d\right)^\dagger \cdot a_{>d} + a_{>d}^\dagger \cdot u\left(P_1, \ldots, P_d\right) + \mathbb{H}_\perp,
\end{aligned}$$

where we have used $-2a_j^\dagger a_k + a_j a_k + a_j^\dagger a_k^\dagger = -4P_jP_k + \delta_{j,k}$ in the second identity. ■

Remark 2.7.4. In the subsequent Lemma 2.7.5, we want to get rid of the term $u\left(P_1,\ldots,P_d\right)^\dagger \cdot a_{>d} + a_{>d}^\dagger \cdot u\left(P_1,\ldots,P_d\right)$ in Eq. (2.7.3) by completing the square, i.e. by applying a shift $a_{>d} \mapsto a_{>d} + w\left(P_1,\ldots,P_d\right)$ where $w(y_1,\ldots,y_d) \in \mathcal{H}_\perp$ is a suitable vector. In the following we are going to construct such a $w(y)$. Let us first define the $\mathbb{R}$-linear map $L : \mathcal{H}_\perp \longrightarrow \mathcal{H}_\perp$

$$z^\dagger \cdot L(w) := z^\dagger \cdot Q_\perp \cdot w + 2\left(w \otimes z\right)^\dagger \cdot G_\perp,$$

for all $z \in \mathcal{H}_\perp$. Furthermore, let us define the real inner product $\langle z, w\rangle_{\mathbb{R}} := \mathfrak{Re}\left[z^\dagger \cdot w\right]$ on $\mathcal{H}_\perp$. Clearly, L is symmetric with respect to this inner product. By Assumption 2.1.3 we have for all $w \in \mathcal{H}_\perp$

$$\langle w, L(w)\rangle_{\mathbb{R}} = \mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}[w] \geqslant \eta\, \|w\|^2, \tag{2.7.4}$$

and consequently we can define $w(y) \in \mathcal{H}_\perp$ for all $y \in \mathbb{R}^d$ as the solution of the equation

$$L \cdot w(y) = -u(y). \tag{2.7.5}$$

We note that $w(y) \in \mathrm{dom}[Q_\perp]$ due to the improved coercivity

$$\langle w, L(w)\rangle_{\mathbb{R}} \geqslant \widetilde{c}\, w^\dagger \cdot Q_\perp \cdot w \tag{2.7.6}$$

where $\widetilde{c}$ is a suitable constant, which follows from the fact that

$$2\left|(w\otimes w)^\dagger \cdot G_\perp\right| \leqslant w^\dagger \cdot \left(\epsilon\, Q_\perp + \epsilon^{-1}c^2\|G_{\mathrm{H}}\|_*^2\right)\cdot w \leqslant \epsilon\, w^\dagger \cdot Q_\perp \cdot w + \frac{c^2\|G_{\mathrm{H}}\|_*^2}{\epsilon\eta}\langle w, L(w)\rangle_{\mathbb{R}}$$

for all $\epsilon > 0$, where c is the constant in Eq. (2.7.2).

Lemma 2.7.5. *Let $w : \mathbb{R}^d \to \mathcal{H}_\perp$ be the function defined by Eq. (2.7.5) and let us define the unitary transformation $\mathcal{R} : \mathcal{F}_0 \longrightarrow \mathcal{F}_0$*

$$\mathcal{R} :=\exp\left[w\left(P_1,\ldots,P_d\right)^\dagger \cdot a_{>d} - a_{>d}^\dagger \cdot w\left(P_1,\ldots,P_d\right)\right].$$

Then there exists a non-negative quadratic function $\eta : \mathbb{R}^d \longrightarrow \mathbb{R}$, s.t.

$$\mathcal{R}\,\mathbb{H}\,\mathcal{R}^{-1} = c_0 + \eta\left(P_1,\ldots,P_d\right) + \mathbb{H}_\perp, \tag{2.7.7}$$

where c_0 and $\mathbb{H}_\perp$ are as in Lemma 2.7.3 and Definition 2.7.1.

Proof. Let us define $\eta(y_1,\ldots,y_d) := \nu(y_1,\ldots,y_d) + \langle w(y_1,\ldots,y_d), u(y_1,\ldots,y_d)\rangle_{\mathbb{R}}$. With η and the vector valued function w at hand, we can rewrite Eq. (2.7.3) as

$$\begin{aligned}\mathbb{H} = c_0 + \eta\left(P_1,\ldots,P_d\right) &+ \Big(a_{>d} - w\left(P_1,\ldots,P_d\right)\Big)^\dagger \cdot Q_\perp \cdot \Big(a_{>d} - w\left(P_1,\ldots,P_d\right)\Big)\\ &+ 2\mathfrak{Re}\left[G_\perp^\dagger \cdot \Big(a_{>d} - w\left(P_1,\ldots,P_d\right)\Big) \otimes \Big(a_{>d} - w\left(P_1,\ldots,P_d\right)\Big)\right].\end{aligned} \tag{2.7.8}$$

Eq. (2.7.7) follows now from the representation of $\mathbb{H}$ in Eq. (2.7.8) and the fact that

$$\mathcal{R}\, a_{>d}\, \mathcal{R}^{-1} = a_{>d} + w\left(P_1,\ldots,P_d\right).$$

In order to see that η is indeed non-negative, note that we can use η and w to complete the square in $\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}[z]$ as well, i.e. for $z = \sum_{j=1}^d \left(t_j + is_j\right) u_j + z_{>d}$ with $t, s \in \mathbb{R}^d$ and $z_{>d} \in \mathcal{H}_\perp$ we can write $\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}[z]$ as

$$\eta(s) + (z_{>d} - w(s))^\dagger \cdot Q_\perp \cdot (z_{>d} - w(s)) + 2\mathfrak{Re}\left[G_\perp^\dagger \cdot (z_{>d} - w(s)) \otimes (z_{>d} - w(s))\right].$$

Therefore, $\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}[z] \geqslant 0$ for all z implies $\eta(s) \geqslant 0$ for all $s \in \mathbb{R}^d$. ■

Proof of Theorem 2.4.4. Since the function η in Lemma 2.7.5 is non-negative, we immediately obtain the lower bound

$$\inf \sigma(\mathbb{H}) \geqslant c_0 + \inf \sigma(\mathbb{H}_\perp) > -\infty.$$

In order to verify the bound from below for the operator $\mathbb{H} - r\mathbb{A}$, where $\mathbb{A}$ is defined in Eq. (2.4.3), we will make use of the improved coercivity

$$\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}[z] \geqslant r_* \left(\sum_{j=1}^{d} s_j^2 + z_{>d}^\dagger \cdot (T+1) \cdot z_{>d} \right), \tag{2.7.9}$$

where r_* is a suitable constant and $z = \sum_{j=1}^{d}(t_j + is_j)u_j + z_{>d}$ with $z_{>d} \in \mathcal{H}_\perp$, which can be verified analogously to Eq. (2.7.6) in Remark 2.7.4. With the definition $\eta_r := r_* - r$ for $r < r_*$ we obtain, in analogy to Assumption 2.1.3,

$$\mathrm{Hess}|_{u_0}\mathcal{E}_{\mathrm{H}}[z] - r \left(\sum_{j=1}^{d} s_j^2 + z_{>d}^\dagger \cdot (T+1) \cdot z_{>d} \right) \geqslant \eta_r \|z\|^2$$

for all z of the form $z = i\sum_{j=1}^{d} s_j u_j + z_{>d}$ with $s_j \in \mathbb{R}$ and $z_{>d} \in \mathcal{H}_\perp$. Therefore we can repeat the proof of the lower bound for the operator $\mathbb{H} - r\mathbb{A}$, which yields

$$\mathbb{H} - r\mathbb{A} \geqslant \inf \sigma(\mathbb{H} - r\mathbb{A}) > -\infty. \tag{2.7.10}$$

Note that this further implies that the Friedrichs extension of the quadratic form $\mathbb{H}$ is well-defined, i.e. $\mathbb{H}$ is semi-bounded and closeable, since $\mathbb{H}$ is comparable to the non-negative selfadjoint operator $\mathbb{A}$, i.e. there exist constants $\alpha_1, \alpha_2, \beta_1, \beta_2 > 0$ with

$$\alpha_1 \mathbb{A} - \beta_1 \leqslant \mathbb{H} \leqslant \alpha_2 \mathbb{A} + \beta_2.$$

In order to verify that there exists an approximate sequence of ground states Ψ_M with $\Psi_M \in \mathcal{F}_{\leqslant M}$ and $\Psi_M \in \mathrm{dom}\left[a_{\geqslant 1}^\dagger \cdot (T+1) \cdot a_{\geqslant 1}\right]$, it is enough to prove that such states are dense in $\mathrm{dom}\left[a_{\geqslant 1}^\dagger \cdot (T+1) \cdot a_{\geqslant 1}\right]$, the domain of the quadratic form which defines the Bogoliubov operator $\mathbb{H}$ by Friedrichs extension, with respect to the norm $\|\Psi\|_{\mathbb{H}}^2 := \langle \mathbb{H} + C \rangle_\Psi$ where $C > -\inf \sigma(\mathbb{H})$. The lower bound follows from Eq. (2.7.10), while the upper bound follows from Eq. (2.7.3) and Inequality (2.7.1). Furthermore, we have

$$\|\Psi\|_{\mathbb{H}}^2 \leqslant \alpha_2 \langle \mathbb{A} \rangle_\Psi + (\beta_2 + C)\|\Psi\|^2 \leqslant \|\Psi\|_\diamond^2,$$

for all $\Psi \in \mathcal{F}_0$, where $\|\Psi\|_\diamond^2 := \alpha_2 \langle a_{\geqslant 1}^\dagger \cdot (T+1) \cdot a_{\geqslant 1} \rangle_\Psi + (\beta_2 + C + \frac{d}{4})\|\Psi\|^2$. Clearly, $\bigcup_M \mathcal{F}_{\leqslant M} \cap \mathrm{dom}\left[a_{\geqslant 1}^\dagger \cdot (T+1) \cdot a_{\geqslant 1}\right]$ is dense in the domain $\mathrm{dom}\left[a_{\geqslant 1}^\dagger \cdot (T+1) \cdot a_{\geqslant 1}\right]$ with respect to the norm $\|.\|_\diamond$ and therefore it is also dense with respect to $\|.\|_{\mathbb{H}}$. ■

2.8 Auxiliary Lemmata

In the following section we will derive various operator estimates involving powers of the operators $p, p', b_{>d}$ and functions of q, with an emphasis on asymptotic results of the form $A_N = o_*(B_N)$, where the $o_*(\cdot)$ notation is introduced in Definition 2.4.10. It is a crucial observation that all of our basic variables q_i, p_j and b_k are of order $o_*(1)$, and therefore the product of a basic variable with an operator A_N should be of order $o_*(A_N)$, which we will verify for specific examples A_N. Let us first discuss an important tool, which we will repeatedly use, given by the following Cauchy–Schwarz inequality for operators.

Lemma 2.8.1. *For any $\lambda \in \mathbb{C}$ with $|\lambda| = 1$, $t > 0$, linear operators $A : \mathcal{H}_1 \longrightarrow \mathcal{H}_2$ and $B : \mathcal{H}_1 \longrightarrow \mathcal{H}_2$, and selfadjoint operator $Q : \mathcal{H}_2 \longrightarrow \mathcal{H}_2$, we have the operator inequality*

$$\mathfrak{Re}\left[\lambda\, A^\dagger \cdot Q \cdot B\right] \leqslant t\, A^\dagger \cdot |Q| \cdot A + t^{-1}\, B^\dagger \cdot |Q| \cdot B. \tag{2.8.1}$$

Furthermore, let A_N, B_N be sequences of linear operators $\mathcal{H}_1 \longrightarrow \mathcal{H}_2$, Q a selfadjoint operator on $\mathcal{H}_2$ and $C_N : \mathcal{H}_1 \longrightarrow \mathcal{H}_1$ a sequence of non-negative operators, which satisfy $A_N^\dagger \cdot |Q| \cdot A_N = O_*\left(C_N\right)$ and $B_N^\dagger \cdot |Q| \cdot B_N = o_*\left(C_N\right)$. Then,

$$\begin{aligned} A_N^\dagger \cdot Q \cdot B_N &= o_*\left(C_N\right), \\ B_N^\dagger \cdot Q \cdot A_N &= o_*\left(C_N\right). \end{aligned}$$

Proof. Let $Q = U|Q|$ be the polar decomposition of Q. Inequality (2.8.1) immediately follows from the inequality

$$0 \leqslant \left(\sqrt{t}\, A - \sqrt{\frac{1}{t}}\lambda\, UB\right)^\dagger \cdot |Q| \cdot \left(\sqrt{t}\, A - \sqrt{\frac{1}{t}}\lambda\, UB\right).$$

By our assumption $A_N^\dagger \cdot |Q| \cdot A_N = O_*\left(C_N\right)$ we know that there exist constants $c, \delta_0 > 0$, such that $\pi_{M,N}\, A_N^\dagger \cdot |Q| \cdot A_N\, \pi_{M,N} \leqslant c\langle C_N \rangle_\Psi$ for all $\frac{M}{N} \leqslant \delta_0$. Furthermore, by our assumption $B_N^\dagger \cdot |Q| \cdot B_N = o_*\left(C_N\right)$, there exists a function $\epsilon : \mathbb{R}^+ \longrightarrow \mathbb{R}^+$ with $\lim_{\delta \to 0} \epsilon(\delta)$, such that $\pi_{M,N}\, B_N^\dagger \cdot |Q| \cdot B_N\, \pi_{M,N} \leqslant \epsilon\left(\frac{M}{N}\right) C_N$. Applying Inequality (2.8.1) with $t := \sqrt{\epsilon\left(\frac{M}{N}\right)}$ yields for all $\lambda \in \mathbb{C}$ with $|\lambda| = 1$ and $\frac{M}{N} \leqslant \delta_0$

$$\pi_{M,N}\, \mathfrak{Re}\left[\lambda\, A_N^\dagger \cdot Q \cdot B_N\right] \pi_{M,N} \leqslant \sqrt{\epsilon\left(\frac{M}{N}\right)}\, C_N.$$

∎

Consider a function $g : \mathbb{R}^d \longrightarrow \mathbb{R}$. The following Lemma states that the operator $g(q)$ depends, up to an exponentially small error, only on the local data of g in an arbitrary small neighborhood $[-\epsilon, \epsilon]^d$ of the origin, i.e. $g(q) = \widetilde{g}(q) + O_*\left(e^{-\delta N}\right)$ in case $g|_{[-\epsilon,\epsilon]^d} = \widetilde{g}|_{[-\epsilon,\epsilon]^d}$. This property plays a key role in the proof of the main technical Theorem 2.4.12, since the involved functions are (somewhat arbitrary) extensions of locally constructed functions with specific properties, which the extensions no longer have, see for example the definition of $f : \mathbb{R}^d \longrightarrow \mathcal{H}_0$ in Definition 2.4.7.

Lemma 2.8.2. *Let $q_1, \ldots, q_d$ be the operators defined in Eq. (2.4.4) and let $g : \mathbb{R}^d \to \mathbb{R}$ be a function such that $g|_{[-\epsilon,\epsilon]^d} = 0$ for some $\epsilon > 0$. Furthermore, assume that g satisfies the growth condition $|g(t)| \leqslant C|t|^{2j}$, with $C > 0$ and $j \in \mathbb{N}$. Then*

$$g\left(q\right) = O_*\left(e^{-\delta N}\right)$$

for some $\delta > 0$.

Proof. Using the elementary estimate $|t|^{2j} = \left(\sum_{r=1}^d t_r^2\right)^j \leqslant d^j \max_{1\leqslant r\leqslant d} t_r^{2j}$ yields

$$|g(t)| \leqslant d^j C \sum_{r=1}^d t_r^{2j}\ \mathbb{1}_{(\epsilon,\infty)}\left(|t_r|\right).$$

In the following we want to verify that there exist constants C, $\delta > 0$ and $\delta_0 > 0$ such that $\langle q_r^{2j}\mathbb{1}_{(\epsilon,\infty)}(|q_r|)\rangle_\Psi \leqslant Ce^{-\delta N}$ for all states $\Psi \in \mathcal{W}_N\mathcal{F}_{\leqslant M}$, $\|\Psi\| = 1$, with $\frac{M}{N} \leqslant \delta_0$ and $r \in \{1,\dots,d\}$. Since $\mathcal{W}_N\, q_r\, \mathcal{W}_N^{-1} = q_r$, it is equivalent to verify this for $\Psi \in \mathcal{F}_{\leqslant M}$ instead. Due to the reflection symmetry $q_r \mapsto -q_r$ of q_r^{2j}, it is furthermore enough to verify that $\langle \mathbb{1}_{(\epsilon,\infty)}(q_r)q_r^{2j}\rangle_\Psi \leqslant Ce^{-\delta N}$ for all states $\Psi \in \mathcal{F}_{\leqslant M}$ with $\frac{M}{N} \leqslant \delta_0$. Note that the operators $q_r := \frac{1}{\sqrt{2N}}\frac{a_r + a_r^\dagger}{\sqrt{2}}$ depend on N. In the following we will make use of the description of the Fock space $\mathcal{F}_{\leqslant M}$ in terms of Hermite polynomials h_n, i.e. for $r \in \{1,\dots,d\}$ and $\Psi \in \mathcal{F}_{\leqslant M}$ there exist states $\Psi_n \in \mathcal{F}_{\leqslant M-n}$ with $a_r\Psi_n = 0$, such that $\Psi = \sum_{n=0}^M h_n\left(\frac{a_r + a_r^\dagger}{\sqrt{2}}\right)\Psi_n$, see for example Eq. (1.26), respectively Exercise 1(ii), in [86]. Furthermore we define the density matrix $\gamma_r(x,y) := \sum_{n_1,n_2=0}^M \langle \Psi_{n_1}, \Psi_{n_2}\rangle h_{n_2}(x)h_{n_1}(y)\frac{1}{\sqrt{\pi}}e^{-\frac{x^2+y^2}{2}}$ on $L^2(\mathbb{R})$. With γ_r at hand we have

$$\langle \mathbb{1}_{(\epsilon,\infty)}(q_r)q_r^{2j}\rangle_\Psi = \int_{\sqrt{2N}\epsilon}^\infty \left(\frac{x}{\sqrt{2N}}\right)^{2j}\gamma_r(x,x)\mathrm{d}x.$$

In order to estimate this quantity, let us define the harmonic oscillator Hamiltonian $H := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2$ on $L^2(\mathbb{R})$. Since γ_r involves only eigenfunctions $h_n(x)e^{-\frac{x^2}{2}}$ of H with $n \leqslant M$, we have the operator inequality $\gamma_r \leqslant e^{2M+1-H}$. Using the Mehler kernel for e^{-H} therefore yields for $c := \frac{1}{\sqrt{2\pi\sinh(2)}}$ and $\lambda := \coth(2) - \mathrm{cosech}(2) > 0$, and all $M \leqslant \epsilon^2\lambda N/2$

$$\int_{\sqrt{2N}\epsilon}^\infty \left(\frac{x}{\sqrt{2N}}\right)^{2j}\gamma_r(x,x)\mathrm{d}x \leqslant c\, e^{\epsilon^2\lambda N+1}\int_{\sqrt{2N}\epsilon}^\infty \left(\frac{x}{\sqrt{2N}}\right)^{2j} e^{-\lambda x^2}\mathrm{d}x = O_{N\to\infty}\left(e^{-\epsilon^2\lambda N}\right).$$

■

The following Lemma is an auxiliary result, which will be useful for the verification of various asymptotic results involving the operator $b_{>d}$.

Lemma 2.8.3. *Recall the operators $\mathcal{W}_N, \mathbb{L}', p_j'$ and $f(q)$ from Definition 2.4.8 and the definition of $\hat{\pi}_{M,N}$ above Eq. (2.5.21). Then, q_j and p_j' commute with $\hat{\pi}_{M,N}$ for $j \in \{1,\dots,d\}$, $\hat{\pi}_{M,N}\mathbb{L}'\Psi = \mathbb{L}'\hat{\pi}_{M,N}\Psi$ for all $\Psi \in \mathcal{W}_N\mathcal{F}_{\leqslant N}$, and $b_k\,\hat{\pi}_{M,N} = \hat{\pi}_{M,N}\, b_k\,\hat{\pi}_{M,N}$ for all $k > d$. Furthermore, we have for all $M \leqslant N$ the estimate*

$$\hat{\pi}_{M,N}\left(b_{>d} + f(q)\right)^\dagger \cdot \left(b_{>d} + f(q)\right)\hat{\pi}_{M,N} \leqslant \frac{M}{N}, \tag{2.8.2}$$

$$\hat{\pi}_{M,N}\, b_{>d}^\dagger \cdot b_{>d}\,\hat{\pi}_{M,N} \leqslant 4. \tag{2.8.3}$$

Proof. Recall $\mathcal{N} := \sum_{j=1}^\infty a_j^\dagger a_j$ and let us define $\mathcal{N}_+ := \sum_{j>d} a_j^\dagger \cdot a_j$. Since $\mathcal{N}_+$ commutes with $\mathbb{L}$ and q_j, p_j for $j \in \{1,\dots,d\}$, we obtain that $\hat{\pi}_{M,N} = \mathcal{W}_N\,\mathbb{1}_{[0,M]}\left(\mathcal{N}_+\right)\mathcal{W}_N^{-1}$ commutes with $q_j = \mathcal{W}_N\, q_j\,\mathcal{W}_N^{-1}$ and $p_j' = \mathcal{W}_N\, p_j\,\mathcal{W}_N^{-1}$. Similarly $\hat{\pi}_{M,N}\mathbb{L}'\Psi = \mathbb{L}'\hat{\pi}_{M,N}\Psi$ for all $\Psi \in \mathcal{W}_N\mathcal{F}_{\leqslant N}$. Making use of the fact that $b_j = \mathcal{W}_N\,\left(b_j - f_j(q)\right)\,\mathcal{W}_N^{-1}$ yields

$$\begin{aligned} b_j\,\hat{\pi}_{M,N} &= \mathcal{W}_N\left(b_j - f_j(q)\right)\mathbb{1}_{[0,M]}\left(\mathcal{N}_+\right)\mathcal{W}_N^{-1} \\ &= \mathcal{W}_N\,\mathbb{1}_{[0,M]}\left(\mathcal{N}_+\right)\left(b_j - f_j(q)\right)\mathbb{1}_{[0,M]}\left(\mathcal{N}_+\right)\mathcal{W}_N^{-1} = \hat{\pi}_{M,N}\, b_j\,\hat{\pi}_{M,N}. \end{aligned}$$

Inequality (2.8.2) follows from $\left(b_{>d} + f(q)\right)^\dagger \cdot \left(b_{>d} + f(q)\right) = \frac{1}{N}\mathcal{W}_N\,\mathcal{N}_+\,\mathcal{W}_N^{-1}$ and

$$\hat{\pi}_{M,N}\ \left(b_{>d} + f(q)\right)^\dagger \cdot \left(b_{>d} + f(q)\right)\ \hat{\pi}_{M,N} = \frac{1}{N}\mathcal{W}_N\,\mathcal{N}_+\mathbb{1}_{[0,M]}\left(\mathcal{N}_+\right)\,\mathcal{W}_N^{-1} \leqslant \frac{M}{N}.$$

In order to verify Inequality (2.8.3), note that $f(t)^\dagger \cdot f(t) \leqslant 1$ for all t. Applying the Cauchy–Schwarz inequality as in 2.8.1 yields

$$\begin{aligned}\hat{\pi}_{M,N}\,b_{>d}^\dagger \cdot b_{>d}\,\hat{\pi}_{M,N} &\leqslant 2\hat{\pi}_{M,N}\left(b_{>d} + f(q)\right)^\dagger \cdot \left(b_{>d} + f(q)\right)\hat{\pi}_{M,N} + 2\hat{\pi}_{M,N}\,f(q)^\dagger \cdot f(q)\,\hat{\pi}_{M,N}\\ &\leqslant 2\frac{M}{N} + 2 \leqslant 4.\end{aligned}$$

■

The proof of the main technical Theorem 2.4.12 consists of two steps: First one has to identify the residuum R_J, which is carried out in the Lemmata 2.5.6 and 2.5.12, and in the second step one has to derive asymptotic results for these residua R_J, which is carried out in the Theorems 2.5.7 and 2.5.16. The following three Lemmata provide asymptotic results for the types of operators most frequently encountered during our analysis of R_J.

Lemma 2.8.4. *Let $\varphi, \Phi : \mathbb{R}^d \longrightarrow \mathbb{R}$ be functions with $|\varphi(t)| \leqslant C|t|^k$ and $|\Phi(t)| \leqslant C(1+|t|^k)$ for some $k \geqslant 1$. Then, $\varphi(q) = o_*(1)$ and $\Phi(q) = O_*(1)$. Furthermore,*

$$\varphi(q)\,b_{>d}^\dagger \cdot b_{>d} = o_*\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right), \tag{2.8.4}$$

$$\Phi(q)\,b_{>d}^\dagger \cdot b_{>d} = O_*\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right). \tag{2.8.5}$$

Proof. In the following, let $0 \leqslant \tau \leqslant 1$ be a smooth function with $\mathrm{supp}\,(\tau) \subset B_1(0)$ and $\tau(t) = 1$ for all $t \in B_{\frac{1}{2}}(0)$, and let $\tau_r(t) := \tau\left(\frac{t}{r}\right)$ for $r > 0$. Clearly $\varphi(q) = \tau_r(q)\varphi(q) + (1-\tau_r(q))\varphi(q)$. By our assumptions we know that $|\tau_r\varphi| \leqslant \epsilon_r$ with $\epsilon_r \underset{r\to 0}{\longrightarrow} 0$ and $(1-\tau_r)\varphi$ is zero in a neighborhood of zero, hence $(1-\tau_r(q))\varphi(q) = O_*\left(e^{-\delta N}\right)$ by Lemma 2.8.2. We conclude that $|\varphi(q)| \leqslant \epsilon_r + O_*\left(e^{-\delta N}\right)$ for all $r > 0$, and consequently $\varphi(q) = o_*(1)$. The corresponding statement for $\Phi(q)$ follows from the fact that $\Phi(q) \leqslant C + \varphi(q)$ with $\varphi(t) := |t|^k$ and $\varphi(q) = o_*(1)$.

Let us write similar to before $\varphi(q)\,b_{>d}^\dagger \cdot b_{>d} = \tau_r(q)\varphi(q)\,b_{>d}^\dagger \cdot b_{>d} + (1-\tau_r(q))\varphi(q)\,b_{>d}^\dagger \cdot b_{>d}$. In order to verify Eq. (2.8.5). First of all $\tau_r(q)\varphi(q)\,b_{>d}^\dagger \cdot b_{>d} \leqslant \epsilon_r b_{>d}^\dagger \cdot b_{>d}$, where we use that q commutes with $b_{>d}$. For the treatment of the second term, recall Inequality (2.8.3) and $\pi_{M,N}(1-\tau_r(q))^2|\varphi_r(q)|^2\pi_{M,N} \leqslant C^2 e^{-2\delta N}$ for $\frac{M}{N} \leqslant \delta$ with $C, \delta > 0$, which follows from Lemma 2.8.2. Hence,

$$\begin{aligned}\pi_{M,N}(1-\tau_r(q))|\varphi(q)|\,b_{>d}^\dagger \cdot b_{>d}\,\pi_{M,N} &= \pi_{M,N}(1-\tau_r(q))|\varphi(q)|\hat{\pi}_{M,N}\,b_{>d}^\dagger \cdot b_{>d}\,\pi_{M,N}\\ &\leqslant \left\|\pi_{M,N}(1-\tau_r(q))|\varphi(q)|\right\|\,\left\|\hat{\pi}_{M,N}\,b_{>d}^\dagger \cdot b_{>d}\,\hat{\pi}_{M,N}\right\| \leqslant 4Ce^{-\delta N}.\end{aligned}$$

We conclude that $\pi_{M,N}\varphi(q)\pi_{M,N} \leqslant 4Ce^{-\delta N} + \epsilon_r b_{>d}^\dagger \cdot b_{>d}$ for $\frac{M}{N} \leqslant \delta$, and therefore $\varphi(q) = o_*\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right)$. The corresponding statement for $\Phi(q)\,b_{>d}^\dagger \cdot b_{>d}$ follows as above. ■

Lemma 2.8.5. *Given $w : \mathbb{R}^d \longrightarrow \mathcal{H}$ with $\|w(t)\| \leqslant c\, |t|^k$ and $W : \mathbb{R}^d \longrightarrow \mathcal{H}$ with $\|W(t)\| \leqslant c\left(1+|t|^k\right)$ for some $c > 0$ and $k \geqslant 1$, we define $X := W(q)^\dagger \cdot b_{>d}$ and $Y := w(q)^\dagger \cdot b_{>d}$. Then, $X^\dagger X$ and $XX^\dagger$ are of order $O_*\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right)$, and $Y^\dagger Y$ and $YY^\dagger$ are of order $o_*\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right)$. Furthermore, for $\Phi : \mathbb{R}^d \longrightarrow \mathbb{R}$ with $|\Phi(t)| \leqslant c\,(1+|t|^j)$, we obtain*

$$\Phi(q)\left(b_{>d}^\dagger \cdot b_{>d}\right)^2 = o_*\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right).$$

Recall the operator p' from Definition 2.4.8. We have

$$(p'-p)^\dagger \cdot (p'-p) = o_*\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right).$$

Proof. Let us define $G(t) := W(t)^\dagger \cdot W(t)$ and $g(t) := w(t)^\dagger \cdot w(t)$. Then we obtain by Lemma 2.8.4 together with the inequality $W(t)\cdot W(t)^\dagger \leqslant G(t)\, 1_{\mathcal{H}}$ the estimate

$$X^\dagger X = b_{>d}^\dagger \cdot W(q)\cdot W(q)^\dagger \cdot b_{>d} \leqslant G(q)\, b_{>d}^\dagger \cdot b_{>d} = O_*\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right).$$

Similarly, $Y^\dagger Y \leqslant g(q)\, b_{>d}^\dagger \cdot b_{>d} = o_*\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right)$. For the reversed order, we use the fact that $\|G(q)\|^2 = O_*(1)$ and $\|g(q)\|^2 = o_*(1)$

$$XX^\dagger = X^\dagger X + \frac{1}{N}\|G(q)\|^2 = O_*\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right),$$

$$YY^\dagger = Y^\dagger Y + \frac{1}{N}\|g(q)\|^2 = o_*\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right).$$

For the next statement, note that we have $\left(b_{>d}^\dagger \cdot b_{>d}\right)^2 = b_{>d}^\dagger \cdot \left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right)\cdot b_{>d}$ and $b_{>d}^\dagger \cdot b_{>d} \leqslant 2(b_{>d}+f(q))^\dagger \cdot (b_{>d}+f(q)) + 2f(q)^\dagger \cdot f(q)$, and consequently

$$\Phi(q)\left(b_{>d}^\dagger \cdot b_{>d}\right)^2 = \Phi(q)\, b_{>d}^\dagger \cdot \left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right)\cdot b_{>d}$$

$$\leqslant 2b_{>d}^\dagger \cdot (b_{>d}+f(q))^\dagger \cdot \Phi(q)\cdot (b_{>d}+f(q))\cdot b_{>d} + 2\Phi(q) f(q)^\dagger \cdot f(q)\, b_{>d}^\dagger \cdot b_{>d} + \frac{\Phi(q)}{N}\, b_{>d}^\dagger \cdot b_{>d}.$$

Note that $2\Phi(q) f(q)^\dagger \cdot f(q)\, b_{>d}^\dagger \cdot b_{>d}$ and $\frac{\Phi(q)}{N}\, b_{>d}^\dagger \cdot b_{>d}$ are of order $o_*\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right)$ by Lemma 2.8.4. For the other term in the inequality above, note that we have the estimate

$$\begin{aligned}
&\pi_{M,N}\, b_{>d}^\dagger \cdot \left[\Phi(q)(b_{>d}+f(q))^\dagger \cdot (b_{>d}+f(q))\right]\cdot b_{>d}\, \pi_{M,N} \\
&= \pi_{M,N}\, b_{>d}^\dagger \cdot \left[\Phi(q)\hat{\pi}_{M,N}(b_{>d}+f(q))^\dagger \cdot (b_{>d}+f(q))\hat{\pi}_{M,N}\right]\cdot b_{>d}\, \pi_{M,N} \\
&\leqslant \frac{M}{N}\, \pi_{M,N}\Phi(q)\, b_{>d}^\dagger \cdot b_{>d}\, \pi_{M,N} \leqslant C\, \frac{M}{N}\pi_{M,N}\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right)\pi_{M,N},
\end{aligned}$$

where we have used that $\pi_{M,N}\Phi(q)\, b_{>d}^\dagger \cdot b_{>d}\, \pi_{M,N} \leqslant C\, \pi_{M,N}\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right)\pi_{M,N}$ for $\frac{M}{N} \leqslant \delta_0 < 1$, see Lemma 2.8.4. In order to verify the last part of the Lemma, let us define the operators $Y_\ell := \partial_\ell f(q)^\dagger \cdot b_{>d}$. From the previous part of this Lemma we know

$$(p'-p)^\dagger \cdot (p'-p) = \sum_{\ell=1}^d \mathfrak{Im}\left[Y_\ell\right]^2 \leqslant \frac{1}{2}\sum_{\ell=1}^d \left(Y_\ell^\dagger Y_\ell + Y_\ell Y_\ell^\dagger\right) = o_*\left(b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}\right).$$

■

For the following Lemma 2.8.6 as well as for the results in Appendix 2.9, it is convenient to define the operator

$$\mathbb{Q}_N := p^\dagger \cdot p + b_{>d}^\dagger \cdot b_{>d} + \frac{1}{N}. \tag{2.8.6}$$

Since $\mathbb{Q}_N \leqslant \mathbb{T}_N$, where $\mathbb{T}_N$ is defined in Eq. (2.4.11), any sequence with $X_N = O_*(\mathbb{Q}_N)$, respectively $X_N = o_*(\mathbb{Q}_N)$, satisfies $X_N = O_*(\mathbb{T}_N)$, respectively $X_N = o_*(\mathbb{T}_N)$, as well.

Lemma 2.8.6. *Let $\varphi : \mathbb{R}^d \longrightarrow \mathbb{R}$ be a function with $|\varphi(t)| \leqslant c\,|t|^k$ and $\Phi : \mathbb{R}^d \longrightarrow \mathbb{R}$ with $|\Phi(t)| \leqslant c\left(1 + |t|^k\right)$ for some constant c and $k \geqslant 1$. Then*

$$(p')^\dagger \cdot \varphi(q) \cdot p' = o_*(\mathbb{Q}_N),$$
$$(p')^\dagger \cdot \Phi(q) \cdot p' = O_*(\mathbb{Q}_N).$$

In case the partial derivatives $\partial_i\varphi(t)$, $\partial_j\Phi(t)$ and $\partial_i\partial_j\Phi(t)$ are bounded by $c\,(1 + |t|^j)$, we also have

$$\varphi(q)\,(p')^\dagger \cdot p'\,\varphi(q) = o_*(\mathbb{Q}_N),$$
$$\Phi(q)\left[(p')^\dagger \cdot p'\right]^2 \Phi(q) = o_*(\mathbb{Q}_N).$$

Proof. Since $p^\dagger \cdot p \leqslant \mathbb{Q}_N$ and $(p' - p)^\dagger \cdot (p' - p) = O_*(\mathbb{Q}_N)$ by Lemma 2.8.5, we obtain $(p')^\dagger \cdot p' = O_*(\mathbb{Q}_N)$ as well, i.e.

$$\pi_{M,N}(p')^\dagger \cdot p'\pi_{M,N} \leqslant C_1\ \pi_{M,N}\mathbb{Q}_N\pi_{M,N}$$

for all M, N with $\frac{M}{N} \leqslant \delta_1 < 1$ where δ_1 and C_1 are suitable constants. By Lemma 2.8.4, we know that $\pi_{M,N}\Phi(q)\pi_{M,N} \leqslant C_2$ for all $\frac{M}{N} \leqslant \delta_2 < 1$ where δ_2 and C_2 are suitable constants, and $\pi_{M,N}\varphi(q)\pi_{M,N} \leqslant \epsilon\left(\frac{M}{N}\right)$ with $\lim_{\delta\to 0}\ \epsilon(\delta) = 0$. Based on the observation that $p'\,\pi_{M,N} = \pi_{M+1,N}\,p'\,\pi_{M,N}$, we obtain for all M, N that satisfy $\frac{M}{N} \leqslant \delta := 2\min\{\delta_1, \delta_2\}$

$$\begin{aligned}\pi_{M,N}\,(p')^\dagger \cdot \Phi(q) \cdot p'\,\pi_{M,N} &= \pi_{M,N}\,(p')^\dagger \cdot \pi_{M+1,N}\Phi(q)\pi_{M+1,N} \cdot p'\,\pi_{M,N}\\ &\leqslant C_1C_2\ \pi_{M,N} \cdot \mathbb{Q}_N \cdot \pi_{M,N}.\end{aligned}$$

Similarly, we have $\pi_{M,N}\,(p')^\dagger \cdot \varphi(q) \cdot p'\,\pi_{M,N} \leqslant C_1\epsilon\left(\frac{M}{N}\right)\ \pi_{M,N}\,\mathbb{Q}_N\,\pi_{M,N}$. Hence, $(p')^\dagger \cdot \Phi(q) \cdot p' = O_*(\mathbb{Q}_N)$ and $(p')^\dagger \cdot \varphi(q) \cdot p' = o_*(\mathbb{Q}_N)$. In case we have a polynomial bound on the partial derivatives as well, let us define $w(t) := \frac{1}{2}\sum_{\ell=1}^d \partial_\ell\varphi(t) \otimes u_\ell$ and $W(t) := \frac{1}{2}\sum_{\ell=1}^d \partial_\ell\Phi(t) \otimes u_\ell$. Using the commutation relation $[ip'_j, q_k] = \frac{\delta_{j,k}}{2N}$, we compute

$$\varphi(q)\ (p')^\dagger \cdot p'\,\varphi(q) = \left(\varphi(q) \cdot ip' + \frac{1}{N}w(q)\right)^\dagger \cdot \left(\varphi(q) \cdot ip' + \frac{1}{N}w(q)\right).$$

From the previous part, we know that $(\varphi(q) \cdot ip')^\dagger \cdot \varphi(q) \cdot ip' = o_*(\mathbb{Q}_N)$. Furthermore, Lemma 2.8.4 tells us that $w(q)^\dagger \cdot w(q) = O_*(1)$, and therefore $\frac{1}{N}w(q)^\dagger \cdot \frac{1}{N}w(q) = o_*(\mathbb{Q}_N)$. Hence, $\varphi(q)\,(p')^\dagger \cdot p'\,\varphi(q)$ is of order $o_*(\mathbb{Q}_N)$ as well. The last estimate in the Lemma can be verified analogously. ■

2.9 Analysis of the Operator Square Root

In the following section we derive asymptotic results for operators involving the square root $\sqrt{1-\mathbb{L}'}$, where $\mathbb{L}'$ is defined in Definition 2.4.8, allowing us to prove a Taylor approximation for the operators $(1-\mathbb{L}')^{\frac{m}{2}}$, see Definition 2.5.5. The easiest case $m=2$ will be discussed in the following Lemma 2.9.1, the case $m=1$ is the content of Lemma 2.9.2 and the case $m=3$ is covered by Corollary 2.9.5.

Lemma 2.9.1. *Recall the operator $\mathbb{Q}_N$ from Eq. (2.8.6) and the function f from Definition 2.4.7, and let us define $g(t) := \sum_{j=1}^d t_j^2 + f(t)^\dagger \cdot f(t)$. Then,*

$$[\mathbb{L}' - g(q)]^2 = o_*(\mathbb{Q}_N)\,. \tag{2.9.1}$$

Proof. Using the transformation laws in Lemma 2.4.9 we obtain

$$\mathbb{L}' - g(q) = f(q)^\dagger \cdot b_{>d} + b_{>d}^\dagger \cdot f(q) + (p')^\dagger \cdot p' + b_{>d}^\dagger \cdot b_{>d} - \frac{d}{2N}.$$

By Lemma 2.8.5, we know that $\left[f(q)^\dagger \cdot b_{>d} + b_{>d}^\dagger \cdot f(q)\right]^2 = o_*(\mathbb{Q}_N)$ and $\left[b_{>d}^\dagger \cdot b_{>d}\right]^2 = o_*(\mathbb{Q}_N)$, and by Lemma 2.8.6 we know that $\left[(p')^\dagger \cdot p'\right]^2 = o_*(\mathbb{Q}_N)$. ■

Lemma 2.9.2. *Let Assumption 2.1.3 hold and recall the function η_1 from Eq. (2.5.7). Then,*

$$\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right]^2 = o_*(\mathbb{Q}_N)\,. \tag{2.9.2}$$

Furthermore for any function $V: \mathbb{R}^d \longrightarrow \mathbb{R}$ with $|V(t)| \leqslant c\left(|t| + |t|^k\right)$ and bounded derivatives $|\partial_{t_i} V(t)| + |\partial_{t_i}\partial_{t_j} V(t)| \leqslant c\left(1 + |t|^k\right)$ for some $k \geqslant 1$, we have

$$V(q)\left[\sqrt{1-\mathbb{L}'} - \eta_1(q) - D_{\mathcal{V}}\big|_q \eta_1\big(b_{\geqslant 1}\big)\right] = o_*(\mathbb{Q}_N)\,. \tag{2.9.3}$$

Proof. Let us define $h(x) := \chi(x)\sqrt{1-x}$, where $\chi: [0,\infty) \longrightarrow [0,1]$ is the function from the definition of η_1 in Eq. (2.5.7), as well as the operator $Q := q^\dagger \cdot q + f(q)^\dagger \cdot f(q)$. By the support properties of χ we have for all $\frac{M}{N} < \frac{1}{2}$ and $\Psi \in \mathcal{W}_N \mathcal{F}_{\leqslant M}$

$$\sqrt{1-\mathbb{L}'}\,\Psi = h(\mathbb{L}')\,\Psi,$$

and therefore it is enough to verify the statements of this Lemma for $h(\mathbb{L}')$ instead of $\sqrt{1-\mathbb{L}'}$. With h at hand, we have $\eta_1(q) = h(\|F(q)\|^2) = h(Q)$ and

$$D_{\mathcal{V}}\big|_q \eta_1(v) = w(q)^\dagger \cdot v + v^\dagger \cdot w(q)$$

with $w(t) := h'\left(\sum_{j=1}^d t_j^2 + f(t)^\dagger \cdot f(t)\right) f(t)$, for all $v \in \mathcal{H}_0$. Hence $w(q) = h'(Q)\,f(q)$. In the following, let $\hat{h}$ be the Fourier transform of the smooth function h, normalized such that $h(x) = \int \hat{h}(z)\, e^{izx}\, \mathrm{d}z$. Then,

$$h(\mathbb{L}') - h(Q) = \int \hat{h}(z)\left(e^{iz\mathbb{L}'} - e^{izQ}\right)\, \mathrm{d}z.$$

In order to investigate the integrand, we use the following integral representation

$$\begin{aligned} e^{iz\mathbb{L}'} - e^{izQ} &= i\int_0^z e^{iy\mathbb{L}'}\left(\mathbb{L}'-Q\right)e^{i(z-y)Q}\,\mathrm{d}y \\ &= i\int_0^z e^{iy\mathbb{L}'}e^{i(z-y)Q}\,\mathrm{d}y\left(\mathbb{L}'-Q\right) + i\int_0^z e^{iy\mathbb{L}'}\left[\mathbb{L}', e^{i(z-y)Q}\right]\,\mathrm{d}y. \end{aligned}$$

Let us define the operators $B_z := i\int_0^z e^{iy\mathbb{L}'}e^{i(z-y)Q}\,\mathrm{d}y$ and $R_z := i\int_0^z e^{iy\mathbb{L}'}\left[\mathbb{L}', e^{i(z-y)Q}\right]\mathrm{d}y$. Clearly, $\|B_z\| \leqslant |z|$. Regarding R_z, note that every term in the definition of $\mathbb{L}'$ commutes with Q, except $(p')\cdot p'$, which satisfies the relation $\left[p'_j, \varphi(q)\right] = \left[p_j, \varphi(q)\right] = \frac{1}{i2N}\left(\partial_j\varphi\right)(q)$. We define the family of functions

$$\varphi_x(t) := e^{ix\left(\sum_{j=1}^d t_j^2 + f(t)^\dagger\cdot f(t)\right)} \tag{2.9.4}$$

and compute

$$\begin{aligned} \left[\mathbb{L}', e^{ixQ}\right] = \left[(p')\cdot p', \varphi_x(q)\right] &= \sum_{j=1}^d \left[\left(p'_j\right)^2, \varphi_x(q)\right] \\ &= \frac{1}{iN}\sum_{j=1}^d \partial_j\varphi_x(q)p'_j - \frac{1}{4N^2}\sum_{j=1}^d \partial_j^2\varphi_x(q). \end{aligned}$$

We have the estimates $|\partial_j\varphi_x(t)| \leqslant c|x|\ |t|$ and $\left|\partial_j^2\varphi_x(t)\right| \leqslant c\left(1+|x|^2\right)\left(1+|t|^2\right)$ for some $c>0$, where we use the fact that $t\mapsto f(t)$ is a $C^2\left(\mathbb{R}^d, \mathcal{H}_0\right)$ function, see Definition 2.4.7. As before, let $\pi_{M,N}$ be the orthogonal projection onto $\mathcal{W}_N\left(\mathcal{F}_{\leqslant M}\right)$. By Lemma 2.8.4

$$\begin{aligned} &\|\partial_j\varphi_x(q)\pi_{M,N}\| \leqslant c|x|\ \|\ |q|\,\pi_{M,N}\| \leqslant \tilde{c}|x|, \\ &\|\partial_j^2\varphi_x(q)\pi_{M,N}\| \leqslant c\left(1+|x|^2\right)\|\left(1+|q|^2\right)\pi_{M,N}\| \leqslant \tilde{c}\left(1+|x|^2\right), \end{aligned}$$

for some constant $\tilde{c}$ and all $x\in\mathbb{R}$ and all $M\leqslant N$. Note that $p'_j\mathcal{W}_N\mathcal{F}_{\leqslant M} \subset \mathcal{W}_N\mathcal{F}_{\leqslant M+1}$ and $\|p'_j\,\pi_{M,N}\| \leqslant \sqrt{\frac{M+1}{N}}$, and consequently we have for all $M\leqslant N-1$

$$\begin{aligned} \|\left[\mathbb{L}', e^{ixQ}\right]\pi_{M,N}\| &\leqslant \frac{2}{N}\sum_{j=1}^d \|\partial_j\varphi_x(q)\,\pi_{M+1,N}\|\ \|p'_j\,\pi_{M,N}\| + \frac{1}{N^2}\sum_{j=1}^d \|\partial_j^2\varphi_x(q)\,\pi_{M,N}\| \\ &\leqslant \frac{d\tilde{c}}{N}|x| + \frac{d\tilde{c}}{4N^2}\left(1+|x|^2\right) \leqslant \frac{2d\tilde{c}}{N}\left(1+|x|^2\right). \end{aligned}$$

Therefore, $\|R_z\pi_{M,N}\| \leqslant \frac{C}{N}\left(1+|z|^3\right)$ for some constant C.

Let us define $B := \int\hat{h}(z)B_z\,\mathrm{d}z$ and $R := \int\hat{h}(z)R_z\,\mathrm{d}z$. From our estimates on B_z, R_z, we deduce $\|B\| \leqslant \int|\hat{h}(z)|\ |z|\ \mathrm{d}z := C_1 < \infty$ and $\|R\,\pi_{M,N}\| \leqslant \frac{C}{N}\int|\hat{h}(z)|\left(1+|z|^3\right)\ \mathrm{d}z := \frac{C_2}{N} < \infty$. Hence, $R^\dagger R = o_*\left(\mathbb{Q}_N\right)$. Since $h\left(\mathbb{L}'\right) - h\left(Q\right) = B\left(\mathbb{L}'-Q\right) + R$, we obtain the estimate

$$\begin{aligned} \left[h\left(\mathbb{L}'\right) - h\left(Q\right)\right]^2 &= \left[B\left(\mathbb{L}'-Q\right)+R\right]^\dagger\left[B\left(\mathbb{L}'-Q\right)+R\right] \\ &\leqslant 2\left(\mathbb{L}'-Q\right)B^\dagger B\left(\mathbb{L}'-Q\right) + 2R^\dagger R \\ &\leqslant 2(C_1)^2\left(\mathbb{L}'-Q\right)^2 + 2R^\dagger R = o_*\left(\mathbb{Q}_N\right), \end{aligned}$$

where we have used that $\left(\mathbb{L}'-Q\right)^2$ is of order $o_*\left(\mathbb{Q}_N\right)$, see Lemma 2.9.1. This proves Eq. (2.9.2).

In order to verify Eq. (2.9.3) let us compute

$$\begin{aligned}
\sqrt{1-\mathbb{L}'} - \eta_1(q) - D_{\mathcal{V}}\big|_q \eta_1\big(b_{\geqslant 1}\big) &= h(\mathbb{L}') - h(Q) - h'(Q)\left(b_{>d}^\dagger \cdot f(q) + f(q)^\dagger \cdot b_{>d}\right) \\
&= \int \hat{h}(z)\left[i\int_0^z e^{iy\mathbb{L}'}(\mathbb{L}'-Q)\, e^{i(z-y)Q}\, \mathrm{d}y - iz\, e^{izQ}\left(f(q)^\dagger \cdot b_{>d} + b_{>d}^\dagger \cdot f(q)\right)\right] \mathrm{d}z \\
&= R + \int \hat{h}(z)\left[i\int_0^z e^{iy\mathbb{L}'} e^{i(z-y)Q} \mathrm{d}y\, (\mathbb{L}'-Q) - iz\, e^{izQ}\left(f(q)^\dagger \cdot b_{>d} + b_{>d}^\dagger \cdot f(q)\right)\right] \mathrm{d}z \\
&= R + i\int \hat{h}(z)\int_0^z \left(e^{iy\mathbb{L}'} - e^{iyQ}\right) e^{i(z-y)Q}\, \mathrm{d}y\, \mathrm{d}z\, (\mathbb{L}'-Q) \qquad (2.9.5)\\
&\quad + i\int \hat{h}(z) z\, e^{izQ}\, \mathrm{d}z \left(\mathbb{L}' - Q - f(q)^\dagger \cdot b_{>d} - b_{>d}^\dagger \cdot f(q)\right).
\end{aligned}$$

Let V be a function that satisfies the assumptions of the Lemma. To complete the proof, we need to verify that $V(q)\left[h(\mathbb{L}') - h(Q) - h'(Q)\left(f(q)^\dagger \cdot b_{>d} + b_{>d}^\dagger \cdot f(q)\right)\right]$ is of order $o_*(\mathbb{Q}_N)$. By Lemma 2.8.4, we know that $|V|^2(q) = o_*(1)$ and from the previous part it is clear that $\pi_{M,N}\, R^\dagger R\, \pi_{M,N} = O_*(\frac{1}{N^2})$. Hence, $V(q)R = o_*(\frac{1}{N})$ and especially $V(q)R = o_*(\mathbb{Q}_N)$. Regarding the second term in Eq. (2.9.5), recall that $e^{iy\mathbb{L}'} - e^{iyQ} = (\mathbb{L}'-Q)\, B_{-y}^\dagger + R_{-y}^\dagger$. Therefore,

$$\begin{aligned}
&\int \hat{h}(z) i\int_0^z \left(e^{iy\mathbb{L}'} - e^{iyQ}\right) e^{i(z-y)Q}\, \mathrm{d}y\, \mathrm{d}z\, (\mathbb{L}'-Q) \\
&\quad = \int \hat{h}(z) i\int_0^z \left[(\mathbb{L}'-Q)\, B_{-y}^\dagger + R_{-y}^\dagger\right] e^{i(z-y)Q}\, \mathrm{d}y\, \mathrm{d}z\, (\mathbb{L}'-Q) \\
&\quad = \left[(\mathbb{L}'-Q)\, \widetilde{B}^\dagger + \widetilde{R}^\dagger\right](\mathbb{L}'-Q),
\end{aligned}$$

with $\widetilde{B} := -i\int \hat{h}(z)\int_0^z e^{i(y-z)Q} B_{-y}\, \mathrm{d}y\, \mathrm{d}z$ and $\widetilde{R} := -i\int \hat{h}(z)\int_0^z e^{i(y-z)Q} R_{-y}\, \mathrm{d}y\, \mathrm{d}z$. In the following we want to verify that $V(q)\left[(\mathbb{L}'-Q)\, \widetilde{B}^\dagger + \widetilde{R}^\dagger\right](\mathbb{L}'-Q) = o_*(\mathbb{Q}_N)$. Since $(\mathbb{L}'-Q)^2 = o_*(\mathbb{Q}_N)$ by Lemma 2.9.1, it is enough to verify that $V(q)\widetilde{R}^\dagger \widetilde{R} V(q)$ and $V(q)(\mathbb{L}'-Q)\, \widetilde{B}^\dagger \widetilde{B}\, (\mathbb{L}'-Q)\, V(q)$ are of order $o_*(\mathbb{Q}_N)$. Recall that we have the identity $R_y = i\int_0^y e^{ix\mathbb{L}'}\left[\mathbb{L}'-Q, e^{i(y-x)Q}\right]\mathrm{d}x = i\int_0^y e^{ix\mathbb{L}'}\left[(p')^\dagger \cdot p', \varphi_x(q)\right]\mathrm{d}x$ with the function φ_x from Eq. (2.9.4). We can further express $[(p')^\dagger \cdot p', \varphi_x(q)]V(q)$ as

$$\sum_{j=1}^d \left(\frac{1}{iN}\partial_j \varphi_x(q) V(q) p_j' - \frac{1}{2N^2}\partial_j \varphi_x(q)\partial_j V(q) - \frac{1}{4N^2}\partial_j^2 \varphi_x(q) V(q)\right).$$

Similar to before, this leads to the estimate $\|R_z V(q)\pi_{M,N}\| \leqslant \frac{\widetilde{C}}{N}(1+|z|^3)$ for some constant $\widetilde{C}$, and consequently $\|\widetilde{R} V(q)\pi_{M,N}\| \leqslant \frac{\widetilde{C}_1}{N}$ for some constant $\widetilde{C}_1$. Hence we have $V(q)\widetilde{R}^\dagger \widetilde{R} V(q) = o_*(\mathbb{Q}_N)$. Regarding the term $V(q)(\mathbb{L}'-Q)\, \widetilde{B}^\dagger \widetilde{B}\, (\mathbb{L}'-Q)\, V(q)$, note that $\|\widetilde{B}\|^2 =: \widetilde{C}_2 < \infty$. Applying the Cauchy–Schwarz yields

$$\begin{aligned}
&V(q)(\mathbb{L}'-Q)\, \widetilde{B}^\dagger \widetilde{B}\, (\mathbb{L}'-Q)\, V(q) \leqslant \widetilde{C}_2\, V(q)(\mathbb{L}'-Q)^2 V(q) \\
&\leqslant 5\widetilde{C}_2 V(q)\left[f(q)^\dagger \cdot b_{>d}\, b_{>d}^\dagger \cdot f(q) + b_{>d}^\dagger \cdot f(q) f(q)^\dagger \cdot b_{>d} + \left((p')^\dagger \cdot p'\right)^2 + \left(b_{>d}^\dagger \cdot b_{>d}\right)^2 + \frac{d^2}{N^2}\right] V(q).
\end{aligned}$$

Let us define the function $w(t) := V(t)f(t)$. By Lemma 2.8.5 we obtain that

$$V(q)\, f(q)^\dagger \cdot b_{>d}\, b_{>d}^\dagger \cdot f(q)\, V(q) = w(q)^\dagger \cdot b_{>d}\, b_{>d}^\dagger \cdot w(q) = o_*\left(\mathbb{Q}_N\right),$$
$$V(q)\, b_{>d}^\dagger \cdot f(q)\; f(q)^\dagger \cdot b_{>d}\, V(q) = b_{>d}^\dagger \cdot w(q)\, w(q)^\dagger \cdot b_{>d} = o_*\left(\mathbb{Q}_N\right),$$

and $V(q)\left(b_{>d}^\dagger \cdot b_{>d}\right)^2 V(q) = o_*\left(\mathbb{Q}_N\right)$. Furthermore, $V(q)\left[(p')^\dagger \cdot p'\right]^2 V(q) = o_*\left(\mathbb{Q}_N\right)$ by Lemma 2.8.6. We conclude that $V(q)\left(\mathbb{L}' - Q\right) \widetilde{B}^\dagger \widetilde{B}\left(\mathbb{L}' - Q\right) V(q) = o_*\left(\mathbb{Q}_N\right)$.

Let us now verify that the final term $\widetilde{V}(q)\left(\mathbb{L}' - Q - b_{>d}^\dagger \cdot f(q) - f(q)^\dagger \cdot b_{>d}\right)$ in Eq. (2.9.5) is of order $o_*\left(\mathbb{Q}_N\right)$, where $\widetilde{V}(t) := V(t) \int \hat{h}(z) iz\; e^{iz\left(\sum_{j=1}^d t_j^2 + f(t)^\dagger \cdot f(t)\right)}\, \mathrm{d}z$. By the definition of $\mathbb{L}'$ and Q, we have the identity

$$\widetilde{V}(q)\left(\mathbb{L}' - Q - f(q)^\dagger \cdot b_{>d} - b_{>d}^\dagger \cdot f(q)\right) = \widetilde{V}(q) b_{>d}^\dagger \cdot b_{>d} + \widetilde{V}(q)\left(p'\right)^\dagger \cdot p' - \frac{d}{2N} V(q).$$

The first term is of order $o_*\left(\mathbb{Q}_N\right)$ by Lemma 2.8.4, the second term is by Lemma 2.8.6 and regarding the last term we know that $\frac{d}{2N} V(q) = o_*\left(\mathbb{Q}_N\right)$ by Lemma 2.8.4. ∎

Before we can verify the Taylor approximation for the operator $(1 - \mathbb{L})^{\frac{3}{2}}$ in Corollary 2.9.5, we need the following two results, which are of independent relevance for the proof of Theorem 2.5.16.

Lemma 2.9.3. *We have* $\left(\mathbb{L}'\right)^2 = o_*(1)$*, and furthermore*

$$\sqrt{1 - \mathbb{L}'}\, \mathbb{Q}_N \sqrt{1 - \mathbb{L}'} = O_*\left(\mathbb{Q}_N\right), \tag{2.9.6}$$
$$\mathbb{L}'\, \mathbb{Q}_N\, \mathbb{L}' = o_*\left(\mathbb{Q}_N\right). \tag{2.9.7}$$

Proof. Note that $\|\mathbb{L}' \pi_{M,N}\| = \frac{M}{N}$ for all $M \leqslant N$, and therefore we immediately obtain $\left(\mathbb{L}'\right)^2 = o_*(1)$. In order to verify Equations (2.9.6) and (2.9.7), it is enough to prove that $\sqrt{1 - \mathbb{L}'}\left(\xi^\dagger \cdot \xi\right)\sqrt{1 - \mathbb{L}'} = O_*\left(\mathbb{Q}_N\right)$ and $\mathbb{L}'\left(\xi^\dagger \cdot \xi\right)\mathbb{L}' = o_*\left(\mathbb{Q}_N\right)$ for $\xi \in \{p', b_{>d}\}$.

The case $\xi = p'$: In order to verify $\sqrt{1 - \mathbb{L}'}\left(\xi^\dagger \cdot \xi\right)\sqrt{1 - \mathbb{L}'} = O_*\left(\mathbb{Q}_N\right)$, observe that we have for all $\Psi \in \mathcal{W}_N \mathcal{F}_{\leqslant N-1}$ the commutation law

$$p_j' \sqrt{1 - \mathbb{L}'}\Psi = \frac{\sqrt{1 - \mathbb{L}' - \frac{1}{N}} + \sqrt{1 - \mathbb{L}' + \frac{1}{N}}}{2} p_j' \Psi + \frac{\sqrt{1 - \mathbb{L}' - \frac{1}{N}} - \sqrt{1 - \mathbb{L}' + \frac{1}{N}}}{2} q_j \Psi.$$

For $M \leqslant N - 2$, let us define the operators $B_{M,N} := \frac{\sqrt{1 - \mathbb{L}' - \frac{1}{N}} + \sqrt{1 - \mathbb{L}' + \frac{1}{N}}}{2} \pi_{M+1,N}$ and $\widetilde{B}_{M,N} := \frac{\sqrt{1 - \mathbb{L}' - \frac{1}{N}} - \sqrt{1 - \mathbb{L}' + \frac{1}{N}}}{2} \pi_{M+1,N}$. Note that $\|B_{M,N}\| \leqslant 1$ and $\|\widetilde{B}_{M,N}\|^2 \leqslant \frac{C}{N^2}$ for all $\frac{M}{N} \leqslant \delta_0$, where C and $0 < \delta < 1$ are suitable constants. Consequently

$$\pi_{M,N} \sqrt{1 - \mathbb{L}'}\; (p')^\dagger \cdot p' \sqrt{1 - \mathbb{L}'} \pi_{M,N} = \left|\left(B_{M,N} \otimes 1_{\mathcal{H}} \cdot p' + \widetilde{B}_{M,N} \otimes 1_{\mathcal{H}} \cdot q\right) \pi_{M,N}\right|^2$$
$$\leqslant 2\left|B_{M,N} \otimes 1_{\mathcal{H}} \cdot p'\, \pi_{M,N}\right|^2 + 2\left|\widetilde{B}_{M,N} \otimes 1_{\mathcal{H}} \cdot q\, \pi_{M,N}\right|^2$$
$$\leqslant \pi_{M,N}\, (p')^\dagger \cdot p'\, \pi_{M,N} + \frac{C(d+1)}{N^2},$$

which concludes the proof of $\sqrt{1-\mathbb{L}'}\,(p')^\dagger \cdot p'\,\sqrt{1-\mathbb{L}'} = O_*\left(\mathbb{Q}_N\right)$. The estimate $\mathbb{L}'\,(p')^\dagger \cdot p'\,\mathbb{L}' = o_*\left(\mathbb{Q}_N\right)$ follows from an analogue commutation law.

The case $\xi = b_{>d}$: In order to verify $\sqrt{1-\mathbb{L}'}\,b_{>d}^\dagger \cdot b_{>d}\sqrt{1-\mathbb{L}'} = O_*\left(\mathbb{Q}_N\right)$, note that $\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right]^2 = o_*\left(\mathbb{Q}_N\right)$ by 2.9.2, i.e. there exists a function ϵ with $\epsilon(\delta) \underset{\delta\to 0}{\longrightarrow} 0$ and $\pi_{M,N}\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right]^2 \pi_{M,N} \leqslant \epsilon\left(\frac{M}{N}\right)\ \pi_{M,N}\,\mathbb{Q}_N\,\pi_{M,N}$. By Lemma 2.8.3, we know that $\hat{\pi}_{M,N}\,b_{>d}^\dagger \cdot b_{>d}\,\hat{\pi}_{M,N} \leqslant C$ for a constant C. Furthermore $\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right]\hat{\pi}_{M,N} = \hat{\pi}_{M,N}\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right]$. Let us define $S := \left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right] b_{>d}^\dagger \cdot b_{>d}\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right]$, and estimate

$$\begin{aligned}\pi_{M,N} S \pi_{M,N} &= \pi_{M,N}\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right]\hat{\pi}_{M,N}\,b_{>d}^\dagger \cdot b_{>d}\,\hat{\pi}_{M,N}\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right]\pi_{M,N}\\ &\leqslant 4\ \pi_{M,N}\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right]^2 \pi_{M,N} \leqslant 4\ \epsilon\left(\frac{M}{N}\right)\ \pi_{M,N}\,\mathbb{Q}_N\,\pi_{M,N}.\end{aligned}$$

Hence, $S = o_*\left(\mathbb{Q}_N\right)$ and therefore

$$\sqrt{1-\mathbb{L}'}\,b_{>d}^\dagger \cdot b_{>d}\sqrt{1-\mathbb{L}'} \leqslant 2\left(S + \eta_1(q)\,b_{>d}^\dagger \cdot b_{>d}\,\eta_1(q)\right) = O_*\left(\mathbb{Q}_N\right).$$

The proof of $\mathbb{L}'\,b_{>d}^\dagger \cdot b_{>d}\,\mathbb{L}' = o_*\left(\mathbb{Q}_N\right)$ can be carried out in a similar fashion. ■

Corollary 2.9.4. *Let X_N be a sequence with $X_N = O_*\left(\mathbb{Q}_N\right)$ and Y_N a sequence with $Y_N = o_*\left(\mathbb{Q}_N\right)$. Then,*

$$\sqrt{1-\mathbb{L}'}X_N\sqrt{1-\mathbb{L}'} = O_*\left(\mathbb{Q}_N\right), \tag{2.9.8}$$

$$\sqrt{1-\mathbb{L}'}Y_N\sqrt{1-\mathbb{L}'} = o_*\left(\mathbb{Q}_N\right), \tag{2.9.9}$$

$$\mathbb{L}'X_N\mathbb{L}' = o_*\left(\mathbb{Q}_N\right). \tag{2.9.10}$$

Proof. The Corollary follows from Lemma 2.9.3 and the fact that $\pi_{M,N}$ commutes with $\sqrt{1-\mathbb{L}'}$ and $\mathbb{L}'$. For the purpose of illustration, let us verify Eq. (2.9.8). By the assumptions of the Corollary we know that there exist constants C and $\delta > 0$, such that $\pi_{M,N}\,X_N\,\pi_{M,N} \leqslant C\pi_{M,N}\,\mathbb{Q}_N\,\pi_{M,N}$. Consequently

$$\begin{aligned}\pi_{M,N}\sqrt{1-\mathbb{L}'}X_N\sqrt{1-\mathbb{L}'}\,\pi_{M,N} &= \sqrt{1-\mathbb{L}'}\pi_{M,N}\,X_N\,\pi_{M,N}\sqrt{1-\mathbb{L}'}\\ &\leqslant C\pi_{M,N}\sqrt{1-\mathbb{L}'}\mathbb{Q}_N\sqrt{1-\mathbb{L}'}\,\pi_{M,N} = O_*\left(\mathbb{Q}_N\right),\end{aligned}$$

where we have used Eq. (2.9.6) from Lemma 2.9.3 in the last equality. ■

Corollary 2.9.5. *Let Assumption 2.1.3 hold and let η_m be the functions from Eq. (2.5.7), with $m \in \{0,\ldots,3\}$. Then*

$$\left[(1-\mathbb{L}')^{\frac{m}{2}} - \eta_m(q)\right]^2 = o_*\left(\mathbb{Q}_N\right).$$

Proof. The case $m=0$ is trivial. The case $m=1$ is the content of Lemma 2.9.2 and the case $m=2$ follows from Lemma 2.9.1. Let us now verify the statement in the case $m=3$.

Using the fact that $\eta_3(t) = \eta_2(t)\eta_1(t)$, we obtain

$$\begin{aligned}(1-\mathbb{L}')\sqrt{1-\mathbb{L}'} - \eta_3(q) &= [(1-\mathbb{L}') - \eta_2(q)]\sqrt{1-\mathbb{L}'} + \eta_2(q)\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right] \\ &= -\left(f(q)^\dagger \cdot b_{>d} + b_{>d}^\dagger \cdot f(q) + (p')^\dagger \cdot p' + b_{>d}^\dagger \cdot b_{>d} - \frac{d}{2N}\right)\sqrt{1-\mathbb{L}'} \\ &\quad + \tau_r(q)\eta_2(q)\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right] + [1-\tau_r(q)]\,\eta_2(q)\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right],\end{aligned}$$

where $\tau : \mathbb{R}^d \longrightarrow \mathbb{R}$ is a function with $\tau|_{B_1(0)} = 0$, $\tau|_{\mathbb{R}^d \setminus B_2(0)} = 1$ and $0 \leqslant \tau \leqslant 1$. Since the function $\widetilde{\eta} = (1-\tau)\eta_2$ is bounded by a constant c, we obtain using Lemma 2.9.2

$$\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right]\widetilde{\eta}^2(q)\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right] \leqslant c\,\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right]^2 = o_*\left(\mathbb{Q}_N\right).$$

Note that $\eta' := (\tau\,\eta_2)^2$ is zero in a neighborhood of zero. Therefore, $\eta'(q) = O_*\left(e^{-\delta N}\right)$ and $\eta_1^2(q)\eta'(q) = O_*\left(e^{-\delta N}\right)$ for some $\delta > 0$ by Lemma 2.8.2. By Corollary 2.9.4, we obtain in particular that $\sqrt{1-\mathbb{L}'}\eta'(q)\sqrt{1-\mathbb{L}'} = o_*\left(\mathbb{Q}_N\right)$. Hence we have the estimate

$$\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right]\eta'(q)\left[\sqrt{1-\mathbb{L}'} - \eta_1(q)\right] \leqslant 2\sqrt{1-\mathbb{L}'}\eta'(q)\sqrt{1-\mathbb{L}'} + 2\eta_1^2(q)\eta'(q) = o_*\left(\mathbb{Q}_N\right).$$

By Lemma 2.8.5, Lemma 2.8.6 and Corollary 2.9.4, we know that the operators

$$\sqrt{1-\mathbb{L}'}\left(b_{>d}^\dagger \cdot f(q) + f(q)^\dagger \cdot b_{>d}\right)^2\sqrt{1-\mathbb{L}'}$$

$\sqrt{1-\mathbb{L}'}\left((p')^\dagger \cdot p'\right)^2\sqrt{1-\mathbb{L}'}$ as well as $\sqrt{1-\mathbb{L}'}\left(b_{>d}^\dagger \cdot b_{>d}\right)^2\sqrt{1-\mathbb{L}'}$ are of order $o_*\left(\mathbb{Q}_N\right)$ as well, and therefore

$$\sqrt{1-\mathbb{L}'}\left(b_{>d}^\dagger \cdot f(q) + f(q)^\dagger \cdot b_{>d} + (p')^\dagger \cdot p' + b_{>d}^\dagger \cdot b_{>d} - \frac{d}{2N}\right)^2\sqrt{1-\mathbb{L}'} = o_*\left(\mathbb{Q}_N\right).$$

We conclude that $(1-\mathbb{L}')\sqrt{1-\mathbb{L}'} - \eta_3(q) = T_1 + T_2 + T_3$ is a sum of terms with $T_i^\dagger T_i = o_*\left(\mathbb{Q}_N\right)$, and therefore $\left[(1-\mathbb{L}')\sqrt{1-\mathbb{L}'} - \eta_3(q)\right]^2 = o_*\left(\mathbb{Q}_N\right)$. ■

CHAPTER 3

The Fröhlich Polaron at Strong Coupling – Part I: The Quantum Correction to the Classical Energy

Abstract. We study the Fröhlich polaron model in $\mathbb{R}^3$, and establish the subleading term in the strong coupling asymptotics of its ground state energy, corresponding to the quantum corrections to the classical energy determined by the Pekar approximation.

3.1 Introduction and Main Results

This is the first part of a study of the asymptotic properties of the Fröhlich polaron, which is a model describing the interaction between an electron and the optical modes of a polar crystal [44]. In the regime of strong coupling between the electron and the optical modes, also called phonons, it is a well known fact [1, 29, 79] that the ground state energy of the Fröhlich polaron is asymptotically given by the minimal Pekar energy [106], which can be considered as the ground state energy of an electron interacting with a classical phonon field. This result is motivated by using appropriately scaled units, see e.g. [116], which demonstrates that the strong coupling regime is a semi-classical limit in the phonon field variables. In such units the Fröhlich Hamiltonian, acting on the space $L^2(\mathbb{R}^3) \otimes \mathcal{F}\left(L^2(\mathbb{R}^3)\right)$, reads

$$\mathbb{H} := -\Delta_x - a\left(w_x\right) - a^\dagger\left(w_x\right) + \mathcal{N}, \tag{3.1.1}$$

where the annihilation and creation operators satisfy the rescaled canonical commutation relations $\left[a(f), a^\dagger(g)\right] = \alpha^{-2}\langle f|g\rangle$ for $f, g \in L^2(\mathbb{R}^3)$ with $\alpha > 0$ being the coupling strength, the interaction is given by $w_x(x') := \pi^{-\frac{3}{2}}|x' - x|^{-2}$ and $\mathcal{N}$ is the corresponding (rescaled) particle number operator, i.e. $\mathcal{N} := \sum_{n=1}^{\infty} a^\dagger(\varphi_n)a(\varphi_n)$ where $\{\varphi_n : n \in \mathbb{N}\}$ is an orthonormal basis of $L^2(\mathbb{R}^3)$. The definition of the Fröhlich Hamiltonian in Eq. (3.1.1) has to be understood in the sense of quadratic forms, see for example [116], due to the ultraviolet singularity in the interaction w_x. By substituting the annihilation and creation operators a and $a^\dagger$ in Eq. (3.1.1) with a (classical) phonon field $\varphi \in L^2(\mathbb{R}^3)$, i.e. replacing $a(f)$ with $\langle f|\varphi\rangle$ and $a^\dagger(f)$ with

$\langle\varphi|f\rangle$, we arrive at the Pekar energy

$$\begin{aligned}\mathcal{E}(\psi,\varphi) : &= \big\langle\psi\big| - \Delta_x - \langle w_x|\varphi\rangle - \langle\varphi|w_x\rangle + \|\varphi\|^2 \big|\psi\big\rangle \\ &= \int |\nabla\psi(x)|^2 \,\mathrm{d}x - \iint w_x(x')\left(\varphi(x') + \overline{\varphi(x')}\right)|\psi(x)|^2 \,\mathrm{d}x'\mathrm{d}x + \int |\varphi(x')|^2 \mathrm{d}x',\end{aligned} \tag{3.1.2}$$

where $\psi \in L^2(\mathbb{R}^3)$ is the wave-function of the electron. We further define the Pekar functional $\mathcal{F}^{\mathrm{Pek}}(\varphi) := \inf_{\|\psi\|=1} \mathcal{E}(\psi,\varphi)$ and the minimal Pekar energy $e^{\mathrm{Pek}} := \inf_\varphi \mathcal{F}^{\mathrm{Pek}}(\varphi)$. It is known that the ground state energy $E_\alpha := \inf\sigma(\mathbb{H})$, as a function of the coupling strength α, is asymptotically given by the minimal Pekar energy e^{Pek} in the limit $\alpha \to \infty$ [1, 29]. More precisely, one has $e^{\mathrm{Pek}} \geqslant E_\alpha = e^{\mathrm{Pek}} + O_{\alpha\to\infty}\left(\alpha^{-\frac{1}{5}}\right)$, as shown in [79]. In this work we are going to verify the prediction in the physics literature [123, 2, 3] that the sub-leading term in this energy asymptotics is actually of order α^{-2} with a rather explicit pre-factor

$$E_\alpha = e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + o_{\alpha\to\infty}\left(\alpha^{-2}\right), \tag{3.1.3}$$

where φ^{Pek} is a minimizer of $\mathcal{F}^{\mathrm{Pek}}$ and H^{Pek} is the Hessian of $\mathcal{F}^{\mathrm{Pek}}$ at φ^{Pek} restricted to real-valued functions $\varphi \in L^2_{\mathbb{R}}(\mathbb{R}^3)$, i.e. H^{Pek} is an operator on $L^2(\mathbb{R}^3)$ defined by

$$\langle\varphi|H^{\mathrm{Pek}}|\varphi\rangle = \lim_{\epsilon\to 0}\frac{1}{\epsilon^2}\left(\mathcal{F}^{\mathrm{Pek}}(\varphi^{\mathrm{Pek}} + \epsilon\varphi) - e^{\mathrm{Pek}}\right) \tag{3.1.4}$$

for all $\varphi \in L^2_{\mathbb{R}}(\mathbb{R}^3)$. The prediction in Eq. (3.1.3) has been verified previously for polaron models either confined to a bounded region of $\mathbb{R}^3$ [40] or to a three-dimensional torus [37]. The methods presented there exhibit substantial problems regarding their extension to the unconfined case, however. In this paper we present a new approach, which is partly based on techniques previously developed in the study of Bose–Einstein condensation and the validity of Bogoliubov's approximation for Bose gases [71, 72, 16] in the mean-field limit. We employ a localization method for the phonon field, which breaks the translation-invariance and effectively reduces the problem to the confined case, allowing for an application of some of the methods developed in [40, 37]. Our main result is the following Theorem 3.1.1 where we verify the lower bound on E_α in Eq. (3.1.3) .

Theorem 3.1.1. *Let E_α be the ground state energy of $\mathbb{H}$ in* (3.1.1)*. For any $s < \frac{1}{29}$*

$$E_\alpha \geqslant e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] - \alpha^{-(2+s)} \tag{3.1.5}$$

for all $\alpha \geqslant \alpha(s)$, where $\alpha(s) > 0$ is a suitable constant.

As an intermediate result, which might be of independent interest, we will establish the existence of a family of approximate ground states, by which we mean states whose energy is given by the right side of (3.1.3), exhibiting complete Bose–Einstein condensation with respect to a minimizer φ^{Pek} of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$. We refer to Theorem 3.3.13 for a precise statement.

In contrast to the lower bound, the proof of the upper bound on E_α in Eq. (3.1.3) is essentially the same as for confined polarons [40, 37] and can be obtained by the same methods. It is also contained as a special case in [91], where it has been verified that the ground state energy $E_\alpha(P)$ as a function of the (conserved) total momentum P can be bounded from above by

$$E_\alpha(P) \leqslant e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \frac{|P|^2}{2\alpha^4 m} + C_\epsilon \alpha^{-\frac{5}{2}+\epsilon}, \tag{3.1.6}$$

where $m := \frac{2}{3}\|\nabla\varphi^{\mathrm{Pek}}\|^2$ and $\epsilon > 0$, with C_ϵ a suitable constant. Since $E_\alpha = E_\alpha(0)$ [50, 30, 93], Theorem 3.1.1 in combination with Eq. (4.1.3) for the specific case $P = 0$ concludes the proof of Eq. (3.1.3). Combining (4.1.3) with Theorem 3.1.1, one further obtains an upper bound on the increment $E_\alpha(P) - E_\alpha$, a quantity related to the effective mass of the polaron [63, 77, 119, 9]. In the second part [18] we will discuss, in analogy to Theorem 3.1.1, the corresponding lower bound on $E_\alpha(P)$.

The proof of Eq. (3.1.3) for confined systems in [40, 37] requires an asymptotically correct local quadratic lower bound on the Pekar functional $\mathcal{F}^{\mathrm{Pek}}(\varphi)$ for configurations close to a minimizer, as well as a sufficiently strong quadratic lower bound valid for all configurations. While our proof of Theorem 3.1.1 makes use of a local quadratic lower bound as well, we believe that in the translation-invariant setting any globally valid quadratic lower bound cannot be sufficiently strong, and therefore new ideas are necessary. As we explain in the following, we circumvent this problem by constructing an approximate ground state Ψ, which is essentially supported close to a minimizer of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$, and consequently we only require a locally valid quadratic lower bound.

Proof strategy of Theorem 3.1.1. Even though we want to verify a lower bound on E_α, let us first discuss how test functions providing an asymptotically correct upper bound are expected to look like. In the following let $(\psi^{\mathrm{Pek}}, \varphi^{\mathrm{Pek}})$ denote a minimizer of the Pekar energy $\mathcal{E}$ defined in Eq. (3.1.2). It has been established in [76] that all other minimizers are given by translations $\varphi_x^{\mathrm{Pek}}(x') := \varphi^{\mathrm{Pek}}(x' - x)$ and $\psi_x^{\mathrm{Pek}}(x') := e^{i\theta}\psi^{\mathrm{Pek}}(x' - x)$ of φ^{Pek} and $e^{i\theta}\psi^{\mathrm{Pek}}$, where θ is an arbitrary phase. W.l.o.g. let us denote in the following by $(\psi^{\mathrm{Pek}}, \varphi^{\mathrm{Pek}})$ the unique minimizer of $\mathcal{E}$ such that φ^{Pek} is radial and ψ^{Pek} is non-negative. Then all the product states of the form $\psi_x^{\mathrm{Pek}} \otimes \Omega_{\varphi_x^{\mathrm{Pek}}}$ with $x \in \mathbb{R}^3$, where $\Omega_{\varphi_x^{\mathrm{Pek}}}$ is the coherent state corresponding to φ_x^{Pek} (defined by $a(w)\Omega_\varphi = \langle w|\varphi\rangle\Omega_\varphi$ for all $w \in L^2(\mathbb{R}^3)$), have the asymptotically correct leading term in the energy $\langle \psi_x^{\mathrm{Pek}} \otimes \Omega_{\varphi_x^{\mathrm{Pek}}} | \, \mathbb{H} \, | \psi_x^{\mathrm{Pek}} \otimes \Omega_{\varphi_x^{\mathrm{Pek}}} \rangle = e^{\mathrm{Pek}}$. By taking convex combinations of these states on the level of density matrices, we can construct a large family of low energy states

$$\Gamma_\mu := \int_{\mathbb{R}^3} |\psi_x^{\mathrm{Pek}} \otimes \Omega_{\varphi_x^{\mathrm{Pek}}}\rangle\langle\psi_x^{\mathrm{Pek}} \otimes \Omega_{\varphi_x^{\mathrm{Pek}}}| \, \mathrm{d}\mu(x)$$

for any given probability measure μ on $\mathbb{R}^3$. Clearly, Γ_μ exhibits the correct leading energy $\langle \mathbb{H} \rangle_{\Gamma_\mu} = e^{\mathrm{Pek}}$. Our proof of the lower bound given in Eq. (3.1.5) relies on the observation that asymptotically as $\alpha \to \infty$, any low energy state Ψ is of the form Γ_μ with a suitable probability measure μ on $\mathbb{R}^3$. Since we only need this statement for the phonon part of Ψ, we will verify the weaker statement

$$\mathrm{Tr}_{\mathrm{electron}}\big[\,|\Psi\rangle\langle\Psi|\,\big] \approx \int_{\mathbb{R}^3} |\Omega_{\varphi_x^{\mathrm{Pek}}}\rangle\langle\Omega_{\varphi_x^{\mathrm{Pek}}}| \, \mathrm{d}\mu(x)$$

instead, see Theorem 3.3.2 for a precise formulation. This statement is analogous to a version of the quantum de Finetti theorem used in [71] in order to verify the Hartree approximation for Bose gases in a general setting. The main technical challenge of this paper will be the construction of approximate ground states Ψ where the corresponding measure is a delta measure, $\mu = \delta_0$, i.e. the construction of states where the phonon part is essentially given by a single coherent state $\Omega_{\varphi^{\mathrm{Pek}}}$. The method presented here is based on a grand-canonical version of the localization techniques previously developed for translation-invariant Bose gases in [16], and in analogy to the concept of Bose–Einstein condensation we say that such states satisfy (complete) condensation with respect to the Pekar minimizer φ^{Pek}. Heuristically this means that only field configurations φ close to the minimizer φ^{Pek} are relevant, hence the translational degree of freedom has been eliminated and the system is effectively confined.

Based on this observation we can adapt the strategy developed for confined polarons in [40, 37], which starts by introducing an ultraviolet regularization in the interaction w_x with the aid of a momentum cut-off Λ, leading to the study of the truncated Hamiltonian $\mathbb{H}_\Lambda$. Using a lower bound on the excitation energy $\mathcal{F}^{\mathrm{Pek}}(\varphi) - e^{\mathrm{Pek}}$ that is, up to a symplectic transformation, quadratic in the field variables φ and valid for all φ close to the minimizer φ^{Pek}, one can bound the truncated Hamiltonian from below by an operator that is, up to a unitary transformation, quadratic in the creation and annihilation operators. The lower bound is only valid, however, if tested against a state satisfying (complete) condensation in φ^{Pek}. Finally an explicit diagonalization of this quadratic operator yields the desired lower bound in Eq. (3.1.5).

The symplectic transformation on the phase space $L^2(\mathbb{R}^3)$, respectively the corresponding unitary transformation on the Hilbert space $\mathcal{F}\left(L^2(\mathbb{R}^3)\right)$, is one of the key novel ingredients in our proof. It turns out to be necessary due to the presence of the translational symmetry, which makes it impossible to find a non-trivial positive semi-definite quadratic lower bound on $\mathcal{F}^{\mathrm{Pek}}(\varphi) - e^{\mathrm{Pek}}$. This issue has already been addressed in the study of a polaron on the three dimensional torus [37], where a different coordinate transformation is used, however. The symplectic/unitary transformation presented in this paper is an adaptation of the one used in the study of translation-invariant Bose gases in [16].

Outline. The paper is structured as follows. In Section 3.2 we will introduce an ultraviolet cut-off as well as a discretization in momentum space, and provide estimates on the energy cost associated with such approximations. Section 3.3 then contains our main technical result Theorem 3.3.13, in which we verify the existence of approximate ground states satisfying (complete) condensation with respect to a minimizer φ^{Pek} of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$. Subsequently we will discuss a large deviation estimate for such condensates in Section 3.4, quantifying the heuristic picture that only configurations close to the point of condensation matter. In Section 3.5 we then discuss properties of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$. In particular, we will discuss quadratic approximations around the minimizer φ^{Pek} as well as lower bounds that are, up to a coordinate transformation, quadratic in φ. Together with the error estimates from Section 3.2 and the large deviation estimate from Section 3.4, applied to the approximate ground state constructed in Section 3.3, this will allow us to verify our main Theorem 3.1.1 in Section 3.6. The subsequent Section 3.7 contains the proof of Theorem 3.3.2, which can be interpreted as a version of the quantum de Finetti theorem adapted to our setting. Finally, Appendices 3.8 and 3.9 contain auxiliary results concerning the Pekar minimizer φ^{Pek} and the projections introduced in Section 3.2, respectively.

3.2 Models with Cut-off

In this section we will estimate the effect of the introduction of an ultraviolet cut-off, as well as a discretization in momentum space, on the ground state energy, following similar ideas as in [79, 40, 37]. We will eventually apply these results for two different levels of coarse graining, a rough scale used in the proof of Theorem 3.3.2 in Section 3.7, which applies to low energy states with energy $e^{\mathrm{Pek}} + o_{\alpha\to\infty}(1)$, and a fine scale precise enough to yield the correct ground state energy up to errors of order $o_{\alpha\to\infty}(\alpha^{-2})$, see the proof of Theorem 3.1.1 in Section 3.6.

Definition 3.2.1. Given parameters $0 < \ell < \Lambda$, let us define for $z \in 2\ell\,\mathbb{Z}^3\backslash\{0\}$ the cubes $C_z := [z_1 - \ell, z_1 + \ell) \times [z_2 - \ell, z_2 + \ell) \times [z_3 - \ell, z_3 + \ell)$, and let $z^1, .., z^N$ be an enumeration of the set of all $z = (z_1, z_2, z_3) \in 2\ell\,\mathbb{Z}^3\backslash\{0\}$ such that $C_z \subset B_\Lambda(0)$, where $B_r(0)$ is the (open) ball of radius r around the origin. Then we define the orthonormal system $e_n \in L^2(\mathbb{R}^3)$ as

$$e_n(x) := \frac{1}{\sqrt{(2\pi)^3 \int_{C_{z^n}} \frac{1}{|k|^2}\,\mathrm{d}k}} \int_{C_{z^n}} \frac{e^{i\,k\cdot x}}{|k|}\,\mathrm{d}k,$$

as well as the translated system $e_{y,n}(x) := e_n(x-y)$ and the orthogonal projection $\Pi^y_{\Lambda,\ell}$ onto the space spanned by $\{e_{y,1}, \ldots, e_{y,N}\}$. Furthermore we denote with Π_Λ the projection onto the spectral subspace of momenta $|k| \leqslant \Lambda$.

Lemma 3.2.2. *Let $w_x(x') := \pi^{-\frac{3}{2}}|x'-x|^{-2}$. Then we obtain for $0 < \ell < \Lambda$ and $x, y \in \mathbb{R}^3$ the following estimate on the L^2 norm*

$$\left\|\Pi_\Lambda w_x - \Pi^y_{\Lambda,\ell} w_x\right\| \lesssim |x-y|\ell\sqrt{\Lambda} + \sqrt{\ell}.$$

Proof. With $\widehat{\cdot}$ denoting Fourier transformation, we have

$$\sqrt{2\pi^2}\,\widehat{\Pi^y_{\Lambda,\ell} w_x}(k) = \sum_{n=1}^{N} \frac{1}{\int_{C_{z^n}} \frac{1}{|k'|^2}\mathrm{d}k'} \int_{C_{z^n}} \frac{e^{ik'\cdot(y-x)}}{|k'|^2}\mathrm{d}k'\,\frac{1}{|k|}\mathbb{1}_{C_{z^n}}(k),$$

where we have used that $\widehat{\Pi_\Lambda w_x}(k) = \frac{1}{\sqrt{2\pi^2}|k|}\mathbb{1}_{B_\Lambda(0)}(k)$. Defining the function $\sigma_n(k,x,y) := \frac{1}{\int_{C_{z^n}} \frac{1}{|k'|^2}\mathrm{d}k'} \int_{C_{z^n}} \frac{e^{ik'\cdot(y-x)} - e^{ik\cdot(y-x)}}{|k'|^2}\mathrm{d}k'$, we further have

$$\sqrt{2\pi^2}\left(\widehat{\Pi^y_{\Lambda,\ell} w_x}(k) - \widehat{\Pi_\Lambda w_x}(k)\right) = \sum_{n=1}^{N} \sigma_n(k,x,y)\frac{1}{|k|}\mathbb{1}_{C_{z^n}}(k) - \frac{1}{|k|}\mathbb{1}_A(k)$$

with $A := B_\Lambda(0)\backslash\left(\bigcup_{n=1}^N C_{z^n}\right)$. Making use of the estimate $|\sigma_n(k,x,y)|^2 \leqslant |y-x|^2 \max_{k'\in C_{z^n}} |k'-k|^2 \leqslant 12|x-y|^2\ell^2$ for $k \in C_{z^n}$, we therefore obtain

$$\sum_{n=1}^{N} \int_{C_{z^n}} |\sigma_n(k,x,y)|^2 \frac{1}{|k|^2}\mathrm{d}k \leqslant 12|x-y|^2\ell^2 \int_{|k|\leqslant\Lambda} \frac{1}{|k|^2}\mathrm{d}k = 48\pi|x-y|^2\ell^2\Lambda.$$

Since $A \subset B_{2\ell} \cup B_\Lambda\backslash B_{\Lambda-4\ell}$ we consequently have $\int_A \frac{1}{|k|^2}\mathrm{d}k \lesssim \ell$. ∎

Definition 3.2.3. For $y \in \mathbb{R}^3$, $0 < \ell < \Lambda$, let us define the cut-off Hamiltonians

$$\mathbb{H}^y_{\Lambda,\ell} := -\Delta_x - a\left(\Pi^y_{\Lambda,\ell} w_x\right) - a^\dagger\left(\Pi^y_{\Lambda,\ell} w_x\right) + \mathcal{N}, \tag{3.2.1}$$

$$\mathbb{H}_\Lambda := -\Delta_x - a\left(\Pi_\Lambda w_x\right) - a^\dagger\left(\Pi_\Lambda w_x\right) + \mathcal{N}. \tag{3.2.2}$$

These Hamiltonians can be interpreted as the restriction of $\mathbb{H}$ (in the quadratic form sense) to states where only the phonon modes in $\Pi^y_{\Lambda,\ell}L^2(\mathbb{R}^3)$, respectively $\Pi_\Lambda L^2(\mathbb{R}^3)$, are occupied. In particular, this implies that $\inf\sigma(\mathbb{H}^y_{\Lambda,\ell}) \geqslant E_\alpha$ as well as $\inf\sigma(\mathbb{H}_\Lambda) \geqslant E_\alpha$. In the following we shall quantify the energy increase due to the introduction of the cut-offs.

Note that the α-dependence of the Hamiltonians $\mathbb{H}$, $\mathbb{H}^y_{\Lambda,\ell}$ and $\mathbb{H}_\Lambda$ only enters through the rescaled canonical commutation relations $\left[a(f), a^\dagger(g)\right] = \alpha^{-2}\langle f|g\rangle$ satisfied by the creation and annihilation operators $a^\dagger$ and a, and we will usually suppress the α dependency in our notation for the sake of readability. In the rest of this paper, we will always assume that α is a parameter satisfying $\alpha \geqslant 1$ and, in case it is not stated otherwise, estimates hold uniformly in this parameter for $\alpha \to \infty$, i.e. we write $X \lesssim Y$ in case there exist constants $C, \alpha_0 > 0$ such that $X \leqslant CY$ for all $\alpha \geqslant \alpha_0$.

The proof of the subsequent Lemma 3.2.4 closely follows the arguments in [80, 79], where it was shown that $\mathbb{H}$ is bounded from below and well approximated by an operator containing only finitely many phonon modes. For the sake of completeness we will illustrate the proof, which is based on the Lieb–Yamazaki commutator method, see [80]. In the following Lemma 3.2.4, we will use the identification $L^2(\mathbb{R}^3)\otimes\mathcal{F}(L^2(\mathbb{R}^3)) \cong L^2(\mathbb{R}^3, \mathcal{F}(L^2(\mathbb{R}^3)))$, in order to represent elements $\Psi \in L^2(\mathbb{R}^3)\otimes\mathcal{F}(L^2(\mathbb{R}^3))$ as functions $x \mapsto \Psi(x)$ with values in $\mathcal{F}(L^2(\mathbb{R}^3))$, allowing us to define the support $\operatorname{supp}(\Psi)$ as the closure of $\{x \in \mathbb{R}^3 : \Psi(x) \neq 0\}$.

Lemma 3.2.4. *We have for all $0 < \ell < \Lambda \leqslant K$ and $L > 0$, and states Ψ with $\operatorname{supp}(\Psi) \subset B_L(y)$ the estimate*

$$\left|\langle\Psi|\mathbb{H}_K - \mathbb{H}^y_{\Lambda,\ell}|\Psi\rangle\right| \lesssim \left(L\ell\sqrt{\Lambda} + \sqrt{\ell} + \sqrt{\frac{1}{\Lambda} - \frac{1}{K}}\right)\langle\Psi| - \Delta_x + \mathcal{N} + 1|\Psi\rangle. \tag{3.2.3}$$

Furthermore, there exists a constant $d > 0$ such that

$$\mathbb{H}_K \geqslant -\frac{d}{t^2} - t\left(\mathcal{N} + \alpha^{-2}\right), \tag{3.2.4}$$

$$\mathbb{H}_K \geqslant -d + \frac{1}{2}\left(-\Delta_x + \mathcal{N}\right) \tag{3.2.5}$$

for all $t > 0$, $K \geqslant 0$ and $\alpha \geqslant 1$.

Proof. Let us define the functions u^n_x by $\widehat{u^n_x}(k) := \frac{1}{\sqrt{2}\pi^2}\mathbb{1}_{B_K(0)\setminus B_\Lambda(0)}(k)\frac{k_n e^{ik\cdot x}}{|k|^3}$. We have $a\left(\partial_{x_n}u^n_x\right) - a^\dagger\left(\partial_{x_n}u^n_x\right) = \left[\partial_{x_n}, a\left(u^n_x\right) - a^\dagger\left(u^n_x\right)\right]$ and

$$\begin{aligned}\pm i\left[\partial_{x_n}, a\left(u^n_x\right) - a^\dagger\left(u^n_x\right)\right] &\leqslant -2\epsilon\partial^2_{x_n} + \frac{1}{\epsilon}\left(a(u^n_x)^\dagger a(u^n_x) + a(u^n_x)a(u^n_x)^\dagger\right)\\ &\leqslant -2\epsilon\,\partial^2_{x_n} + \frac{\|u^n_x\|^2}{\epsilon}\left(2\mathcal{N} + \alpha^{-2}\right) = 2\|u^n_x\|\left(-\partial^2_{x_n} + \mathcal{N} + \frac{1}{2}\alpha^{-2}\right),\end{aligned}$$

where we have applied the Cauchy–Schwarz inequality in the first line and used the specific choice $\epsilon := \|u^n_x\|$ in the last identity. Note that the L^2-norm $\|u^n_x\|$ is independent of x, and furthermore we can express $\pm\left(\mathbb{H}^y_{\Lambda,\ell} - \mathbb{H}_K\right)$ as

$$\begin{aligned}&\pm a\left(\Pi_\Lambda w_x - \Pi^y_{\Lambda,\ell}w_x\right) \pm a^\dagger\left(\Pi_\Lambda w_x - \Pi^y_{\Lambda,\ell}w_x\right) \pm i\sum_{n=1}^{3}\left(a\left(\partial_{x_n}u^n_x\right) - a^\dagger\left(\partial_{x_n}u^n_x\right)\right)\\ &\leqslant 2\left\|\Pi_\Lambda w_x - \Pi^y_{\Lambda,\ell}w_x\right\|(1 + \mathcal{N}) + 2\max_{n\in\{1,2,3\}}\|u^n_x\|\left(-\Delta_x + 3\mathcal{N} + \frac{3}{2}\alpha^{-2}\right).\end{aligned}$$

This concludes the proof of Eq. (3.2.3), since we have $\|\Pi_\Lambda w_x - \Pi^y_{\Lambda,\ell} w_x\| \lesssim L\ell\sqrt{\Lambda} + \sqrt{\ell}$ for all $x \in \operatorname{supp}(\Psi)$ by Lemma 3.2.2 and $\|u^n_x\|^2 \lesssim \frac{1}{\Lambda} - \frac{1}{K}$. The other statements in Eqs. (3.2.4) and (3.2.5) can be verified similarly, using the decomposition $\Pi_K w_x = \Pi_{K'} w_x + \sum_{n=1}^3 \frac{1}{i}\partial_{x_n} g^n_x$ with $\widehat{g^n_x}(k) := \frac{1}{\sqrt{2\pi^2}} \mathbb{1}_{B_K(0)\setminus B_{K'}(0)}(k) \frac{k_n e^{ik\cdot x}}{|k|^3}$ where $K' \leqslant K$ is large enough such that $\|g^n_x\| < \frac{1}{12}$. ∎

The subsequent Theorem 3.2.5 is a direct consequence of the results in [40] and [97, 37], where multiple Lieb–Yamazaki bounds as well as a suitable Gross transformation are used in order to verify that the energy cost of introducing an ultraviolet cut-off $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ with $\sigma > 0$ is only of order $o_{\alpha\to\infty}(\alpha^{-2})$. Combined with an application of the IMS localization formula, as was also done in [79], one obtains the following.

Theorem 3.2.5. *Given a constant $0 < \sigma \leqslant \frac{1}{4}$, let us introduce the momentum cut-off $\Lambda := \alpha^{\frac{4}{5}(1+\sigma)}$ as well as the space cut-off $L := \alpha^{1+\sigma}$. Then there exists a sequence of states $\Psi^\diamond_\alpha$ satisfying $\langle \Psi^\diamond_\alpha | \mathbb{H}_\Lambda | \Psi^\diamond_\alpha \rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$ and $\operatorname{supp}(\Psi^\diamond_\alpha) \subset B_L(0)$, where E_α is the ground state energy of $\mathbb{H}$.*

Proof. We start by arguing that

$$\inf \sigma(\mathbb{H}_\Lambda) - E_\alpha \lesssim \Lambda^{-\frac{5}{2}} + \alpha^{-1}\Lambda^{-\frac{3}{2}} + \alpha^{-2}\Lambda^{-\frac{1}{2}} \tag{3.2.6}$$

for large α. An analogous bound was shown in [40, Prop. 7.1] in the confined case, where additional powers of $\ln \Lambda$ appear due to complications coming from the boundary. In the translation-invariant setting on a torus, (3.2.6) is shown [37, Prop. 4.5], and that proof applies verbatim also in the unconfined case considered here (as has been worked out also in [97]).

By our choice of $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$, we immediately obtain $\inf \sigma(\mathbb{H}_\Lambda) - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$. Hence there exists a state Ψ satisfying $\langle \Psi | \mathbb{H}_\Lambda | \Psi \rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$. In order to construct a state which is furthermore supported on the ball $B_L(0)$, let χ be a non-negative $H^1(\mathbb{R}^3)$ function with $\int \chi(y)^2 \mathrm{d}y = 1$ and $\operatorname{supp}(\chi) \subset B_1(0)$. We define $\Psi_y(x) := L^{-\frac{3}{2}} \chi(L^{-1}(x-y)) \Psi(x)$ for $y \in \mathbb{R}^3$ and compute, using the IMS identity,

$$\begin{aligned}\int \langle \Psi_y | \mathbb{H}_\Lambda | \Psi_y \rangle \, \mathrm{d}y &= \langle \Psi | \mathbb{H}_\Lambda | \Psi \rangle + L^{-3} \iint \left| \nabla_x \chi\left(L^{-1}(x-y)\right)\right|^2 \mathrm{d}y \, \|\Psi(x)\|^2 \mathrm{d}x \\ &= \langle \Psi | \mathbb{H}_\Lambda | \Psi \rangle + L^{-2} \|\nabla \chi\|^2 = E_\alpha + O_{\alpha\to\infty}\left(\alpha^{-2(1+\sigma)}\right),\end{aligned}$$

see also [79] where an explicit choice of χ is used. Since $\int \|\Psi_y\|^2 \mathrm{d}y = 1$, there clearly exists a $y \in \mathbb{R}^3$ such that the state $\Psi^\diamond_\alpha := \|\Psi_y\|^{-1} \Psi_y$ satisfies $\langle \Psi^\diamond_\alpha | \mathbb{H}_\Lambda | \Psi^\diamond_\alpha \rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$. By the translation invariance of $\mathbb{H}_\Lambda$ we can assume that $y = 0$. ∎

3.3 Construction of a Condensate

The purpose of this section is to construct a sequence of approximate ground states Ψ_α, i.e. states with $\langle \Psi_\alpha | \mathbb{H}_\Lambda | \Psi_\alpha \rangle = E_\alpha + o_{\alpha\to\infty}(\alpha^{-2})$ and Λ as in Theorem 3.2.5, that additionally satisfy complete condensation with respect to a minimizer φ^{Pek} of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$, i.e. the phonon part of Ψ_α is in a suitable sense close to a coherent state $\Omega_{\varphi^{\mathrm{Pek}}}$ with $\Omega_{\varphi^{\mathrm{Pek}}} := e^{\alpha^2 a^\dagger(\varphi^{\mathrm{Pek}}) - \alpha^2 a(\varphi^{\mathrm{Pek}})} \Omega$, where Ω is the vacuum in $\mathcal{F}(L^2(\mathbb{R}^3))$, see Lemma 3.3.12 and Theorem 3.3.13. The construction will be based on various localization procedures of the phonon field with respect to operators of the form $\widehat{F}$ defined in the subsequent Definition 3.3.1. Before we start with the localization procedures, we will discuss an asymptotic formula for the expectation value $\langle \Psi_\alpha|\widehat{F}|\Psi_\alpha\rangle$ in Theorem 3.3.2 as well as the energy cost of localizing with respect to such an operator $\widehat{F}$ in Lemma 3.3.3.

Definition 3.3.1. Given a function $F : \mathcal{M}(\mathbb{R}^3) \longrightarrow \mathbb{R}$, where $\mathcal{M}(\mathbb{R}^3)$ is the set of finite (Borel) measures on $\mathbb{R}^3$, let us define the operator $\widehat{F}$ acting on the Fock space $\mathcal{F}(L^2(\mathbb{R}^3)) = \bigoplus_{n=0}^{\infty} L^2_{\mathrm{sym}}(\mathbb{R}^{3\times n})$ as $\widehat{F} \bigoplus_{n=0}^{\infty} \Psi_n := \bigoplus_{n=0}^{\infty} F^n \Psi_n$, where

$$(F^n\Psi_n)(x^1,\dots,x^n) := F\left(\alpha^{-2}\sum_{k=1}^{n}\delta_{x^k}\right)\Psi_n(x^1,\dots,x^n)$$

and $F_0\Psi_0 = F(0)\Psi_0$, i.e. $\widehat{F}$ acts component-wise on $\bigoplus_{n=0}^{\infty} L^2_{\mathrm{sym}}(\mathbb{R}^{3\times n})$ by multiplication with the real valued function $(x^1,\dots,x^n) \mapsto F\left(\alpha^{-2}\sum_{k=1}^n \delta_{x^k}\right)$.

In order to keep the notation simple, we will allow $F : \mathcal{M}(\mathbb{R}^3) \longrightarrow \mathbb{R}$ to act on non-negative $L^1(\mathbb{R}^3)$ functions $q : \mathbb{R}^3 \longrightarrow [0,\infty)$ as well by identifying them with the corresponding measure $\lambda \in \mathcal{M}(\mathbb{R}^3)$ defined as $\frac{\mathrm{d}\lambda}{\mathrm{d}x} = q(x)$.

Before we discuss the asymptotic formula for the expectation value $\langle \Psi_\alpha|\widehat{F}|\Psi_\alpha\rangle$, let us introduce a family of cut-off functions $\chi^\epsilon(a \leqslant f(x) \leqslant b)$ where $\epsilon \geqslant 0$ determines the sharpness of the cut-off. In the following let $\alpha, \beta : \mathbb{R} \longrightarrow [0,1]$ be C^∞ functions such that $\alpha^2 + \beta^2 = 1$, $\mathrm{supp}(\alpha) \subset (-\infty, 1)$ and $\mathrm{supp}(\beta) \subset (-1,\infty)$. For a given function $f : X \longrightarrow \mathbb{R}$ and constants $-\infty \leqslant a < b \leqslant \infty$, let us define the function $\chi^\epsilon(a \leqslant f \leqslant b) : X \longrightarrow [0,1]$ as

$$\chi^\epsilon(a \leqslant f(x) \leqslant b) := \begin{cases} \alpha\left(\frac{f(x)-b}{\epsilon}\right)\beta\left(\frac{f(x)-a}{\epsilon}\right), & \text{for } \epsilon > 0 \\ \mathbb{1}_{[a,b]}(f(x)), & \text{for } \epsilon = 0. \end{cases} \tag{3.3.1}$$

Note that $\sum_{j\in J} \chi^\epsilon(a_j \leqslant f(x) \leqslant b_j)^2 = 1$ in case the intervals $[a_j, b_j)$ are a disjoint partition of $\mathbb{R}$ with $-\infty \leqslant a_j < b_j \leqslant \infty$.

Similarly, we define the operator $\chi^\epsilon(a \leqslant T \leqslant b) := \int \chi^\epsilon(a \leqslant t \leqslant b)\,\mathrm{d}E(t)$, where T is a self-adjoint operator and E is the spectral measure with respect to T. Furthermore we will write $\chi(a \leqslant f \leqslant b)$, respectively $\chi(a \leqslant T \leqslant b)$, in case $\epsilon = 0$ as well as $\chi^\epsilon(a \leqslant \cdot)$ and $\chi^\epsilon(\cdot \leqslant b)$ in case $b = \infty$ or $a = -\infty$, respectively.

The proof of the following Theorem 3.3.2 will be carried out in Section 3.7. It is reminiscent of the quantum de-Finetti Theorem, and establishes in addition that for low energy states phonon field configurations are necessarily close to the set of Pekar minimizers given by $\{\varphi_x^{\mathrm{Pek}}\}_{x\in\mathbb{R}^3}$.

Theorem 3.3.2. *Given $m \in \mathbb{N}, C > 0$ and $g \in L^2(\mathbb{R}^3)$, we can find a constant $T > 0$ such that for all $\alpha \geqslant 1$ and states Ψ satisfying $\chi(\mathcal{N} \leqslant C)\Psi = \Psi$ and $\langle \Psi|\mathbb{H}_K|\Psi\rangle \leqslant e^{\mathrm{Pek}} + \delta e$ with $\delta e \geqslant 0$ and $K \geqslant \alpha^{\frac{8}{29}}$, there exists a probability measure μ on $\mathbb{R}^3$, with the property*

$$\left|\left\langle \Psi|\widehat{F}|\Psi\right\rangle - \int_{\mathbb{R}^3} F\left(|\varphi_x^{\mathrm{Pek}}|^2\right)\mathrm{d}\mu(x)\right| \leqslant T\|f\|_\infty \max\left\{\sqrt{\delta e}, \alpha^{-\frac{2}{29}}\right\} \tag{3.3.2}$$

for all $F : \mathcal{M}(\mathbb{R}^3) \longrightarrow \mathbb{R}$ of the form $F(\rho) = \int \dots \int f(x_1, \dots, x_m)\, \mathrm{d}\rho(x_1) \dots \mathrm{d}\rho(x_m)$ with bounded $f : \mathbb{R}^{3\times m} \longrightarrow \mathbb{R}$, and furthermore

$$\left| \left\langle \Psi \middle| W_g^{-1} \mathcal{N} W_g \middle| \Psi \right\rangle - \int_{\mathbb{R}^3} \left\| \varphi_x^{\mathrm{Pek}} - g \right\|^2 \mathrm{d}\mu(x) \right| \leqslant T \max\left\{ \sqrt{\delta e}, \alpha^{-\frac{2}{29}} \right\}, \qquad (3.3.3)$$

where W_g is the Weyl operator characterized by $W_g^{-1} a(h) W_g = a(h) - \langle h|g\rangle$.

In the subsequent Lemma 3.3.3 we introduce a generalized IMS-type estimate quantifying the energy cost of localizing with respect to an $\widehat{F}$-operator, similar to the generalized IMS results in [78, Theorem A.1] and [72, Proposition 6.1]. In order to formulate the result, let us define for a given subset $\Omega \subset \mathcal{M}(\mathbb{R}^3)$ and a (quadratic) partition of unity $\mathcal{P} = \{F_j : \mathcal{M}(\mathbb{R}^3) \longrightarrow \mathbb{R} : j \in J\}$, i.e. $0 \leqslant F_j \leqslant 1$ and $\sum_{j\in J} F_j^2 = 1$, the variation of this partition on Ω as

$$V_\Omega(\mathcal{P}) := \alpha^4 \sup_{\rho\in\Omega, y\in\mathbb{R}^3} \sum_{j\in J} \left| F_j\left(\rho + \alpha^{-2}\delta_y\right) - F_j(\rho) \right|^2.$$

Lemma 3.3.3. *There exists a constant $c > 0$, such that for any partition of unity $\mathcal{P} = \{F_j : \mathcal{M}(\mathbb{R}^3) \longrightarrow \mathbb{R} : j \in J\}$, $\Omega \subset \mathcal{M}(\mathbb{R}^3)$, $K > 0$, $\alpha \geqslant 1$ and state Ψ with $\widehat{\mathbb{1}_\Omega}\Psi = \Psi$*

$$\left| \sum_{j\in J} \left\langle \widehat{F_j}\Psi \middle| \mathbb{H}_K \middle| \widehat{F_j}\Psi \right\rangle - \langle \Psi | \mathbb{H}_K | \Psi \rangle \right| \leqslant c\sqrt{K}\alpha^{-4} V_\Omega(\mathcal{P}) \left\langle \Psi \middle| \sqrt{\mathcal{N} + \alpha^{-2}} \middle| \Psi \right\rangle. \qquad (3.3.4)$$

Furthermore given $M > 0$, there exists a constant $c' > 0$ such that we have for any $\varphi \in L^2(\mathbb{R}^3)$ satisfying $\|\varphi\| \leqslant M$, partition of unity $\{f_j : \mathbb{R} \longrightarrow \mathbb{R} : j \in J\}$, $K \geqslant 1$, $\alpha \geqslant 1$ and state Ψ

$$\left| \sum_{j\in J} \langle \Psi_j | \mathbb{H}_K | \Psi_j \rangle - \langle \Psi | \mathbb{H}_K | \Psi \rangle \right| \leqslant c' \sqrt{K} \alpha^{-4} V_{\mathcal{M}(\mathbb{R}^3)}(\mathcal{P}') \left\langle \Psi \middle| \sqrt{\mathcal{N} + 1} \middle| \Psi \right\rangle,$$

where we define $\Psi_j := f_j\left(W_\varphi^{-1} \mathcal{N} W_\varphi\right) \Psi$ with W_φ being the corresponding Weyl operator and $\mathcal{P}' := \{F_j' : \mathcal{M}(\mathbb{R}^3) \longrightarrow \mathbb{R} : j \in J\}$ with $F_j'(\rho) := f_j(\int \mathrm{d}\rho)$.

Proof. By applying the IMS identity, we obtain

$$\sum_{j\in J} \widehat{F_j} \mathbb{H}_K \widehat{F_j} - \mathbb{H}_K = \frac{1}{2} \sum_{j\in J} \left[\left[\widehat{F_j}, \mathbb{H}_K \right], \widehat{F_j} \right] = - \sum_{j\in J} \mathfrak{Re} \left[\left[\widehat{F_j}, a(\Pi_K w_x) \right], \widehat{F_j} \right],$$

where we have used the fact that F_j commutes with $-\Delta_x$ and $\mathcal{N}$ in the last identity. Since a state Ψ is a function with values in $\mathcal{F}(L^2(\mathbb{R}^3)) = \bigoplus_{n=0}^{\infty} L^2_{\mathrm{sym}}(\mathbb{R}^{3\times n})$, we can represent it as $\Psi = \bigoplus_{n=0}^{\infty} \Psi_n$ where $\Psi_n(y, x^1, \dots, x^n)$ is a function of the electron variable y and the n phonon coordinates $x^k \in \mathbb{R}^3$. In order to simplify the notation, we will suppress the dependence on the electron variable y in our notation. By an explicit computation, we obtain $\left[\left[\widehat{F}, a(v) \right], \widehat{F} \right] \bigoplus_{n=0}^{\infty} \Psi_n = - \bigoplus_{n=0}^{\infty} \sqrt{\frac{n+1}{\alpha^2}} \Psi_n'$ with

$$\Psi_n'(x^1, \dots, x^n) = \int \left[F\left(\alpha^{-2} \sum_{k=1}^{n+1} \delta_{x^k} \right) - F\left(\alpha^{-2} \sum_{k=1}^{n} \delta_{x^k} \right) \right]^2 v(x^{n+1}) \Psi_{n+1}(x^1, \dots, x^{n+1}) \mathrm{d}x^{n+1},$$

for $v \in L^2(\mathbb{R}^3)$ and $F : \mathcal{M}(\mathbb{R}^3) \longrightarrow \mathbb{R}$. By the definition of $V_\Omega(\mathcal{P})$ we obtain that

$$\sigma(x^1,\dots,x^{n+1}) := \sum_{j\in J}\left[F_j\Big(\alpha^{-2}\sum_{k=1}^{n+1}\delta_{x^k}\Big) - F_j\Big(\alpha^{-2}\sum_{k=1}^{n}\delta_{x^k}\Big)\right]^2 \leqslant \alpha^{-4}V_\Omega(\mathcal{P})$$

for all $x^{n+1} \in \mathbb{R}^3$ and every $(x^1,\dots,x^n) \in \mathbb{R}^{3n}$ with $\alpha^{-2}\sum_{k=1}^n \delta_{x^k} \in \Omega$. Hence we can estimate $\left|\left\langle \Psi\middle|\sum_{j\in J}\mathfrak{Re}\left[\left[\widehat{F}_j, a(v)\right], \widehat{F}_j\right]\middle|\Psi\right\rangle\right|$, using the notation $X = (x^1,\dots,x^n)$, by

$$\begin{aligned}
&\sum_{n=0}^{\infty}\sqrt{\frac{n+1}{\alpha^2}}\int|\Psi_n(X)|\int\sigma(X,x^{n+1})|v(x_{n+1})\Psi_{n+1}(X,x_{n+1})|\mathrm{d}x_{n+1}\mathrm{d}X\\
&\quad\leqslant \alpha^{-5}V_\Omega(\mathcal{P})\sum_{n=0}^{\infty}\sqrt{n+1}\int|\Psi_n(X)|\int|v(x_{n+1})\Psi_{n+1}(X,x_{n+1})|\mathrm{d}x^{n+1}\mathrm{d}X\\
&\quad\leqslant \alpha^{-5}V_\Omega(\mathcal{P})\,\|v\|\sum_{n=0}^{\infty}\sqrt{n+1}\|\Psi_n\|\,\|\Psi_{n+1}\| \leqslant \alpha^{-4}V_\Omega(\mathcal{P})\,\|v\|\left\langle\Psi\middle|\sqrt{\mathcal{N}+\alpha^{-2}}\middle|\Psi\right\rangle.
\end{aligned}$$

This concludes the proof of Eq. (3.3.4), using the concrete choice $v := \Pi_K w_x$, since $\|\Pi_K w_x\|^2 = \frac{1}{2\pi^2}\int_{|k|\leqslant K}\frac{1}{|k|^2} = \frac{2}{\pi}K$.

In order to verify the second statement we apply the unitary transformation W_φ to the operator $\mathbb{X} := \sum_{j\in J} f_j\left(W_\varphi^{-1}\mathcal{N}W_\varphi\right)\mathbb{H}_K f_j\left(W_\varphi^{-1}\mathcal{N}W_\varphi\right) - \mathbb{H}_K$ and compute

$$\begin{aligned}
W_\varphi\mathbb{X}\,W_\varphi^{-1} &= \frac{1}{2}\sum_{j\in J}\left[\left[f_j(\mathcal{N}), W_\varphi\mathbb{H}_K W_\varphi^{-1}\right], f_j(\mathcal{N})\right]\\
&= \sum_{j\in J}\mathfrak{Re}\left[\left[f_j(\mathcal{N}), a(\varphi-\Pi_K w_x)\right], f_j(\mathcal{N})\right] = \sum_{j\in J}\mathfrak{Re}\left[\left[\widehat{F}'_j, a(v)\right], \widehat{F}'_j\right],
\end{aligned}$$

where we defined $v := \varphi - \Pi_K w_x$ and applied the definition $F'_j(\rho) = f_j\left(\int\mathrm{d}\rho\right)$. We know from the previous estimates that

$$\pm\sum_{j\in J}\mathfrak{Re}\left[\left[f_j(\mathcal{N}), a(v)\right], f_j(\mathcal{N})\right] \leqslant \alpha^{-4}V_{\mathcal{M}(\mathbb{R}^3)}(\mathcal{P}')\,\|v\|\sqrt{\mathcal{N}+\alpha^{-2}}.$$

Clearly $\|v\| \leqslant \|\varphi\| + \|\Pi_K w_x\| \lesssim \sqrt{K}$ for $K \geqslant 1$, and consequently

$$\begin{aligned}
&\left|\sum_{j\in J}\langle\Psi_j|\mathbb{H}_K|\Psi_j\rangle - \langle\Psi|\mathbb{H}_K|\Psi\rangle\right| \lesssim \sqrt{K}\alpha^{-4}V_{\mathcal{M}(\mathbb{R}^3)}(\mathcal{P}')\left\langle\Psi\middle|\sqrt{W_\varphi^{-1}\mathcal{N}W_\varphi+\alpha^{-2}}\middle|\Psi\right\rangle\\
&\qquad\lesssim \sqrt{K}\alpha^{-4}V_{\mathcal{M}(\mathbb{R}^3)}(\mathcal{P}')\left\langle\Psi\middle|\sqrt{\mathcal{N}+1}\middle|\Psi\right\rangle,
\end{aligned}$$

where we have used that $W_\varphi^{-1}\mathcal{N}W_\varphi \leqslant 2\left(\mathcal{N}+\|\varphi\|^2\right)$ and the operator-monotonicity of the square root. ■

In the following let $L := \alpha^{1+\sigma}$ and $\Lambda := \alpha^{\frac{4}{5}(1+\sigma)}$ with $0 < \sigma \leqslant \frac{1}{4}$, and let $\Psi_\alpha^\bullet$ be a sequence of states satisfying $\operatorname{supp}(\Psi_\alpha^\bullet) \subset B_L(0)$ and $\widetilde{E}_\alpha - E_\alpha \lesssim \alpha^{-\frac{4}{29}}$, where

$$\widetilde{E}_\alpha := \langle\Psi_\alpha^\bullet|\mathbb{H}_\Lambda|\Psi_\alpha^\bullet\rangle. \tag{3.3.5}$$

The exponent $\frac{4}{29}$ is chosen for convenience, as it allows to simplify the right hand side of Eq. (3.3.2) to $\|f\|_\infty \alpha^{-\frac{2}{29}}$ (using that $E_\alpha \leqslant e^{\mathrm{Pek}}$). For the proof of Theorem 3.1.1 we shall use the specific choice $\Psi_\alpha^\diamond$ from Theorem 3.2.5 for $\Psi_\alpha^\bullet$, but it will be useful in the second part to have the first two localization procedures in Lemma 3.3.4 and 3.3.5 formulated for a more general sequence $\Psi_\alpha^\bullet$.

In the following Eq. (3.3.6) and Eq. (3.3.10), we will apply localizations procedures to the given sequence $\Psi_\alpha^\bullet$ in order to construct states having additional useful properties, which we will use in Lemma 3.3.12 in order to construct a sequence of approximate ground states satisfying complete condensation. Furthermore we will quantify the energy cost of these localizations by $\langle \Psi_\alpha | \mathbb{H}_\Lambda | \Psi_\alpha \rangle - \widetilde{E}_\alpha \lesssim \alpha^{-3}$ in the Lemmata 3.3.4 and 3.3.5. In Theorem 3.3.13 we will then apply a final localization procedure, in order to lift the (weak) condensation from Lemma 3.3.12 to a strong one, following the argument in [72].

Having Lemma 3.3.3 at hand, we can verify our first localization result in Lemma 3.3.4, which allows us to restrict our attention to states Ψ'_α having a (rescaled) particle number $\mathcal{N}$ between some fixed constants c_- and c_+. To be precise, for given c_-, c_+ and ϵ' we use the function $F_*(\rho) := \chi^{\epsilon'}\left(c_- + \epsilon' \leqslant \int \mathrm{d}\rho \leqslant c_+ - \epsilon'\right)$ in order to define the states

$$\Psi'_\alpha := Z_\alpha^{-1} \widehat{F}_* \Psi_\alpha^\bullet, \tag{3.3.6}$$

with the corresponding normalization constants $Z_\alpha := \|\widehat{F}_* \Psi_\alpha^\bullet\|$. By construction we have $\chi\left(c_- \leqslant \mathcal{N} \leqslant c_+\right) \Psi'_\alpha = \Psi'_\alpha$ as well as $\mathrm{supp}\left(\Psi'_\alpha\right) \subset B_L(0)$. In the following Lemma 3.3.4 we derive an upper bound on the energy of Ψ'_α, and in addition we will investigate the large α behavior of Z_α, which will be useful in the second part.

Lemma 3.3.4. *Let $\Psi_\alpha^\bullet$ be the sequence introduced above Eq. (3.3.5). Then there exist α-independent constants $c_-, c_+, \epsilon' > 0$ such that the corresponding states Ψ'_α defined in Eq. (3.3.6) satisfy $\langle \Psi'_\alpha | \mathbb{H}_\Lambda | \Psi'_\alpha \rangle - \widetilde{E}_\alpha \lesssim \alpha^{-\frac{7}{2}}$. Furthermore, $Z_\alpha \underset{\alpha\to\infty}{\longrightarrow} 1$.*

Proof. In the following let F_* be the function defined above Eq. (3.3.6) and let us complete it to a quadratic partition of unity $\mathcal{P} := \{F_-, F_*, F_+\}$ with the aid of the functions $F_-(\rho) := \chi^{\epsilon'}\left(\int \mathrm{d}\rho \leqslant c_- + \epsilon'\right)$ and $F_+(\rho) := \chi^{\epsilon'}\left(c_+ - \epsilon' \leqslant \int \mathrm{d}\rho\right)$. Making use of Lemma 3.3.3 and $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)} \leqslant \alpha$, we then obtain

$$\begin{aligned} &Z_{\alpha,-}^2 \langle \Psi_{\alpha,-} | \mathbb{H}_\Lambda | \Psi_{\alpha,-} \rangle + Z_\alpha^2 \langle \Psi'_\alpha | \mathbb{H}_\Lambda | \Psi'_\alpha \rangle + Z_{\alpha,+}^2 \langle \Psi_{\alpha,+} | \mathbb{H}_\Lambda | \Psi_{\alpha,+} \rangle \\ &\qquad \leqslant \langle \Psi_\alpha^\bullet | \mathbb{H}_\Lambda | \Psi_\alpha^\bullet \rangle + c\, \alpha^{-\frac{7}{2}} V_{\mathcal{M}(\mathbb{R}^3)}(\mathcal{P}) \left\langle \Psi_\alpha^\bullet \middle| \sqrt{\mathcal{N} + \alpha^{-2}} \middle| \Psi_\alpha^\bullet \right\rangle, \end{aligned} \tag{3.3.7}$$

where $\Psi_{\alpha,\pm} := Z_{\alpha,\pm}^{-1} \widehat{F}_{(\pm)} \Psi_\alpha^\bullet$, with corresponding normalization factors $Z_{\alpha,\pm} := \|\widehat{F}_{(\pm)} \Psi_\alpha^\bullet\|$. By Eq. (3.2.5) there exists a constant d s.t. $\left\langle \Psi_\alpha^\bullet \middle| \mathcal{N} \middle| \Psi_\alpha^\bullet \right\rangle \leqslant \left\langle \Psi_\alpha^\bullet \middle| 2\mathbb{H}_\Lambda + d \middle| \Psi_\alpha^\bullet \right\rangle \lesssim d + \alpha^{-\frac{4}{29}}$, where we have used the assumption $\left\langle \Psi_\alpha^\bullet \middle| \mathbb{H}_\Lambda \middle| \Psi_\alpha^\bullet \right\rangle = \widetilde{E}_\alpha \leqslant \widetilde{E}_\alpha - E_\alpha \lesssim \alpha^{-\frac{4}{29}}$. The first derivative of the functions $\chi^{\epsilon'}(\cdot \leqslant c_- + \epsilon'), \chi^{\epsilon'}(c_- + \epsilon' \leqslant \cdot \leqslant c_+ - \epsilon')$ and $\chi^{\epsilon'}(\cdot \leqslant c_+ - \epsilon')$ is uniformly bounded by some ϵ'-dependent constant D, and consequently we have for all finite measures ρ and $\rho' := \rho + \alpha^{-2}\delta_y$ with $y \in \mathbb{R}^3$, and $\diamond \in \{-, *, +\}$,

$$|F_\diamond(\rho') - F_\diamond(\rho)| \leqslant D \left| \int \mathrm{d}\rho' - \int \mathrm{d}\rho \right| = D\alpha^{-2}.$$

This implies that $V_{\mathcal{M}(\mathbb{R}^3)}(\mathcal{P}) \lesssim 1$, and therefore the right hand side of Eq. (3.3.7) is bounded by $\langle \Psi_\alpha^\bullet | \mathbb{H}_\Lambda | \Psi_\alpha^\bullet \rangle + C\alpha^{-\frac{7}{2}}$ for a suitable $C > 0$. Since $Z_{\alpha,-}^2 + Z_\alpha^2 + Z_{\alpha,+}^2 = 1$, this means that at least one of the terms $\langle \Psi_{\alpha,-}|\mathbb{H}_\Lambda|\Psi_{\alpha,-}\rangle, \langle \Psi'_\alpha|\mathbb{H}_\Lambda|\Psi'_\alpha\rangle$ or $\langle \Psi_{\alpha,+}|\mathbb{H}_\Lambda|\Psi_{\alpha,+}\rangle$ is bounded from above by $\langle \Psi^\bullet_\alpha|\mathbb{H}_\Lambda|\Psi^\bullet_\alpha\rangle + C\alpha^{-\frac{7}{2}} = \widetilde{E}_\alpha + C\alpha^{-\frac{7}{2}}$. We can however rule out that $\langle \Psi_{\alpha,-}|\mathbb{H}_\Lambda|\Psi_{\alpha,-}\rangle$, respectively $\langle \Psi_{\alpha,+}|\mathbb{H}_\Lambda|\Psi_{\alpha,+}\rangle$, satisfy this upper bound for all small c_-, ϵ' and large α, c_+, since $\widetilde{E}_\alpha \leqslant E_\alpha + C'\alpha^{-\frac{4}{29}} \leqslant e^{\mathrm{Pek}} + C'\alpha^{-\frac{4}{29}} < \frac{e^{\mathrm{Pek}}}{2} < 0$ for α large enough and a suitable C', and since we have by Eqs. (3.2.4) and (3.2.5) for all $t > 0$

$$\langle \Psi_{\alpha,-}|\mathbb{H}_\Lambda|\Psi_{\alpha,-}\rangle \geqslant \langle \Psi_{\alpha,-}|-\frac{d}{t^2} - t\big(\mathcal{N} + \alpha^{-2}\big)|\Psi_{\alpha,-}\rangle \geqslant -\frac{d}{t^2} - t\big(c_- + 2\epsilon' + \alpha^{-2}\big) \geqslant -\frac{e^{\mathrm{Pek}}}{2}, \tag{3.3.8}$$

$$\langle \Psi_{\alpha,+}|\mathbb{H}_\Lambda|\Psi_{\alpha,+}\rangle \geqslant \langle \Psi_{\alpha,+}| - d + \frac{1}{2}\mathcal{N}|\Psi_{\alpha,+}\rangle \geqslant -d + \frac{1}{2}(c_+ - 2\epsilon') \geqslant 0, \tag{3.3.9}$$

where the last inequality in Eq. (3.3.8), respectively Eq. (3.3.9), holds for small c_-, ϵ' and large α, c_+ with the concrete choice $t := \left(\frac{d}{c_- + 2\epsilon' + \alpha^{-2}}\right)^{\frac{1}{3}}$. Using again that the right hand side of Eq. (3.3.7) is bounded by $\langle \Psi^\bullet_\alpha|\mathbb{H}_\Lambda|\Psi^\bullet_\alpha\rangle + C\alpha^{-\frac{7}{2}}$ together with Eqs. (3.3.8) and (3.3.9), and the fact that $\mathbb{H}_\Lambda \geqslant E_\alpha$ and $E_\alpha \leqslant e^{\mathrm{Pek}}$, yields furthermore

$$(1 - Z_\alpha^2)\left(E_\alpha - \frac{e^{\mathrm{Pek}}}{2}\right) + Z_\alpha^2 E_\alpha \leqslant (1 - Z_\alpha^2)\frac{e^{\mathrm{Pek}}}{2} + Z_\alpha^2 E_\alpha \leqslant \widetilde{E}_\alpha + C\alpha^{-\frac{7}{2}},$$

and therefore $-(1 - Z_\alpha^2)\frac{e^{\mathrm{Pek}}}{2} \leqslant \widetilde{E}_\alpha - E_\alpha + C\alpha^{-\frac{7}{2}} \underset{\alpha\to\infty}{\longrightarrow} 0$. Since $e^{\mathrm{Pek}} < 0$, this immediately implies $Z_\alpha \underset{\alpha\to\infty}{\longrightarrow} 1$. ∎

Regarding the next localization step in Lemma 3.3.5, let us introduce for given R and $\epsilon > 0$ satisfying $R > 2\epsilon$ the function $K_R(\rho) := \iint \chi^\epsilon(R - \epsilon \leqslant |x - y|)\, \mathrm{d}\rho(x)\mathrm{d}\rho(y)$, which measures how sharply the mass of the measure ρ is concentrated. It will be convenient in the second part to have K_R defined for arbitrary $\epsilon \geqslant 0$ even though we only need it for $\epsilon = 0$ in the following. We also define the function $F_R(\rho) := \chi^{\frac{\delta}{3}}\left(K_R(\rho) \leqslant \frac{2\delta}{3}\right)$ for $R, \delta > 0$, as well as the states

$$\Psi''_\alpha := Z_{R,\alpha}^{-1}\widehat{F}_R\Psi'_\alpha, \tag{3.3.10}$$

where Ψ'_α is as in Lemma 3.3.4 and $Z_{R,\alpha} := \|\widehat{F}_R\Psi'_\alpha\|$. Since Ψ'_α satisfies $\mathrm{supp}(\Psi'_\alpha) \subset B_L(0)$, we have $\mathrm{supp}(\Psi''_\alpha) \subset B_L(0)$ as well. Furthermore $\chi\left(\widehat{K}_R \leqslant \delta\right)\Psi''_\alpha = \Psi''_\alpha$. Heuristically this means that we can restrict our attention to phonon configurations that concentrate in a ball of fixed radius R.

Lemma 3.3.5. *Let Ψ'_α be the sequence from Lemma 3.3.4, and let $\epsilon \geqslant 0$ and $\delta > 0$ be given constants. Then there exists a α independent $R > 0$, such that the states Ψ''_α defined in Eq. (3.3.10) satisfy $\langle \Psi''_\alpha|\mathbb{H}_\Lambda|\Psi''_\alpha\rangle - \widetilde{E}_\alpha \lesssim \alpha^{-\frac{7}{2}}$, where $\widetilde{E}_\alpha$ is defined in Eq. (3.3.5). Furthermore, $Z_{R,\alpha} \underset{\alpha\to\infty}{\longrightarrow} 1$.*

Proof. Since $\mathcal{P} := \{F_R, G_R\}$ with $G_R := \sqrt{1 - F_R^2} = \chi^{\frac{\delta}{3}}\left(\frac{2\delta}{3} \leqslant K_R(\rho)\right)$ is a partition of unity, we obtain by Lemma 3.3.3

$$\langle \widehat{F}_R\Psi'_\alpha|\mathbb{H}_\Lambda|\widehat{F}_R\Psi'_\alpha\rangle + \langle \widehat{G}_R\Psi'_\alpha|\mathbb{H}_\Lambda|\widehat{G}_R\Psi'_\alpha\rangle \leqslant \langle \Psi'_\alpha|\mathbb{H}_\Lambda|\Psi'_\alpha\rangle + c\,\alpha^{-\frac{7}{2}} V_\Omega(\mathcal{P})\langle \Psi'_\alpha|\sqrt{c_+ + \alpha^{-2}}\,|\Psi'_\alpha\rangle \tag{3.3.11}$$

with $\Omega := \{\rho : \int \mathrm{d}\rho \leqslant c_+\}$, where we have used $\chi(\mathcal{N} \leqslant c_+)\,\Psi'_\alpha = \Psi'_\alpha$ and $\Lambda \leqslant \alpha$. Since $\frac{\mathrm{d}}{\mathrm{d}x}\chi^{\frac{\delta}{3}}\left(\frac{2\delta}{3} \leqslant x\right)$ and $\frac{\mathrm{d}}{\mathrm{d}x}\chi^{\frac{\delta}{3}}\left(x \leqslant \frac{2\delta}{3}\right)$ are bounded by some δ-dependent constant D, we have for all $\rho \in \Omega$ and $\rho' := \rho + \alpha^{-2}\delta_z$ with $z \in \mathbb{R}^3$, and $R > 2\epsilon$, the estimate

$$|F_R(\rho') - F_R(\rho)| \leqslant D\,|K_R(\rho') - K_R(\rho)| = 2D\alpha^{-2}\int \chi^\epsilon(R - \epsilon \leqslant |y - z|)\,\mathrm{d}\rho(y)$$
$$\leqslant 2D\alpha^{-2}c_+,$$

and the same result holds for G_R. Therefore we have by Eq. (3.3.11) and Lemma 3.3.4

$$\langle \widehat{F}_R\Psi'_\alpha|\mathbb{H}_\Lambda|\widehat{F}_R\Psi'_\alpha\rangle + \langle \widehat{G}_R\Psi'_\alpha|\mathbb{H}_\Lambda|\widehat{G}_R\Psi'_\alpha\rangle \leqslant \langle \Psi'_\alpha|\mathbb{H}_\Lambda|\Psi'_\alpha\rangle + C_1\alpha^{-\frac{7}{2}} \leqslant \widetilde{E}_\alpha + C_2\alpha^{-\frac{7}{2}} \tag{3.3.12}$$

for suitable constants $C_1, C_2 > 0$. Since $\|\widehat{F}_R\Psi'_\alpha\|^2 + \|\widehat{G}_R\Psi'_\alpha\|^2 = 1$, this means that we either have $\langle \Psi''_\alpha|\mathbb{H}_\Lambda|\Psi''_\alpha\rangle \leqslant \widetilde{E}_\alpha + C_2\alpha^{-\frac{7}{2}}$ or $\langle \widetilde{\Psi}_\alpha|\mathbb{H}_\Lambda|\widetilde{\Psi}_\alpha\rangle \leqslant \widetilde{E}_\alpha + C_2\alpha^{-\frac{7}{2}}$, where $\widetilde{\Psi}_\alpha := \|\widehat{G}_R\Psi'_\alpha\|^{-1}\widehat{G}_R\Psi'_\alpha$. In the following we are going to rule out the second case for R and α large enough, to be precise we are going to verify $\langle \widetilde{\Psi}_\alpha|\mathbb{H}_\Lambda|\widetilde{\Psi}_\alpha\rangle > \widetilde{E}_\alpha + d\alpha^{-\frac{4}{29}}$ for any $d > 0$ and large enough R and α by contradiction. In order to do this, let us assume $\langle \widetilde{\Psi}_\alpha|\mathbb{H}_\Lambda|\widetilde{\Psi}_\alpha\rangle \leqslant \widetilde{E}_\alpha + d\alpha^{-\frac{4}{29}}$. Since $\widetilde{E}_\alpha \leqslant E_\alpha + C\alpha^{-\frac{4}{29}} \leqslant e^{\mathrm{Pek}} + C\alpha^{-\frac{4}{29}}$ by assumption for a suitable constant C, $\widetilde{\Psi}_\alpha$ satisfies the assumptions of Theorem 3.3.2 with $\delta e := (d + C)\alpha^{-\frac{4}{29}}$. Hence there exists a measure μ such that Eq. (3.3.2) holds. By the support properties of G_R we obtain

$$\frac{\delta}{3} \leqslant \langle \widetilde{\Psi}_\alpha|\widehat{K}_R|\widetilde{\Psi}_\alpha\rangle = \int K_R\left(\left|\varphi^{\mathrm{Pek}}_x\right|^2\right)\mathrm{d}\mu + O_{\alpha\to\infty}\left(\alpha^{-\frac{2}{29}}\right) \tag{3.3.13}$$
$$= K_R\left(\left|\varphi^{\mathrm{Pek}}\right|^2\right) + O_{\alpha\to\infty}\left(\alpha^{-\frac{2}{29}}\right). \tag{3.3.14}$$

Since $\lim_{R\to\infty} K_R\left(\left|\varphi^{\mathrm{Pek}}\right|^2\right) = 0$, Eq. (3.3.13) is a contradiction for large R and α, and consequently we have $\langle \widetilde{\Psi}_\alpha|\mathbb{H}_\Lambda|\widetilde{\Psi}_\alpha\rangle > \widetilde{E}_\alpha + d\alpha^{-\frac{4}{29}}$ for such R and α. In combination with Eq. (3.3.12) this furthermore yields

$$Z^2_{R,\alpha}E_\alpha + (1 - Z^2_{R,\alpha})\left(E_\alpha + d\alpha^{-\frac{4}{29}}\right) \leqslant Z^2_{R,\alpha}E_\alpha + (1 - Z^2_{R,\alpha})\left(\widetilde{E}_\alpha + d\alpha^{-\frac{4}{29}}\right) \leqslant \widetilde{E}_\alpha + C_2\alpha^{-\frac{7}{2}},$$

and therefore $1 - Z^2_{R,\alpha} \leqslant \frac{\alpha^{\frac{4}{29}}}{d}\left(\widetilde{E}_\alpha - E_\alpha + C_2\alpha^{-\frac{7}{2}}\right) \leqslant \frac{1}{d} + \frac{C_2}{d}\alpha^{\frac{4}{29} - \frac{7}{2}}$. Since this holds for any $d > 0$ and α large enough, we conclude that $Z_{R,\alpha} \underset{\alpha\to\infty}{\longrightarrow} 1$. ∎

The previous localizations in the Lemmas 3.3.4 and 3.3.5 will allow us to control the energy cost of the main localization in the proof of Lemma 3.3.12. Before we come to Lemma 3.3.12 we need to define the regularized median m_q in Definition 3.3.8 and verify Lemma 3.3.10, which provides an upper bound on the variation $V_\Omega(\mathcal{P})$ for partitions $\mathcal{P} = \{F_j : j \in J\}$ of the form $F_j(\rho) = f_j(m_q(\rho))$. The following auxiliary Lemmas 3.3.6 , 3.3.7 and 3.3.9 will be useful in proving Lemma 3.3.10.

Lemma 3.3.6. *Let us define the set Ω_{reg} as the set of all $\rho \in \mathcal{M}(\mathbb{R}^3)$ satisfying*

$$\int_{x_i = t} \mathrm{d}\rho(x) \leqslant \alpha^{-2}$$

for all $t \in \mathbb{R}$ and $i \in \{1, 2, 3\}$. Then $\widehat{\mathbb{1}_{\Omega_{\mathrm{reg}}}}\Psi = \Psi$ for all $\Psi \in \mathcal{F}(L^2(\mathbb{R}^3))$.

Proof. For given $x = (x^1, \dots, x^n) \in \mathbb{R}^{3\times n}$, let us define the measure $\rho_x := \alpha^{-2}\sum_{k=1}^n \delta_{x^k}$. Note that $\rho_x \notin \Omega_{\mathrm{reg}}$ if and only if there exists an $i \in \{1,2,3\}$ such that $x_i^k = x_i^{k'}$ for indices $k \neq k'$. Clearly the set of all such $x \in \mathbb{R}^{3\times n}$ has Lebesgue measure zero. Hence the multiplication operator by the function $(x^1, \dots, x^n) \mapsto \mathbb{1}_{\Omega_{\mathrm{reg}}}(\rho_x)$ is equal to the identity on $L^2_{\mathrm{sym}}(\mathbb{R}^{3\times n})$, which concludes the proof according to Definition 3.3.1. ■

Lemma 3.3.7. *Let ν, ν' be finite measures on $\mathbb{R}$ such that $\nu(\{t\}) \leqslant \epsilon$ and $\nu'(\{t\}) \leqslant \epsilon$ for all $t \in \mathbb{R}$, and let $x^\kappa(\nu)$ be the κ-quantile of the measure ν with $0 \leqslant \kappa \leqslant 1$, to be precise $x^\kappa(\nu)$ is the supremum over all numbers $t \in \mathbb{R}$ satisfying $\int_{-\infty}^t \mathrm{d}\nu \leqslant \kappa \int \mathrm{d}\nu$, where we use the convention that the boundaries are included in the domain of integration $\int_a^b f \mathrm{d}\nu := \int_{[a,b]} f \mathrm{d}\nu$. Then*

$$\Big| \int_{-\infty}^{x^\kappa(\nu')} \mathrm{d}\nu - \int_{-\infty}^{x^\kappa(\nu)} \mathrm{d}\nu \Big| \leqslant 2\|\nu' - \nu\|_{\mathrm{TV}} + \epsilon,$$

where $\|\nu' - \nu\|_{\mathrm{TV}} := \sup_{\|f\|_\infty = 1} \left| \int f\,\mathrm{d}\nu' - \int f\,\mathrm{d}\nu \right|$.

Proof. We estimate

$$\int_{-\infty}^{x^\kappa(\nu')} \mathrm{d}\nu - \int_{-\infty}^{x^\kappa(\nu)} \mathrm{d}\nu \leqslant \int_{-\infty}^{x^\kappa(\nu')} \mathrm{d}\nu - \kappa \int \mathrm{d}\nu \leqslant \int_{-\infty}^{x^\kappa(\nu')} \mathrm{d}\nu' + \|\nu' - \nu\|_{\mathrm{TV}} - \kappa \int \mathrm{d}\nu$$
$$\leqslant \kappa \int \mathrm{d}\nu' + \epsilon + \|\nu' - \nu\|_{\mathrm{TV}} - \kappa \int \mathrm{d}\nu \leqslant 2\|\nu' - \nu\|_{\mathrm{TV}} + \epsilon,$$

where we have used $\int_{-\infty}^{x^\kappa(\nu)} \mathrm{d}\nu \geqslant \kappa \int \mathrm{d}\nu$ and $\int_{-\infty}^{x^\kappa(\nu')} \mathrm{d}\nu' \leqslant \kappa \int \mathrm{d}\nu' + \epsilon$. The bound from below can be obtained by interchanging the role of ν and ν'. ■

Definition 3.3.8. Let $x^\kappa(\nu)$ be the κ-quantile of a measure ν on $\mathbb{R}$ defined in Lemma 3.3.7 and let us denote $K_q(\nu) := [x^{\frac{1}{2}-q}(\nu), x^{\frac{1}{2}+q}(\nu)]$ for $0 < q < \frac{1}{2}$. Then we define

$$m_q(\nu) := \frac{1}{\int_{K_q(\nu)} \mathrm{d}\nu} \int_{K_q(\nu)} t\,\mathrm{d}\nu(t) \in \mathbb{R} \tag{3.3.15}$$

for $\nu \neq 0$ and $m_q(0) := 0$. Furthermore we define for a measure ρ on $\mathbb{R}^3$ the regularized median as $m_q(\rho) := \Big(m_q(\rho_1), m_q(\rho_2), m_q(\rho_3)\Big) \in \mathbb{R}^3$, where ρ_1, ρ_2 and ρ_3 are the marginal measures of ρ defined by $\rho_i(A) := \rho([x_i \in A])$.

Note that $x^\kappa(\nu)$ is the largest value, such that both $\int_{-\infty}^{x^\kappa(\nu)} \mathrm{d}\nu \geqslant \kappa \int \mathrm{d}\nu$ and $\int_{x^\kappa(\nu)}^{\infty} \mathrm{d}\nu \geqslant (1-\kappa)\int \mathrm{d}\nu$ hold. As an immediate consequence, we obtain that the expression in Eq. (3.3.15) is well-defined for $\nu \neq 0$ and $0 < q < \frac{1}{2}$, since

$$\int_{K_q(\nu)} \mathrm{d}\nu = \int_{-\infty}^{x^{\frac{1}{2}+q}(\nu)} \mathrm{d}\nu + \int_{x^{\frac{1}{2}-q}(\nu)}^{\infty} \mathrm{d}\nu - \int \mathrm{d}\nu \geqslant 2q \int \mathrm{d}\nu > 0. \tag{3.3.16}$$

Lemma 3.3.9. *Given constants $R, c > 0$ and $0 < \delta < \frac{c^2}{2}$, let ρ satisfy $c \leqslant \int \mathrm{d}\rho$ and $\iint_{|x-y|\geqslant R} \mathrm{d}\rho(x)\mathrm{d}\rho(y) \leqslant \delta$ and let q be a constant satisfying $0 < q \leqslant \frac{1}{2} - \frac{\delta}{c^2}$. Then we have for all $i \in \{1,2,3\}$ that $x^{\frac{1}{2}}(\rho_i) - R \leqslant x^{\frac{1}{2}-q}(\rho_i) \leqslant x^{\frac{1}{2}+q}(\rho_i) \leqslant x^{\frac{1}{2}}(\rho_i) + R$.*

Proof. Since x^κ is translation covariant, i.e. $x^\kappa(\nu(\cdot - t)) = x^\kappa(\nu) + t$, we can assume w.l.o.g. that $x^{\frac{1}{2}}(\rho_i) = 0$ for $i \in \{1,2,3\}$. Then

$$\delta \geqslant \iint\limits_{|x-y|\geqslant R} \mathrm{d}\rho(x)\mathrm{d}\rho(y) \geqslant 2\int_{x_i\geqslant 0}\mathrm{d}\rho(x)\int_{y_i\leqslant -R}\mathrm{d}\rho(y) \geqslant \int \mathrm{d}\rho\int_{y_i\leqslant -R}\mathrm{d}\rho(y) \geqslant c\int_{y_i\leqslant -R}\mathrm{d}\rho(y),$$

where we have used that $x^{\frac{1}{2}}(\rho_i) = 0$ and $\int \mathrm{d}\rho \geqslant c$ in the last two inequalities. Hence

$$\int_{y_i\leqslant -R}\mathrm{d}\rho(y) \leqslant \frac{\delta}{c} \leqslant \frac{\delta}{c^2}\int \mathrm{d}\rho \leqslant \kappa\int \mathrm{d}\rho$$

for all $\kappa \geqslant \frac{\delta}{c^2}$ and consequently we have $-R \leqslant x^\kappa(\rho_i)$ for all such κ by the definition of $x^\kappa(\rho_i)$. Similarly we obtain $x^\kappa(\rho_i) \leqslant R$ for all κ satisfying $\kappa \leqslant 1 - \frac{\delta}{c^2}$. Therefore $|x^{\frac{1}{2}\pm q}(\rho_i)| \leqslant R$ for $q \leqslant \frac{1}{2} - \frac{\delta}{c^2}$. ■

Lemma 3.3.10. *Given constants $R, c > 0$ and $0 < \delta < \frac{c^2}{2}$, let Ω be the set of $\rho \in \Omega_{\mathrm{reg}}$ satisfying $c \leqslant \int \mathrm{d}\rho$ and $\iint\limits_{|x-y|\geqslant R} \mathrm{d}\rho(x)\mathrm{d}\rho(y) \leqslant \delta$. Then*

$$\left|m_q\left(\rho + \alpha^{-2}\delta_x\right) - m_q\left(\rho\right)\right| \lesssim \frac{R}{c\alpha^2 q}$$

for all $\rho \in \Omega$, $x \in \mathbb{R}^3$ and $0 < q < \frac{1}{2} - \frac{\delta}{c^2}$, where m_q is defined in Definition 3.3.8.

Proof. Since m_q acts translation covariant on any $\rho \neq 0$, i.e. $m_q(\rho(\cdot - y)) = m_q(\rho) + y$, we can assume w.l.o.g. that $x^{\frac{1}{2}}(\rho_i) = 0$ for $i \in \{1,2,3\}$. By Lemma 3.3.9 we therefore obtain $|x^{\frac{1}{2}\pm q}(\rho_i)| \leqslant R$ for $\rho \in \Omega$ and $0 < q \leqslant \frac{1}{2} - \frac{\delta}{c^2}$. Note that the marginal measures ρ_i and ρ_i', where $\rho' := \rho + \alpha^{-2}\delta_x$, satisfy $\rho_i(\{y\}) \leqslant \alpha^{-2}$ and $\rho_i'(\{y\}) \leqslant 2\alpha^{-2}$ by our assumption $\rho \in \Omega_{\mathrm{reg}}$. Therefore $x^{\kappa_*}(\rho_i) \leqslant x^\kappa(\rho_i') \leqslant x^{\kappa^*}(\rho_i)$ for $\rho \in \Omega$ and $\kappa > 0$, with $\kappa_* := \kappa - 2\frac{1}{c}\alpha^{-2}$ and $\kappa^* := \kappa + 3\frac{1}{c}\alpha^{-2}$. In particular, this implies $|x^{\frac{1}{2}\pm q}(\rho_i')| \leqslant R$ for $0 < q < 1/2 - \delta/c^2$ and α large enough. In the following it will be convenient to write the difference $m_q(\rho_i') - m_q(\rho_i)$ as

$$\left(\frac{1}{\int_{K_q(\rho_i')}\mathrm{d}\rho_i'} - \frac{1}{\int_{K_q(\rho_i)}\mathrm{d}\rho_i}\right)\int_{K_q(\rho_i')} t\,\mathrm{d}\rho_i'(t) + \frac{1}{\int_{K_q(\rho_i)}\mathrm{d}\rho_i}\left(\int_{K_q(\rho_i')} t\,\mathrm{d}\rho_i'(t) - \int_{K_q(\rho_i)} t\,\mathrm{d}\rho_i(t)\right). \tag{3.3.17}$$

Making use of $\int_{K_q(\rho_i)}\mathrm{d}\rho_i \geqslant 2qc$, see Eq. (3.3.16), and $K_q(\rho_i') \subset [-R, R]$ for all $\rho \in \Omega$, we can estimate the individual terms in Eq. (3.3.17) by

$$\left|\left(\frac{1}{\int_{K_q(\rho_i')}\mathrm{d}\rho_i'} - \frac{1}{\int_{K_q(\rho_i)}\mathrm{d}\rho_i}\right)\int_{K_q(\rho_i')} t\,\mathrm{d}\rho_i'(t)\right| \leqslant R\frac{\left|\int_{K_q(\rho_i')}\mathrm{d}\rho_i' - \int_{K_q(\rho_i)}\mathrm{d}\rho_i\right|}{2qc},$$

$$\left|\frac{1}{\int_{K_q(\rho_i)}\mathrm{d}\rho_i}\left(\int_{K_q(\rho_i')} t\,\mathrm{d}\rho_i'(t) - \int_{K_q(\rho_i)} t\,\mathrm{d}\rho_i(t)\right)\right| \leqslant \frac{\left|\int_{K_q(\rho_i')} t\,\mathrm{d}\rho_i'(t) - \int_{K_q(\rho_i)} t\,\mathrm{d}\rho_i(t)\right|}{2qc}.$$

Note that $K_q(\rho_i)$ is contained in $[-R, R]$ as well and consequently t is bounded by R on the subset $K_q(\rho_i) \cup K_q(\rho_i')$. In order to verify the statement of the Lemma, it is therefore sufficient to prove that $\left|\int_{K_q(\rho_i')} f(t)\,\mathrm{d}\rho_i'(t)-\int_{K_q(\rho_i)} f(t)\,\mathrm{d}\rho_i(t)\right| \lesssim \alpha^{-2}\|f\|_\infty$ for an arbitrary measurable and bounded $f:\mathbb{R}\to\mathbb{R}$. We estimate

$$\left|\int_{K_q(\rho_i')} f(t)\,\mathrm{d}\rho_i'(t)-\int_{K_q(\rho_i)} f(t)\,\mathrm{d}\rho_i(t)\right| \leqslant \left|\int_{K_q(\rho_i')} f(t)\,\mathrm{d}\rho_i'(t)-\int_{K_q(\rho_i')} f(t)\,\mathrm{d}\rho_i(t)\right|$$
$$+\left|\int_{K_q(\rho_i')} f(t)\,\mathrm{d}\rho_i(t)-\int_{K_q(\rho_i)} f(t)\,\mathrm{d}\rho_i(t)\right| \leqslant \|f\|_\infty\left(\|\rho_i'-\rho_i\|_{\mathrm{TV}}+\int_{K_q(\rho_i')\Delta K_q(\rho_i)}\mathrm{d}\rho_i\right),$$

where $A\Delta B := (A\cup B)\setminus(A\cap B)$ is the symmetric difference. Note that $\|\rho_i'-\rho_i\|_{\mathrm{TV}}=\alpha^{-2}$. Furthermore we can estimate the expression $\int_{K_q(\rho_i')\Delta K_q(\rho_i)}\mathrm{d}\rho_i$ by

$$\left|\int_{-\infty}^{x^{\frac{1}{2}-q}(\rho_i')}\mathrm{d}\rho_i-\int_{-\infty}^{x^{\frac{1}{2}-q}(\rho_i)}\mathrm{d}\rho_i\right|+\left|\int_{-\infty}^{x^{\frac{1}{2}+q}(\rho_i')}\mathrm{d}\rho_i-\int_{-\infty}^{x^{\frac{1}{2}+q}(\rho_i)}\mathrm{d}\rho_i\right|.$$

Since the distributions ρ_i and ρ_i' satisfy the assumptions of Lemma 3.3.7 with $\epsilon := 2\alpha^{-2}$, we conclude that every term in the sum above is bounded by $2\|\rho'-\rho\|_{\mathrm{TV}}+\epsilon = 4\alpha^{-2}$. ■

Before we state the central Lemma 3.3.12, let us verify in the subsequent Lemma 3.3.11 that low energy states with a localized median necessarily satisfy (complete) condensation with respect to a minimizer of the Pekar functional.

Lemma 3.3.11. *Given a constant $C>0$, there exists a constant $T>0$, such that*

$$\left\langle\Psi\middle|W_{\varphi^{\mathrm{Pek}}}^{-1}\mathcal{N}W_{\varphi^{\mathrm{Pek}}}\middle|\Psi\right\rangle \leqslant T\left(\alpha^{-\frac{2}{29}}+q+\epsilon\right)$$

for all states Ψ satisfying $\langle\Psi|\mathbb{H}_K|\Psi\rangle \leqslant e^{\mathrm{Pek}}+\alpha^{-\frac{4}{29}}$ with $K\geqslant\alpha^{\frac{8}{29}}$ and $\widehat{\mathbb{1}_{\Omega^*}}\Psi=\Psi$, where Ω^* is the set of all ρ satisfying $\int\mathrm{d}\rho\leqslant C$ and $|m_q(\rho)|\leqslant\epsilon$ with $q,\epsilon>0$.

Proof. Let us begin by defining the functions

$$P_i^\epsilon(\rho) := \left(\frac{1}{2}\int\mathrm{d}\rho\right)^2-\int_{x_i\leqslant\epsilon}\mathrm{d}\rho(x)\int_{y_i\geqslant-\epsilon}\mathrm{d}\rho(y). \tag{3.3.18}$$

Observe that $|m_q(\rho)|\leqslant\epsilon$ implies $-\epsilon\leqslant x^{\frac{1}{2}+q}(\rho_i)$ and $x^{\frac{1}{2}-q}(\rho_i)\leqslant\epsilon$ for all such ρ which additionally satisfy $\rho\neq 0$, see Definition 3.3.8. Therefore $P_i^\epsilon(\rho)\leqslant\left(\int\mathrm{d}\rho\right)^2\left(\frac{1}{4}-\left(\frac{1}{2}-q\right)^2\right)\lesssim q$ for all $\rho\in\Omega^*$, and consequently the measure μ from Theorem 3.3.2 corresponding to the state Ψ satisfies $\int P_i^\epsilon\left(\left|\varphi_x^{\mathrm{Pek}}\right|^2\right)\mathrm{d}\mu(x)\leqslant\left\langle\Psi\middle|\widehat{P}_i^\epsilon\middle|\Psi\right\rangle+D\alpha^{-\frac{2}{29}}\lesssim q+\alpha^{-\frac{2}{29}}$ for a suitable $D>0$, where we have used Eq. (3.3.2) in the first inequality. Furthermore we know that $\|\varphi_x^{\mathrm{Pek}}-\varphi^{\mathrm{Pek}}\|^2\lesssim\sum_{i=1}^3 P_i^\epsilon\left(\left|\varphi_x^{\mathrm{Pek}}\right|^2\right)+\epsilon$ by Lemma 3.8.3, hence

$$\int\|\varphi_x^{\mathrm{Pek}}-\varphi^{\mathrm{Pek}}\|^2\,\mathrm{d}\mu(x)\lesssim\sum_{i=1}^3\int P_i^\epsilon\left(\left|\varphi_x^{\mathrm{Pek}}\right|^2\right)\mathrm{d}\mu(x)+\epsilon\lesssim q+\alpha^{-\frac{2}{29}}+\epsilon.$$

Therefore Eq. (3.3.3) immediately concludes the proof of Eq. (3.3.19). ■

Lemma 3.3.12. *Given* $0 < \sigma \leqslant \frac{1}{4}$, *let* Λ *and* L *be as in Theorem 3.2.5. Then there exist states* Ψ'''_α *satisfying* $\langle \Psi'''_\alpha | \mathbb{H}_\Lambda | \Psi'''_\alpha \rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$, $\operatorname{supp}(\Psi'''_\alpha) \subset B_{4L}(0)$ *and*

$$\left\langle \Psi'''_\alpha \middle| W^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \middle| \Psi'''_\alpha \right\rangle \lesssim \alpha^{-\frac{2}{29}}, \tag{3.3.19}$$

where $W_{\varphi^{\mathrm{Pek}}}$ *is the Weyl operator corresponding to the Pekar minimizer* φ^{Pek}.

Proof. It is clearly sufficient to consider only the case $\alpha \geqslant \alpha_0$ for a suitable (large) α_0, since we can always re-define $\Psi'''_\alpha := \Psi$ for $\alpha < \alpha_0$ where Ψ is an arbitrary state satisfying $\operatorname{supp}(\Psi) \subset B_{4L}(0)$. In the following let us use the concrete choice $\Psi^\bullet_\alpha := \Psi^\diamond_\alpha$ for the sequence in Eq. (3.3.5), where $\Psi^\diamond_\alpha$ is defined in in Theorem 3.2.5, which is a valid choice since it satisfies the assumptions $\operatorname{supp}(\Psi^\diamond_\alpha) \subset B_L(0)$ and $\widetilde{E}_\alpha - E_\alpha \lesssim \alpha^{-2(1+\sigma)} \leqslant \alpha^{-\frac{4}{29}}$. Furthermore let $\{\chi_z : z \in \mathbb{Z}^3\}$ be a smooth (quadratic) partition of unity on $\mathbb{R}^3$, i.e. $0 \leqslant \chi_z \leqslant 1$ and $\sum_{z\in\mathbb{Z}^3} \chi_z^2 = 1$, with $\chi_z(x) = \chi_0(x-z)$ and $\operatorname{supp}(\chi_0) \subset B_1(0)$. Then we define for $z \in \mathbb{Z}^3$ and $u, v \geqslant \frac{2}{29}$ with $u + v \leqslant \frac{1}{4}$ the function $F_z(\rho) := \chi_z\big(\alpha^u\, m_{\alpha^{-v}}(\rho)\big)$, as well as the states

$$\Psi_{\alpha,z} := Z^{-1}_{\alpha,z} \widehat{F}_z \Psi''_\alpha \tag{3.3.20}$$

with $Z_{\alpha,z} := \|\widehat{F}_z \Psi''_\alpha\|$ and Ψ''_α as in Lemma 3.3.5 for $\epsilon = 0$ and $0 < \delta < \frac{c^2}{2}$, where $c := c_-$ is as in Lemma 3.3.4. Applying Lemma 3.3.3 with respect to $\mathcal{P} := \{F_z : z \in \mathbb{Z}^3\}$, where the functions F_z are defined above Eq. (3.3.20) and Ω is defined as the set of all $\rho \in \Omega_{\mathrm{reg}}$ satisfying $c_- \leqslant \int \mathrm{d}\rho \leqslant c_+$ and $\iint_{|x-y|\geqslant R} \mathrm{d}\rho(x)\mathrm{d}\rho(y) \leqslant \delta$, yields

$$\sum_{z\in\mathbb{Z}^3} Z^2_{\alpha,z} \langle \Psi_{\alpha,z} | \mathbb{H}_\Lambda | \Psi_{\alpha,z} \rangle \leqslant \langle \Psi''_\alpha | \mathbb{H}_\Lambda | \Psi''_\alpha \rangle + c\alpha^{-\frac{7}{2}} V_\Omega(\mathcal{P}) \sqrt{c_+ + \alpha^{-2}}, \tag{3.3.21}$$

where we used Lemma 3.3.6, $\Lambda \leqslant \alpha$ and $\widehat{\mathbb{1}_\Omega} \Psi''_\alpha = \Psi''_\alpha$ by the definition of Ψ''_α in Eq. (3.3.10). Since the support of χ_z only overlaps with the support of finitely many other $\chi_{z'}$, we obtain for $v > 0$ and α large enough

$$\begin{aligned} V_\Omega(\mathcal{P}) &\lesssim \alpha^4 \sup_{\rho\in\Omega, y\in\mathbb{R}^3} \sup_{z\in\mathbb{Z}^3} \left|\chi_z\big(\alpha^u m_{\alpha^{-v}}(\rho + \alpha^{-2}\delta_y)\big) - \chi_z\big(\alpha^u m_{\alpha^{-v}}(\rho)\big)\right|^2 \\ &\lesssim \alpha^{2u+4} \sup_{\rho\in\Omega, y\in\mathbb{R}^3} \left| m_{\alpha^{-v}}(\rho + \alpha^{-2}\delta_y) - m_{\alpha^{-v}}(\rho) \right|^2 \lesssim \alpha^{2(u+v)}, \end{aligned}$$

where we have used $\sup_{z\in\mathbb{Z}^3} |\chi_z(y) - \chi_z(x)| \leqslant \|\nabla\chi_0\|_\infty |y-x|$ in the first inequality and Lemma 3.3.10 in the second one. Combining this with Eq. (3.3.21) and the fact that $u+v \leqslant \frac{1}{4}$ yields

$$\sum_{z\in\mathbb{Z}^3} Z^2_{\alpha,z} \langle \Psi_{\alpha,z} | \mathbb{H}_\Lambda | \Psi_{\alpha,z} \rangle - \langle \Psi''_\alpha | \mathbb{H}_\Lambda | \Psi''_\alpha \rangle \lesssim \alpha^{-3}. \tag{3.3.22}$$

Since $\sum_{z\in\mathbb{Z}^3} Z^2_{\alpha,z} = 1$, this in particular means that there exists a $z_\alpha \in \mathbb{Z}^3$ such that $\langle \Psi_{\alpha,z_\alpha} | \mathbb{H}_\Lambda | \Psi_{\alpha,z_\alpha} \rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$, and by the translation invariance of $\mathbb{H}_\Lambda$ we obtain $\langle \Psi'''_\alpha | \mathbb{H}_\Lambda | \Psi'''_\alpha \rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$ where $\Psi'''_\alpha = \mathcal{T}_{-\alpha^{-u} z_\alpha} \Psi_{\alpha,z_\alpha}$. Using the fact that $\mathbb{1}_{\Omega^*} \Psi'''_\alpha = \Psi'''_\alpha$, where Ω^* is the set of all ρ satisfying $\int \mathrm{d}\rho \leqslant c_+$ and $|m_{\alpha^{-v}}(\rho)| \leqslant \alpha^{-u}$, together with Lemma 3.3.11, immediately concludes the proof of Eq. (3.3.19).

Finally let us verify that $\operatorname{supp}(\Psi'''_\alpha) \subset B_{4L}(0)$. By the definition of $\Psi'''_\alpha = \mathcal{T}_{-\alpha^{-u} z_\alpha} \Psi_{\alpha,z_\alpha}$, and the fact that $\operatorname{supp}(\Psi_{\alpha,z_\alpha}) \subset B_L(0)$, it is clear that $\operatorname{supp}(\Psi'''_\alpha) \subset B_L(-w_\alpha)$ with

$w_\alpha := \alpha^{-u} z_\alpha$. In the following we show that $|w_\alpha| \leqslant 3L$ by contradiction for α large enough, and therefore $\operatorname{supp}(\Psi'''_\alpha) \subset B_{L+|w_\alpha|}(0) \subset B_{4L}(0)$. Assuming $|w_\alpha| > 3L$, we obtain $\operatorname{supp}(\Psi'''_\alpha) \subset \mathbb{R}^3 \backslash B_{2L}(0)$ and Corollary 3.9.7 consequently yields $\langle \Psi'''_\alpha | \mathbb{H}_\Lambda | \Psi'''_\alpha \rangle \geqslant E_\alpha + \langle \Psi'''_\alpha | \mathcal{N}_{B_L(0)} | \Psi'''_\alpha \rangle - \sqrt{\frac{D}{L}}$, where $\mathcal{N}_{B_L(0)}$ denotes the number operator in the ball $B_L(0)$ (as defined in Cor. 3.9.7). Defining $\varphi_L(x) := \chi(|x| \leqslant L)\, \varphi^{\mathrm{Pek}}(x)$, we further have

$$\begin{aligned}\langle \Psi'''_\alpha | \mathcal{N}_{B_L(0)} | \Psi'''_\alpha \rangle &= \left\langle \Psi'''_\alpha \middle| W^{-1}_{\varphi^{\mathrm{Pek}}} \left(\mathcal{N}_{B_L(0)} + a(\varphi_L) + a^\dagger(\varphi_L) + \|\varphi_L\|^2 \right) W_{\varphi^{\mathrm{Pek}}} \middle| \Psi'''_\alpha \right\rangle \\ &\geqslant -\left\langle \Psi'''_\alpha \middle| W^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \middle| \Psi'''_\alpha \right\rangle + \frac{1}{2}\|\varphi_L\|^2 \geqslant -D' \alpha^{-\frac{2}{29}} + \frac{1}{2}\|\varphi_L\|^2\end{aligned}$$

for a suitable constant D', where we have used the operator inequality $\mathcal{N}_{B_L(0)} + a(\varphi_L) + a^\dagger(\varphi_L) + \|\varphi_L\|^2 \geqslant -\mathcal{N} + \frac{1}{2}\|\varphi_L\|^2$ as well as Eq. (3.3.19). Therefore we obtain

$$\langle \Psi'''_\alpha | \mathbb{H}_\Lambda | \Psi'''_\alpha \rangle - E_\alpha \geqslant \frac{1}{2}\|\varphi_L\|^2 - D'\alpha^{-\frac{2}{29}} - \sqrt{\frac{D}{L}} \underset{\alpha \to \infty}{\longrightarrow} \frac{1}{2}\|\varphi^{\mathrm{Pek}}\|^2 > 0,$$

where we have used that $L = \alpha^{1+\sigma} \underset{\alpha\to\infty}{\longrightarrow} \infty$. This, however, is a contradiction to $\langle \Psi'''_\alpha | \mathbb{H}_\Lambda | \Psi'''_\alpha \rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$. ∎

Following the method in [72], we are going to lift the weak condensation derived in Lemma 3.3.12 to a strong one in the subsequent Theorem 3.3.13, which represents the main result of this section.

Theorem 3.3.13. *Given $0 < \sigma \leqslant \frac{1}{4}$ and $h < \frac{2}{29}$, let Λ and L be as in Theorem 3.2.5. Then there exist states Ψ_α with $\langle \Psi_\alpha | \mathbb{H}_\Lambda | \Psi_\alpha \rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$ and $\operatorname{supp}(\Psi_\alpha) \subset B_{4L}(0)$, satisfying*

$$\chi\left(W^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \leqslant \alpha^{-h} \right) \Psi_\alpha = \Psi_\alpha \tag{3.3.23}$$

for large enough α.

Proof. Using the states Ψ'''_α from Lemma 3.3.12, we define for $0 < \epsilon < \frac{1}{2}$

$$\Psi_\alpha := Z_\alpha^{-1} \chi^\epsilon \left(\alpha^h W^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \leqslant \frac{1}{2} \right) \Psi'''_\alpha$$

where Z_α is a normalizing constant. Clearly the states Ψ_α satisfy the strong condensation property $\chi\left(W^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \leqslant \alpha^{-h} \right) \Psi_\alpha = \Psi_\alpha$. In order to control the energy cost of the localization with respect to the operator $W^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} W_{\varphi^{\mathrm{Pek}}}$, note that the partition $\mathcal{P}' := \{F', G'\}$ with $F'(\rho) := \chi^\epsilon\left(\alpha^h \int \mathrm{d}\rho \leqslant \frac{1}{2}\right)$ and $G'(\rho) := \chi^\epsilon\left(\frac{1}{2} \leqslant \alpha^h \int \mathrm{d}\rho\right)$ satisfies

$$\kappa := V_{\mathcal{M}(\mathbb{R}^3)}(\mathcal{P}') \lesssim \alpha^4 \sup_{\rho, x \in \mathbb{R}^3} \left| \alpha^h \int \mathrm{d}\left(\rho + \alpha^{-2}\delta_x\right) - \alpha^h \int \mathrm{d}\rho \right|^2 = \alpha^{2h},$$

where we used $\left|\chi^\epsilon\left(y \leqslant \frac{1}{2}\right) - \chi^\epsilon\left(x \leqslant \frac{1}{2}\right)\right| \leqslant \left\| \frac{\mathrm{d}}{\mathrm{d}x}\chi^\epsilon\left(\cdot \leqslant \frac{1}{2}\right)\right\|_\infty |y - x|$ and the corresponding estimate for $\chi^\epsilon\left(\frac{1}{2} \leqslant \cdot\right)$. Therefore we obtain by Lemma 3.3.3, using $\Lambda \leqslant \alpha$,

$$\begin{aligned} Z_\alpha^2 \langle \Psi_\alpha | \mathbb{H}_\Lambda | \Psi_\alpha \rangle + (1 - Z_\alpha^2) \langle \widetilde{\Psi}_\alpha | \mathbb{H}_\Lambda | \widetilde{\Psi}_\alpha \rangle &\leqslant \langle \Psi'''_\alpha | \mathbb{H}_\Lambda | \Psi'''_\alpha \rangle + c'\, \alpha^{-\frac{7}{2}} \kappa \left\langle \Psi''' \middle| \sqrt{\mathcal{N} + 1} \middle| \Psi''' \right\rangle \\ &\leqslant E_\alpha + O_{\alpha\to\infty}\left(\alpha^{-2(1+\sigma)}\right) + O_{\alpha\to\infty}\left(\alpha^{2h - \frac{7}{2}}\right) = E_\alpha + O_{\alpha\to\infty}\left(\alpha^{-2(1+\sigma)}\right), \end{aligned} \tag{3.3.24}$$

with $\widetilde{\Psi}_\alpha := \sqrt{1-Z_\alpha^2}^{-1}\chi^\epsilon\left(\frac{1}{2}\leqslant \alpha^h W_{\varphi^{\mathrm{Pek}}}^{-1}\mathcal{N}W_{\varphi^{\mathrm{Pek}}}\right)\Psi_\alpha'''$. Making use of the trivial lower bound $E_\alpha \leqslant \langle\widetilde{\Psi}_\alpha|\mathbb{H}_\Lambda|\widetilde{\Psi}_\alpha\rangle$, Eq. (3.3.24) implies $\langle\Psi_\alpha|\mathbb{H}_\Lambda|\Psi_\alpha\rangle \leqslant E_\alpha + Z_\alpha^{-2}O_{\alpha\to\infty}\left(\alpha^{-2(1+\sigma)}\right)$, which concludes the proof since

$$1-Z_\alpha^2 = \left\langle \Psi_\alpha'''\middle|\chi^\epsilon\left(\frac{1}{2}\leqslant \alpha^h W_{\varphi^{\mathrm{Pek}}}^{-1}\mathcal{N}W_{\varphi^{\mathrm{Pek}}}\right)^2\middle|\Psi_\alpha'''\right\rangle$$
$$\leqslant \frac{1}{\frac{1}{2}-\epsilon}\alpha^h\left\langle\Psi_\alpha'''\middle|W_{\varphi^{\mathrm{Pek}}}^{-1}\mathcal{N}W_{\varphi^{\mathrm{Pek}}}\middle|\Psi_\alpha'''\right\rangle \lesssim \frac{1}{\frac{1}{2}-\epsilon}\alpha^h\alpha^{-\frac{2}{29}} \underset{\alpha\to\infty}{\longrightarrow} 0.$$

■

3.4 Large Deviation Estimates for Strong Condensates

In this Section we will derive a large deviation principle for states with suitably small particle number (compared to α^2), which can be interpreted as complete condensation with respect to the vacuum. We will show that such states are, up to an error which is exponentially small in α^2, contained in the spectral subspace $\left|a(f)+a^\dagger(f)\right|\leqslant\epsilon$, see Eq. (3.4.6). Note that taking the point of condensation to be the vacuum is not a real restriction, since this is the case after applying a suitable Weyl transformation. Before we can formulate the main result of this section in Proposition 3.4.2, we need to introduce some notation.

For $0<\sigma<\frac{1}{4}$ let us define $\Lambda := \alpha^{\frac{4}{5}(1+\sigma)}$, $\ell := \alpha^{-4(1+\sigma)}$ and

$$\Pi := \Pi^0_{\Lambda,\ell}, \tag{3.4.1}$$

see Definition 3.2.1, and let us identify $\mathcal{F}\left(\Pi L^2(\mathbb{R}^3)\right)$ with $L^2\big(\mathbb{R}^N\big)$ using the representation of real functions $\varphi=\sum_{n=1}^N\lambda_n\varphi_n\in\Pi L^2(\mathbb{R}^3)$ by points $\lambda=(\lambda_1,\dots,\lambda_N)\in\mathbb{R}^N$, where $N:=\dim \Pi L^2(\mathbb{R}^3)$ and $\{\varphi_1,\dots,\varphi_N\}$ is a real orthonormal basis of $\Pi L^2(\mathbb{R}^3)$. We choose this identification such that the annihilation operators $a_n := a(\varphi_n)$ read

$$a_n = \lambda_n + \frac{1}{2\alpha^2}\partial_{\lambda_n}, \tag{3.4.2}$$

where λ_n is the multiplication operator by the function $\lambda\mapsto\lambda_n$ on $L^2\big(\mathbb{R}^N\big)$. From the construction one readily checks that $N\lesssim(\Lambda/\ell)^3\leqslant\alpha^p$ for suitable $p>0$.

In the following we will verify a large deviation principle for the density function $\rho(\lambda):=\gamma(\lambda,\lambda)$ corresponding to a density matrix γ on $\mathcal{F}\left(\Pi L^2(\mathbb{R}^3)\right)$ that satisfies the strong condensation condition

$$\chi\left(\sum_{n=1}^N a_n^\dagger a_n\leqslant\alpha^{-h}\right)\gamma=\gamma \tag{3.4.3}$$

for some $h>0$. This result is comparable to [16, Lemma C.2]. For this purpose, we define a convenient norm $|\cdot|_\diamond$ on $\mathbb{R}^N$ in the subsequent Definition.

Definition 3.4.1. Let $|\lambda|:=\sqrt{\sum_{n=1}^N\lambda_n^2}$ denote the standard norm on $\mathbb{R}^N$ and let us define the norm $|\cdot|_\diamond$ on $\mathbb{R}^N$, using the identification $\varphi=\sum_{n=1}^N\lambda_n\varphi_n$, as

$$|\lambda|_\diamond := 2\sup_{x\in\mathbb{R}^3}\sqrt{\int_{B_1(x)}\left|\left((-\Delta)^{-\frac{1}{2}}\varphi\right)(y)\right|^2\mathrm{d}y}. \tag{3.4.4}$$

The norm $|\cdot|_\diamond$ will again appear naturally in Section 3.5 where we investigate properties of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$ (see Eq. (3.5.2) and the subsequent comment).

Proposition 3.4.2. *Let $0 < s < \min\left\{\frac{h}{2}, \frac{1}{5}(1-4\sigma)\right\}$ and $D > 0$. Then there exist constants $\beta, \alpha_0 > 0$, such that we have for all $\alpha \geqslant \alpha_0$, $\epsilon \geqslant D\alpha^{-s}$ and γ satisfying Eq. (3.4.3)*

$$\int_{|\lambda|_\diamond \geqslant \epsilon} \left(1 + |\lambda|^2\right) \rho(\lambda) \mathrm{d}\lambda \leqslant e^{-\beta \epsilon^2 \alpha^2}, \tag{3.4.5}$$

where $\rho(\lambda) := \gamma(\lambda, \lambda)$ is the density function corresponding to the state γ. Furthermore for all $\zeta \in \mathbb{R}^N$ and $\beta < \frac{1}{|\zeta|^2}$, there exists a constant $\alpha(\beta, |\xi|)$ such that

$$\int_{|\langle \zeta|\lambda\rangle| \geqslant \epsilon} \left(1 + |\lambda|^2\right) \rho(\lambda) \mathrm{d}\lambda \leqslant e^{-\beta \epsilon^2 \alpha^2} \tag{3.4.6}$$

for all $\alpha \geqslant \alpha(\beta, |\xi|)$ and $\epsilon \geqslant D\alpha^{-s}$.

The restriction to the finite dimensional space $\Pi L^2(\mathbb{R}^3)$ will be essential in the proof of Proposition 3.4.2, to be precise we will make use of the fact that $N \lesssim \alpha^p$ for a suitable $p > 0$, which in particular implies that $N \lesssim e^{\alpha^t}$, uniformly in α, for any $t > 0$. Before we prove Proposition 3.4.2, we first need auxiliary results concerning the $|\cdot|_\diamond$ norm.

Definition 3.4.3. For $x \in \mathbb{R}^3$ and $r > 0$, let us define $T_x\lambda := -2\chi\left(|\cdot - x| \leqslant 1\right)(-\Delta)^{-\frac{1}{2}} \varphi$ and $T_{\geqslant r}\lambda := -2\chi\left(|\cdot| \geqslant r\right)(-\Delta)^{-\frac{1}{2}} \varphi$ with the above identification $\varphi = \sum_{n=1}^N \lambda_n \varphi_n$. Furthermore let us define the operators $A_x := \sqrt{T_x^\dagger T_x}$ and $A_{\geqslant r} := \sqrt{T_{\geqslant r}^\dagger T_{\geqslant r}}$, as well as the constant $\beta_0 := \inf_{x \in \mathbb{R}^3} \|A_x\|^{-2}$.

Using the operators A_x we can write $|\lambda|_\diamond = \sup_{x \in \mathbb{R}^3} |A_x \lambda|$, which is bounded by

$$|\lambda|_\diamond \leqslant 65 \max\left\{\sup_{z \in \mathbb{Z}^3 : |z| \leqslant r+1} |A_z \lambda|, \, |A_{\geqslant r}\lambda|\right\} \tag{3.4.7}$$

for any $r > 0$. In order to see this, note that for any $y \in \mathbb{R}^3$ there exists a $z \in \mathbb{Z}^3$ with $|y - z| < 1$. In case $y \in B_r(0) \cap B_1(x)$, where $x \in \mathbb{R}^3$, we see that z satisfies $|z| \leqslant r + 1$ and $|x - z| < 2$. Denoting the set of such z by $M(x, r) \subset \mathbb{Z}^3$, we obtain $B_1(x) \subset \bigcup_{z \in M(x,r)} B_1(z) \cup (\mathbb{R}^3 \backslash B_r(0))$. Consequently

$$|\lambda|_\diamond \leqslant \sup_x \sum_{z \in M(x,r)} |A_z\lambda| + |A_{\geqslant r}\lambda| \leqslant \sup_x \Big(|M(x,r)| + 1\Big) \max_x \Big\{\sup_{z \in M(x,r)} |A_z\lambda|, \, |A_{\geqslant r}\lambda|\Big\}.$$

This concludes the proof of Eq. (3.4.7), since there are at most 64 elements $z \in \mathbb{Z}^3$ satisfying $|x - z| < 2$.

Lemma 3.4.4. *The constant β_0 from Definition 3.4.3 is positive, uniformly in α, and $\|A_x\|_{\mathrm{HS}} \lesssim \Lambda$ uniformly in $x \in \mathbb{R}^3$, where Λ is defined above Eq. (3.4.1). Furthermore there exists a constant $v > 0$ such that $\|A_{\geqslant r}\|_{\mathrm{HS}} \lesssim \frac{\alpha^v}{\sqrt{r}}$ for all $\alpha \geqslant 1$ and $r > 0$.*

Proof. Note that the space $\Pi L^2(\mathbb{R}^3)$ is contained in the spectral subspace $-\Delta \leqslant \Lambda^2$, hence $\Pi \leqslant (1+\Lambda^2)(1-\Delta)^{-1}$, and therefore

$$\|A_x\|_{\mathrm{HS}}^2 = 4\left\|\chi\left(|\cdot - x| \leqslant 1\right)(-\Delta)^{-\frac{1}{2}}\Pi\right\|_{\mathrm{HS}}^2 \leqslant 4\left(1+\Lambda^2\right)\left\|\chi\left(|\cdot - x| \leqslant 1\right)(-\Delta)^{-\frac{1}{2}}(1-\Delta)^{-\frac{1}{2}}\right\|_{\mathrm{HS}}^2$$
$$= 4\left(1+\Lambda^2\right)\left\|\chi\left(|\cdot| \leqslant 1\right)(-\Delta)^{-\frac{1}{2}}(1-\Delta)^{-\frac{1}{2}}\right\|_{\mathrm{HS}}^2.$$

Applying Eq. (3.9.5) with $\psi = \chi(|.| \leqslant 1)$ yields that $\chi(|\cdot| \leqslant 1)(-\Delta)^{-\frac{1}{2}}(1-\Delta)^{-\frac{1}{2}}$ is Hilbert-Schmidt, hence $\|A_x\|_{\mathrm{HS}} \lesssim \Lambda$. In order to prove the uniform lower bound $\beta_0 > 0$, it is enough to verify the boundedness of $\chi(|.| \leqslant 1) f(-\Delta)$, where $f(t) := \frac{\chi(|t| \leqslant 1)}{\sqrt{t}}$. An explicit computation in Fourier space yields for $\varphi \in L^2(\mathbb{R}^3)$

$$\langle \varphi | f(-\Delta)\chi(|.| \leqslant 1) f(-\Delta)|\varphi\rangle = \int_{|k|\leqslant 1}\int_{|k|\leqslant 1} \frac{\widehat{\chi(|\cdot| \leqslant 1)}(k-k')\overline{\widehat{\varphi}(k)}\widehat{\varphi}(k')}{|k|\,|k'|}\mathrm{dkdk}$$
$$\leqslant \left\|\widehat{\chi(|\cdot| \leqslant 1)}\right\|_\infty \left|\int_{|k|\leqslant 1}\frac{|\widehat{\varphi}(k)|}{|k|}\mathrm{dk}\right|^2 \lesssim \|\varphi\|^2.$$

Finally we are going to verify $\|A_{\geqslant r}\|_{\mathrm{HS}} \lesssim \frac{\alpha^v}{\sqrt{r}}$, using that

$$\|A_{\geqslant r}\|_{\mathrm{HS}} = 2\sqrt{\sum_{n=1}^N \left\|\chi(|\cdot| \geqslant r)(-\Delta)^{-\frac{1}{2}}\varphi_n\right\|^2} \lesssim \sqrt{N}\frac{\alpha^v}{\sqrt{r}}$$

for a suitable constant $v > 0$ by Corollary 3.9.2, where N is the dimension of $\Pi L^2(\mathbb{R}^3)$. This concludes the proof, since $N \lesssim \alpha^p$ for some $p > 0$. ∎

Proof of Proposition 3.4.2. Making use of Eq. (3.4.7) and defining $\epsilon_* := \frac{\epsilon}{65}$, we obtain

$$\int_{|\lambda|_\diamond \geqslant \epsilon}\left(1+|\lambda|^2\right)\rho(\lambda)\mathrm{d}\lambda \leqslant \sum_{|z|\leqslant r+1}\int_{|A_z\lambda|\geqslant \epsilon_*}\left(1+|\lambda|^2\right)\rho(\lambda)\mathrm{d}\lambda + \int_{|A_{\geqslant r}\lambda|\geqslant \epsilon_*}\left(1+|\lambda|^2\right)\rho(\lambda)\mathrm{d}\lambda,$$

where the sum runs over $z \in \mathbb{Z}^3$ with $|z| \leqslant r+1$. In the following we are going to verify that every contribution of the form $\int_{|A_x\lambda|\geqslant \epsilon_*}(1+|\lambda|^2)\rho(\lambda)\mathrm{d}\lambda$ is exponentially small uniformly in $x \in \mathbb{R}^3$. As a consequence of Eq. (3.4.3), we have for $t \geqslant 0$ the estimate

$$\gamma \leqslant \chi\left(\sum_{n=1}^N a_n^\dagger a_n \leqslant \alpha^{-h}\right) \leqslant e^{t\left(\alpha^{-h} - \sum_{n=1}^N a_n^\dagger a_n\right)}.$$

By our assumption on s, there exists a h' such that $2s < h' < h$. Consequently we obtain for $t := \alpha^{2+(h-h')}$, using Mehler's kernel,

$$\rho(\lambda) = \gamma(\lambda,\lambda) \leqslant e^{\alpha^{2-h'}} e^{-t\sum_{n=1}^N a_n^\dagger a_n}(\lambda,\lambda) = e^{\alpha^{2-h'}}\left(\frac{1}{1-e^{-\alpha^{h-h'}}}\right)^N \left(\frac{\alpha^2 w_\alpha}{\pi}\right)^{\frac{N}{2}} e^{-\alpha^2 w_\alpha |\lambda|^2}, \tag{3.4.8}$$

with $w_\alpha := \coth\left(\alpha^{h-h'}\right) - \mathrm{cosech}\left(\alpha^{h-h'}\right)$. Since $Ne^{-\alpha^{h-h'}} \underset{\alpha\to\infty}{\longrightarrow} 0$, it is clear that $\left(\frac{1}{1-e^{-\alpha^{h-h'}}}\right)^N$ is bounded uniformly in α. Since $w_\alpha \geqslant 0$ is strictly increasing in α, we can choose

$0 < \beta' < \beta_0 \inf_{\alpha \geqslant 1} w_\alpha$, where β_0 is the constant from Definition 3.4.3. Consequently $\|\frac{\beta'}{w_\alpha}|A_x|^2\| < 1$ uniformly in $x \in \mathbb{R}^3$ and $\alpha \geqslant 1$, and in particular $\left(1 - \frac{\beta'}{w_\alpha}|A_x|^2\right)^{-1}$ is a bounded operator. Hence we obtain for $x \in \mathbb{R}^3$

$$\int_{|A_x\lambda| \geqslant \epsilon_*} \left(1 + |\lambda|^2\right) \rho(\lambda) \mathrm{d}\lambda \lesssim e^{\alpha^{2-h'}} \left(\frac{\alpha^2 w_\alpha}{\pi}\right)^{\frac{N}{2}} \int_{|A_x\lambda| \geqslant \epsilon_*} \left(1 + |\lambda|^2\right) e^{-\alpha^2 w_\alpha |\lambda|^2} \mathrm{d}\lambda$$
$$\leqslant e^{\alpha^{2-h'}} \left(\frac{\alpha^2 w_\alpha}{\pi}\right)^{\frac{N}{2}} \int_{\mathbb{R}^N} \left(1 + |\lambda|^2\right) e^{-\alpha^2 \left(w_\alpha |\lambda|^2 + \beta' \epsilon_*^2 - \beta' |A_x \lambda|^2\right)} \mathrm{d}\lambda$$
$$= e^{\alpha^{2-h'}} \frac{w_\alpha + \alpha^{-2} \mathrm{Tr} \left(1 - \frac{\beta'}{w_\alpha}|A_x|^2\right)^{-1}}{w_\alpha \det \sqrt{1 - \frac{\beta'}{w_\alpha}|A_x|^2}} \, e^{-\beta' \epsilon_*^2 \alpha^2}.$$

Furthermore, for a suitable, x-independent, constant μ

$$e^{\alpha^{2-h'}} \frac{w_\alpha + \alpha^{-2} \mathrm{Tr} \left(1 - \frac{\beta'}{w_\alpha}|A_x|^2\right)^{-1}}{w_\alpha \det \sqrt{1 - \frac{\beta'}{w_\alpha}|A_x|^2}} \lesssim e^{\alpha^{2-h'}} \frac{\alpha^p}{\det \sqrt{1 - \frac{\beta'}{w_\alpha}|A_x|^2}}$$
$$= e^{\alpha^{2-h'} + p \ln \alpha - \frac{1}{2} \mathrm{Tr} \ln \left(1 - \frac{\beta'}{w_\alpha}|A_x|^2\right)} \leqslant e^{\alpha^{2-h'} + p \ln \alpha + \mu \|A_x\|_{\mathrm{HS}}^2} \leqslant e^{\alpha^{2-h'} + p \ln \alpha + \mu C \Lambda^2}, \tag{3.4.9}$$

where we have used the rough estimate $w_\alpha + \alpha^{-2} \mathrm{Tr} \left(1 - \frac{\beta'}{w_\alpha}|A_x|^2\right)^{-1} \lesssim 1 + \alpha^{-2} N \lesssim \alpha^p$ for a suitable exponent $p > 0$ in the first inequality and Lemma 3.4.4 in the last inequality. Note that the exponent in Eq. (3.4.9) is of order $\alpha^{\max\left\{2-h', \frac{8}{5}(1+\sigma)\right\}} \ll \epsilon_*^2 \alpha^2$ since $\Lambda^2 = \alpha^{\frac{8}{5}(1+\sigma)}$ and $\epsilon \geqslant D\alpha^{-s}$ with $s < \min\left\{\frac{h'}{2}, \frac{1}{5}(1 - 4\sigma)\right\}$.

Defining $r := \alpha^{2q}$ with $q > v$, where v is the constant from Lemma 3.4.4 and making use of the fact that the number of $z \in \mathbb{Z}^3$ with $|z| \leqslant r + 1$ is of order $r^3 = \alpha^{6q}$, we obtain

$$\sum_{|z| \leqslant r+1} \int_{|A_z\lambda| \geqslant \epsilon_*} \left(1 + |\lambda|^2\right) \rho(\lambda) \mathrm{d}\lambda \, \mathrm{d}x \lesssim \alpha^{6q} e^{\alpha^{2-h'} + p \ln \alpha + \mu C \Lambda^2 - \beta' \epsilon_*^2 \alpha^2} \leqslant e^{-\beta \epsilon_*^2 \alpha^2}$$

for $\beta < \beta'$ and α large enough. We have $\|A_{\geqslant r}\|_{\mathrm{HS}} \underset{\alpha \to \infty}{\longrightarrow} 0$ by Lemma 3.4.4 and our choice $r = \alpha^{2q}$ with $q > v$. Using Eq. (3.4.8), and an argument similar to the one in Eq. (3.4.9), we can therefore estimate $\int_{|A_{\geqslant r}\lambda| \geqslant \epsilon_*} \left(1 + |\lambda|^2\right) \rho(\lambda) \mathrm{d}\lambda$ by

$$\int_{|A_{\geqslant r}\lambda| \geqslant \epsilon_*} \left(1 + |\lambda|^2\right) \rho(\lambda) \mathrm{d}\lambda \lesssim e^{\alpha^{2-h'}} \left(\frac{\alpha^2 w_\alpha}{\pi}\right)^{\frac{N}{2}} \int_{|A_{\geqslant r}\lambda| \geqslant \epsilon_*} \left(1 + |\lambda|^2\right) e^{-\alpha^2 w_\alpha |\lambda|^2} \mathrm{d}\lambda$$
$$\lesssim e^{\alpha^{2-h'}} \frac{\alpha^p}{\det \sqrt{1 - \frac{\beta'}{w_\alpha}|A_{\geqslant r}|^2}} \, e^{-\beta' \epsilon_*^2 \alpha^2} \lesssim e^{\alpha^{2-h'} + p \ln \alpha + \mu \|A_{\geqslant r}\|_{\mathrm{HS}}^2 - \beta' \epsilon_*^2 \alpha^2}.$$

Again we observe that the exponent $\alpha^{2-h'} + p \ln \alpha + \mu \|A_{\geqslant r}\|_{\mathrm{HS}}^2$ is small compared to $\epsilon_*^2 \alpha^2$, which concludes the proof of Eq. (3.4.5).

The proof of Eq. (3.4.6) can be carried out analogously with the help of the operator $A_\zeta \lambda := \langle \zeta | \lambda \rangle \frac{\zeta}{\|\zeta\|}$ using the fact that $\|A_\zeta\|_{\mathrm{HS}} = \|A_\zeta\| = |\zeta|$ and the assumption $\beta < \frac{1}{|\xi|^2}$. More precisely we obtain for $\beta < \beta' < \frac{1}{|\xi|^2}$

$$\int_{|\langle\zeta|\lambda\rangle|\geqslant\epsilon} \left(1+|\lambda|^2\right)\rho(\lambda)\mathrm{d}\lambda \lesssim e^{\alpha^{2-h'}}\left(\frac{\alpha^2 w_\alpha}{\pi}\right)^{\frac{N}{2}}\int_{|A_\zeta\lambda|\geqslant\epsilon}\left(1+|\lambda|^2\right)e^{-\alpha^2 w_\alpha|\lambda|^2}\mathrm{d}\lambda$$
$$\lesssim e^{\alpha^{2-h'}}\frac{\alpha^p}{\det\sqrt{1-\frac{\beta'}{w_\alpha}|A_\zeta|^2}}\,e^{-\beta'\epsilon^2\alpha^2} \lesssim e^{\alpha^{2-h'}+p\ln\alpha+\mu\|A_\zeta\|_{\mathrm{HS}}^2-\beta'\epsilon^2\alpha^2} \leqslant e^{-\beta\epsilon^2\alpha^2}.$$

■

3.5 Properties of the Pekar Functional

In this section we are going to discuss essential properties of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$, and we are going to verify an asymptomatically sharp quadratic approximation for $\mathcal{F}^{\mathrm{Pek}}(\varphi)$, which is valid for all field configurations φ close to a minimizer φ^{Pek}. It has been proven in [40] that a suitable quadratic approximation of $\mathcal{F}^{\mathrm{Pek}}$ holds for all configurations φ satisfying $\|V_{\varphi-\varphi^{\mathrm{Pek}}}\| \ll 1$, where

$$V_\varphi := -2\,(-\Delta)^{-\frac{1}{2}}\,\mathfrak{Re}\,\varphi. \tag{3.5.1}$$

In the following we are showing that this result is still valid, in case we substitute the L^2-norm with the weaker $\|\cdot\|_\diamond$ norm, which is a hybrid between the L^2 and the L^∞ norm defined as

$$\|V\|_\diamond := \sup_{x\in\mathbb{R}^3}\sqrt{\int_{B_1(x)}|V(y)|^2\,\mathrm{d}y}, \tag{3.5.2}$$

where $B_1(x)$ is the unit ball centered at $x\in\mathbb{R}^3$. This will be the content of Lemma 3.5.2 and Theorem 3.5.4, respectively. We have $\|V_\varphi\|_\diamond = |\lambda|_\diamond$ for $\varphi = \sum_{n=1}^N \lambda_n\varphi_n$, where $|\cdot|_\diamond$ is the norm defined in Eq. (3.4.4). Before we come to the proof of Lemma 3.5.2, we first need the subsequent auxiliary Lemma 3.5.1.

Lemma 3.5.1. *There exists a constant $C>0$ such that the operator inequality*

$$V^2 \leqslant C\|V\|_\diamond^2\,(1-\Delta)^2 \tag{3.5.3}$$

holds for all (measurable) $V:\mathbb{R}^3\longrightarrow\mathbb{R}$, where V^2 is interpreted as a multiplication operator.

Proof. As a first step, we are going to verify that Eq. (3.5.3) holds in case we use the L^2 norm $\|V\|$ instead of $\|V\|_\diamond$. This follows from $V^2 \leqslant \|V(1-\Delta)^{-1}\|_{\mathrm{HS}}^2\,(1-\Delta)^2$, where $\|\cdot\|_{\mathrm{HS}}$ is the Hilbert-Schmidt norm, and

$$\left\|V(1-\Delta)^{-1}\right\|_{\mathrm{HS}}^2 = \int\int V(x)^2K(y-x)^2\,\mathrm{d}x\mathrm{d}y = \int K(y)^2\mathrm{d}y\,\|V\|^2$$

with $K(y-x)$ being the kernel of the operator $(1-\Delta)^{-1}$. Note that $C' := \int K(y)^2\mathrm{d}y$ is finite, which concludes the first step. In order to obtain the analogue statement for $\|V\|_\diamond$, let χ be a smooth, non-negative, function with $\mathrm{supp}\,(\chi)\subset B_1(0)$ and $\int_{\mathbb{R}^3}\chi(y)^2\,\mathrm{d}y = 1$.

Defining $\chi_y(x) := \chi(x-y)$ for $y \in \mathbb{R}^3$ and using the previously derived inequality $V^2 \leqslant C'\|V\|^2 (1-\Delta)^2$, which holds for any $V \in L^2(\mathbb{R}^3)$, we obtain

$$V^2 = \int \chi_y V^2 \chi_y \,\mathrm{d}y = \int \chi_y \left(\mathbb{1}_{B_1(y)} V\right)^2 \chi_y \,\mathrm{d}y \leqslant C' \int \|\mathbb{1}_{B_1(y)} V\|^2 \chi_y (1-\Delta)^2 \chi_y \,\mathrm{d}y$$
$$\leqslant C'\|V\|_\diamond^2 \int \chi_y (1-\Delta)^2 \chi_y \,\mathrm{d}y = C'\|V\|_\diamond^2 \int \left|(1-\Delta)\chi_y\right|^2 \mathrm{d}y,$$

where $|A|^2 = A^\dagger A$. Furthermore $(1-\Delta)\chi_y = \chi_y(1-\Delta) - 2(\nabla\chi_y)\nabla - (\Delta\chi_y)$, which yields together with a Cauchy–Schwarz inequality the estimate

$$\int \left|(1-\Delta)\chi_y\right|^2 \mathrm{d}y \leqslant 3\int \left((1-\Delta)\chi_y^2(1-\Delta) - 4\nabla\left|\nabla\chi_y\right|^2\nabla + |\Delta\chi_y|^2\right)\mathrm{d}y$$
$$= 3(1-\Delta)^2 - 12\,\nabla\left(\int \left|\nabla\chi_y^2\right| \mathrm{d}y\right)\nabla + 3\int |\Delta\chi_y|^2 \mathrm{d}y \lesssim (1-\Delta)^2,$$

where we have used that $\int |\nabla\chi(y)|^2 \,\mathrm{d}y$ and $\int |\Delta\chi(y)|^2 \,\mathrm{d}y$ are finite. ∎

In the following we are going to use that we can write the Pekar energy as

$$\mathcal{F}^{\mathrm{Pek}}(\varphi) = \|\varphi\|^2 + \inf\sigma\left(-\Delta + V_\varphi\right), \tag{3.5.4}$$

where V_φ is defined in Eq. (3.5.1). As an immediate consequence of Eq. (3.5.3) we have $\pm V \leqslant \sqrt{C}\|V\|_\diamond (1-\Delta)$ and consequently there exists a $\delta_0 > 0$ and a contour $\mathcal{C} \subset \mathbb{C}$, such that $\mathcal{C}$ separates the ground state energy $\inf\sigma(-\Delta+V)$ from the excitation spectrum of $H_V := -\Delta + V$ for all V with $\|V - V_{\varphi^{\mathrm{Pek}}}\|_\diamond < \delta_0$, see also [40]. This allows us to further identify $\mathcal{F}^{\mathrm{Pek}}(\varphi)$ as

$$\mathcal{F}^{\mathrm{Pek}}(\varphi) = \|\varphi\|^2 + \mathrm{Tr}\int_{\mathcal{C}} \frac{z}{z - H_{V_\varphi}} \frac{\mathrm{d}z}{2\pi i} \tag{3.5.5}$$

for all φ satisfying $\|V_{\varphi-\varphi^{\mathrm{Pek}}}\|_\diamond < \delta_0$. Following the strategy in [40], we will use Eq. (3.5.5) to compare $\mathcal{F}^{\mathrm{Pek}}(\varphi)$ with $e^{\mathrm{Pek}} = \mathcal{F}^{\mathrm{Pek}}(\varphi^{\mathrm{Pek}})$. Before we do this let us introduce the operators

$$K^{\mathrm{Pek}} := 1 - H^{\mathrm{Pek}} = 4(-\Delta)^{-\frac{1}{2}}\,\psi^{\mathrm{Pek}} \frac{1 - |\psi^{\mathrm{Pek}}\rangle\langle\psi^{\mathrm{Pek}}|}{H_{V^{\mathrm{Pek}}} - \mu^{\mathrm{Pek}}}\psi^{\mathrm{Pek}}(-\Delta)^{-\frac{1}{2}}, \tag{3.5.6}$$
$$L^{\mathrm{Pek}} := 4(-\Delta)^{-\frac{1}{2}}\,\psi^{\mathrm{Pek}}(1-\Delta)^{-1}\psi^{\mathrm{Pek}}(-\Delta)^{-\frac{1}{2}}, \tag{3.5.7}$$

where H^{Pek} is defined in Eq. (3.1.4), $\mu^{\mathrm{Pek}} := e^{\mathrm{Pek}} - \|\varphi^{\mathrm{Pek}}\|^2$ and ψ^{Pek} is the, non-negative, ground state of the operator $H_{V^{\mathrm{Pek}}}$ with $V^{\mathrm{Pek}} := V_{\varphi^{\mathrm{Pek}}}$, which we interpret as a multiplication operator in Eqs. (3.5.6) and (3.5.7). The following Lemma 3.5.2 can be proved in the same way as [40, Proposition 3.3], using Lemma 3.5.1.

Lemma 3.5.2. *There exist constants $c, \delta_0 > 0$ such that for all φ with $\|V_{\varphi-\varphi^{\mathrm{Pek}}}\|_\diamond < \delta_0$*

$$\left|\mathcal{F}^{\mathrm{Pek}}(\varphi) - e^{\mathrm{Pek}} - \langle\varphi-\varphi^{\mathrm{Pek}}|1-K^{\mathrm{Pek}}|\varphi-\varphi^{\mathrm{Pek}}\rangle\right| \leqslant c\|V_{\varphi-\varphi^{\mathrm{Pek}}}\|_\diamond \langle\varphi-\varphi^{\mathrm{Pek}}|L^{\mathrm{Pek}}|\varphi-\varphi^{\mathrm{Pek}}\rangle. \tag{3.5.8}$$

Proof. By taking δ_0 small enough, we can assume for all V with $\|V_{\varphi-\varphi^{\mathrm{Pek}}}\|_\diamond < \delta_0$ that

$$\sup_{z\in\mathcal{C}} \left\| V_{\varphi-\varphi^{\mathrm{Pek}}} \frac{1}{z - H_{V^{\mathrm{Pek}}}} \right\|_{\mathrm{op}} < 1, \tag{3.5.9}$$

where $\|\cdot\|_{\mathrm{op}}$ denotes the operator norm. This immediately follows from

$$\left\| V_{\varphi-\varphi^{\mathrm{Pek}}} \frac{1}{H_{V^{\mathrm{Pek}}}-z} \right\|_{\mathrm{op}}^2 \lesssim \left\| \left(V_\varphi - V^{\mathrm{Pek}}\right)(1-\Delta)^{-1} \right\|_{\mathrm{op}}^2 \leqslant C \|V_{\varphi-\varphi^{\mathrm{Pek}}}\|_\diamond^2,$$

where we used Eq. (3.5.3) and the fact that the spectrum of $H_{V^{\mathrm{Pek}}}$ has a positive distance to the contour $\mathcal{C}$, allowing us to bound the operator norm of $(1-\Delta)\frac{1}{H_{V^{\mathrm{Pek}}}-z}$ uniformly in $z \in \mathcal{C}$. Given Eq. (3.5.9), it has been verified in the proof of [40, Proposition 3.3] that

$$\left| \|\varphi\|^2 + \mathrm{Tr} \int_{\mathcal{C}} \frac{z}{z-H_{V_\varphi}} \frac{\mathrm{d}z}{2\pi i} - e^{\mathrm{Pek}} - \langle \varphi - \varphi^{\mathrm{Pek}} | 1 - K^{\mathrm{Pek}} | \varphi - \varphi^{\mathrm{Pek}} \rangle \right|$$
$$\lesssim \epsilon \langle \varphi - \varphi^{\mathrm{Pek}} | L^{\mathrm{Pek}} | \varphi - \varphi^{\mathrm{Pek}} \rangle$$

for $\epsilon := \sup_{z\in\mathcal{C}} \left\{ \left\|\frac{A}{1-A}\right\|_{\mathrm{op}} + \left\|\frac{B}{1-B}\right\|_{\mathrm{op}} + \left\|(1-\Delta)^{\frac{1}{2}} \frac{1}{z-H_{V^{\mathrm{Pek}}}} \frac{A}{1-A} (1-\Delta)^{\frac{1}{2}}\right\|_{\mathrm{op}} \right\}$, where we denote $A := \left(V_{\varphi-\varphi^{\mathrm{Pek}}}\right)\frac{1}{z-H_{V^{\mathrm{Pek}}}}$ and $B := \left(1 - |\psi^{\mathrm{Pek}}\rangle\langle\psi^{\mathrm{Pek}}|\right) A^\dagger$. In the following we want to verify that $\epsilon \lesssim \|V_{\varphi-\varphi^{\mathrm{Pek}}}\|_\diamond$, which concludes the proof by Eq. (3.5.5). Since $(1-\Delta)\frac{1}{z-H_{V^{\mathrm{Pek}}}}$ is uniformly bounded in z, $\left\|\frac{A}{1-A}\right\|_{\mathrm{op}} \leqslant \frac{\|A\|_{\mathrm{op}}}{1-\|A\|_{\mathrm{op}}} \lesssim \left\| \left(V_{\varphi-\varphi^{\mathrm{Pek}}}\right)(1-\Delta)^{-1} \right\|_{\mathrm{op}} \lesssim \|V_{\varphi-\varphi^{\mathrm{Pek}}}\|_\diamond$ by Eq. (3.5.3). Similarly $\left\|\frac{B}{1-B}\right\|_{\mathrm{op}} \lesssim \|V_{\varphi-\varphi^{\mathrm{Pek}}}\|_\diamond$. Regarding the final term in the definition of ϵ, note that $(1-\Delta)^{\frac{1}{2}}\frac{1}{z-H_{V^{\mathrm{Pek}}}}(1-\Delta)^{\frac{1}{2}}$ is uniformly bounded in z, and therefore

$$\left\|(1-\Delta)^{\frac{1}{2}} \frac{1}{z-H_{V^{\mathrm{Pek}}}} \frac{A}{1-A} (1-\Delta)^{\frac{1}{2}}\right\|_{\mathrm{op}} \lesssim \left\|(1-\Delta)^{-\frac{1}{2}} \frac{A}{1-A} (1-\Delta)^{\frac{1}{2}}\right\|_{\mathrm{op}} = \left\|\frac{A'}{1-A'}\right\|_{\mathrm{op}},$$

with $A' := (1-\Delta)^{-\frac{1}{2}} A (1-\Delta)^{\frac{1}{2}}$. Furthermore $\left\|\frac{A'}{1-A'}\right\|_{\mathrm{op}} \leqslant \frac{\|A'\|_{\mathrm{op}}}{1-\|A'\|_{\mathrm{op}}}$ and

$$\|A'\|_{\mathrm{op}} \lesssim \left\|(1-\Delta)^{-\frac{1}{2}} \left(V_{\varphi-\varphi^{\mathrm{Pek}}}\right)(1-\Delta)^{-\frac{1}{2}}\right\|_{\mathrm{op}} \leqslant \left\| \left(V_{\varphi-\varphi^{\mathrm{Pek}}}\right)(1-\Delta)^{-1} \right\|_{\mathrm{op}} \lesssim \|V_{\varphi-\varphi^{\mathrm{Pek}}}\|_\diamond.$$

■

Lemma 3.5.2 gives a lower bound on $\mathcal{F}^{\mathrm{Pek}}\left(\varphi^{\mathrm{Pek}}+\xi\right) - e^{\mathrm{Pek}}$ in terms of a quadratic function $\xi \mapsto \langle \xi | 1 - \left(K^{\mathrm{Pek}} + \epsilon L^{\mathrm{Pek}}\right) | \xi \rangle$ for ξ satisfying $\|V_\xi\|_\diamond < \min\{\frac{\epsilon}{c}, \delta_0\}$. Due to the translation invariance of $\mathcal{F}^{\mathrm{Pek}}$, this lower bound is however insufficient, since we have for all $\xi \in \mathrm{span}\{\partial_{y_1}\varphi^{\mathrm{Pek}}, \partial_{y_2}\varphi^{\mathrm{Pek}}, \partial_{y_3}\varphi^{\mathrm{Pek}}\}\backslash\{0\}$

$$\langle \xi | 1 - \left(K^{\mathrm{Pek}} + \epsilon L^{\mathrm{Pek}}\right) | \xi \rangle = \mathrm{Hess}|_{\varphi^{\mathrm{Pek}}} \mathcal{F}^{\mathrm{Pek}}[\xi] - \epsilon \langle \xi | L^{\mathrm{Pek}} | \xi \rangle = -\epsilon \langle \xi | L^{\mathrm{Pek}} | \xi \rangle < 0, \tag{3.5.10}$$

i.e. the quadratic lower bound is not even non-negative. In order to improve this lower bound, we will introduce a suitable coordinate transformation τ in Definition 3.5.3. Before we can formulate Definition 3.5.3 we need some auxiliary preparations.

In the following let Π be the projection defined in Eq. (3.4.1) and let us define the real orthonormal system

$$\varphi_n := \frac{\Pi \partial_{y_n} \varphi^{\mathrm{Pek}}}{\|\Pi \partial_{y_n} \varphi^{\mathrm{Pek}}\|} \tag{3.5.11}$$

for $n \in \{1,2,3\}$, which we complete to a real orthonormal basis $\{\varphi_1,..,\varphi_N\}$ of $\Pi L^2(\mathbb{R}^3)$. Furthermore let us write $\varphi_x^{\text{Pek}}(y) := \varphi^{\text{Pek}}(y-x)$ for the translations of φ^{Pek} and let us define the map $\omega : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ as

$$\omega(x) := \left(\langle \varphi_n | \varphi_x^{\text{Pek}} \rangle\right)_{n=1}^{3} \in \mathbb{R}^3. \tag{3.5.12}$$

Since $\varphi^{\text{Pek}} \in H^1(\mathbb{R}^3)$, ω is differentiable. Moreover, since φ^{Pek} is invariant under the action of $O(3)$ and since the operator Π commutes with the reflections $y_i \to -y_i$ and permutations $y_i \leftrightarrow y_j$, it is clear that $\omega(0) = 0$. By the same argument we see that $D|_0\omega$ has full rank and therefore there exists a local inverse $t \mapsto x_t$ for $|t| < \delta_*$ and a suitable constant $\delta_* > 0$.

Definition 3.5.3. We define the map $\tau : \Pi L^2(\mathbb{R}^3) \longrightarrow \Pi L^2(\mathbb{R}^3)$ as

$$\tau(\varphi) := \varphi - f(t^\varphi),$$

where $t^\varphi := \big(\langle \varphi_1|\varphi\rangle, \langle \varphi_2|\varphi\rangle, \langle \varphi_3|\varphi\rangle\big) \in \mathbb{R}^3$ and $f(t)$ is defined as

$$f(t) := \chi\big(|t| < \delta_*\big) \left(\Pi\varphi_{x_t}^{\text{Pek}} - \sum_{n=1}^{3} t_n \varphi_n\right).$$

The map τ is constructed in a way such that it "flattens" the manifold of Pekar minimizers $\{\varphi_x^{\text{Pek}} : x \in \mathbb{R}^3\}$. More precisely, we have that $\tau\left(\Pi\varphi_x^{\text{Pek}}\right)$ is for all small enough $x \in \mathbb{R}^3$ an element of the linear space spanned by $\{\varphi_1, \varphi_2, \varphi_3\}$. A similar construction appears in [16] and, in a somewhat different way, in [37].

Recall the operators K^{Pek} and L^{Pek} from Eqs. (3.5.6) and (3.5.7), and let T_x be the translation operator defined by $(T_x\varphi)(y) := \varphi(y-x)$. Then we define the operators $K_x^{\text{Pek}} := T_x\, K^{\text{Pek}}\, T_{-x}$ and $L_x^{\text{Pek}} := T_x\, L^{\text{Pek}}\, T_{-x}$, as well as for $|t| < \epsilon$ with $\epsilon < \delta_*$

$$J_{t,\epsilon} := \pi\Big(1 - (1+\epsilon)\left(K_{x_t}^{\text{Pek}} + \epsilon L_{x_t}^{\text{Pek}}\right)\Big)\pi, \tag{3.5.13}$$

where $\pi : L^2(\mathbb{R}^3) \longrightarrow L^2(\mathbb{R}^3)$ is the orthogonal projection onto the subspace spanned by $\{\varphi_4, \dots, \varphi_N\}$. Furthermore we define $J_{t,\epsilon} := \pi$ for $|t| \geqslant \epsilon$. In contrast to the operator $1 - \left(K^{\text{Pek}} + \epsilon L^{\text{Pek}}\right)$ from Eq. (3.5.10), the operator $J_{t,\epsilon}$ is non-negative for ϵ small enough, as will be shown in Lemma 3.9.5. With the operator $J_{t,\epsilon}$ and the transformation τ at hand we can formulate a strong lower bound for $\mathcal{F}^{\text{Pek}}(\varphi) - e^{\text{Pek}}$ in the subsequent Theorem 3.5.4, where we use the shorthand notation $J_{t,\epsilon}\big[\varphi\big] := \langle\varphi|J_{t,\epsilon}|\varphi\rangle$.

Theorem 3.5.4. *There exist constants $C > 0$, $0 < \epsilon_0 \leqslant \delta_*$ and $0 < D \leqslant 1$ such that*

$$\mathcal{F}^{\text{Pek}}(\varphi) \geqslant e^{\text{Pek}} + J_{t^\varphi,\epsilon}\big[\tau(\varphi)\big] - \frac{C}{\epsilon}\left\|(1-\Pi)\,\varphi_{x_{t^\varphi}}^{\text{Pek}}\right\|^2 \tag{3.5.14}$$

for all $0 < \epsilon < \epsilon_0$ and $\varphi \in \Pi L^2(\mathbb{R}^3)$ satisfying $\left\|V_{\varphi-\varphi^{\text{Pek}}}\right\|_\diamond < \epsilon D$ and $|t^\varphi| < \epsilon D$, where $J_{t,\epsilon}$ is defined in Eq. (3.5.13).

Proof. In the following we use the abbreviation $t := t^\varphi$. Since $\left\|V_{\varphi^{\text{Pek}}-\varphi_x^{\text{Pek}}}\right\|_\diamond \lesssim |x|$ and $|x_t| \lesssim |t|$ for $|t| \leqslant \frac{\delta_*}{2}$, we have for all φ satisfying $\left\|V_{\varphi-\varphi^{\text{Pek}}}\right\|_\diamond < D\epsilon$ and $|t| < \min\{D\epsilon, \frac{\delta_*}{2}\}$

$$\left\|V_{T_{-x_t}\varphi-\varphi^{\text{Pek}}}\right\|_\diamond = \left\|V_{\varphi-\varphi_{x_t}^{\text{Pek}}}\right\|_\diamond \leqslant \left\|V_{\varphi-\varphi^{\text{Pek}}}\right\|_\diamond + \left\|V_{\varphi^{\text{Pek}}-\varphi_{x_t}^{\text{Pek}}}\right\|_\diamond \lesssim \left\|V_{\varphi-\varphi^{\text{Pek}}}\right\|_\diamond + |t| \lesssim D\epsilon.$$

By taking D small enough we obtain $\left\|V_{T_{-x_t}\varphi-\varphi^{\mathrm{Pek}}}\right\|_\diamond \leqslant \frac{\epsilon}{c}$ where c is the constant from Lemma 3.5.2. Let us define $\epsilon_0 := \min\left\{c\delta_0, \frac{\delta_*}{2D}, \delta_*\right\}$. Using the translation-invariance of $\mathcal{F}^{\mathrm{Pek}}$ and applying Lemma 3.5.2 yields

$$\begin{aligned}
\mathcal{F}^{\mathrm{Pek}}(\varphi)-e^{\mathrm{Pek}} &= \mathcal{F}^{\mathrm{Pek}}(T_{-x_t}\varphi)-e^{\mathrm{Pek}} \geqslant \langle T_{-x_t}\varphi-\varphi^{\mathrm{Pek}}|1-\left(K^{\mathrm{Pek}}+\epsilon L^{\mathrm{Pek}}\right)|T_{-x_t}\varphi-\varphi^{\mathrm{Pek}}\rangle \\
&= \langle \varphi-\varphi^{\mathrm{Pek}}_{x_t}|1-\left(K^{\mathrm{Pek}}_{x_t}+\epsilon L^{\mathrm{Pek}}_{x_t}\right)|\varphi-\varphi^{\mathrm{Pek}}_{x_t}\rangle \\
&\geqslant \|\varphi-\Pi\varphi^{\mathrm{Pek}}_{x_t}\|^2-\langle \varphi-\varphi^{\mathrm{Pek}}_{x_t}|K^{\mathrm{Pek}}_{x_t}+\epsilon L^{\mathrm{Pek}}_{x_t}|\varphi-\varphi^{\mathrm{Pek}}_{x_t}\rangle \\
&\geqslant \|\varphi-\Pi\varphi^{\mathrm{Pek}}_{x_t}\|^2-(1+\epsilon)\langle \varphi-\Pi\varphi^{\mathrm{Pek}}_{x_t}|K^{\mathrm{Pek}}_{x_t}+\epsilon L^{\mathrm{Pek}}_{x_t}|\varphi-\Pi\varphi^{\mathrm{Pek}}_{x_t}\rangle \\
&\quad -\left(1+\epsilon^{-1}\right)\langle (1-\Pi)\,\varphi^{\mathrm{Pek}}_{x_t}|K^{\mathrm{Pek}}_{x_t}+\epsilon L^{\mathrm{Pek}}_{x_t}|\,(1-\Pi)\,\varphi^{\mathrm{Pek}}_{x_t}\rangle, \qquad (3.5.15)
\end{aligned}$$

where we have used the positivity of K^{Pek}_x and L^{Pek}_x, and the Cauchy–Schwarz inequality in the last estimate. Note that by construction of x_t as the local inverse of the function ω from Eq. (3.5.12), we have $\langle\varphi_n|\varphi-\Pi\varphi^{\mathrm{Pek}}_{x_t}\rangle = 0$ for $n\in\{1,2,3\}$ and therefore

$$\varphi-\Pi\varphi^{\mathrm{Pek}}_{x_t} = \pi\left(\varphi-\Pi\varphi^{\mathrm{Pek}}_{x_t}\right) = \pi\left(\varphi-f(t)\right) = \pi\left(\tau\left(\varphi\right)\right)$$

with π being defined below Eq. (3.5.13), where we used $|t|<\delta_*$. This concludes the proof with $C := (1+\epsilon_0)\left(\|K\|_{\mathrm{op}}+\epsilon_0\|L\|_{\mathrm{op}}\right)$. ■

3.6 Proof of Theorem 3.1.1

In the following we will combine the results of the previous sections in order to prove the lower bound on the ground state energy E_α in Theorem 3.1.1. We start by verifying the subsequent Lemma 3.6.1, which provides a lower bound on E_α in terms of an operator that is, up to a coordinate transformation τ and a non-negative term, a harmonic oscillator.

Let us again use the identification $\mathcal{F}\left(\Pi L^2(\mathbb{R}^3)\right)\cong L^2\left(\mathbb{R}^N\right)$ utilizing the representation of real functions $\varphi=\sum_{n=1}^N\lambda_n\varphi_n\in\Pi L^2(\mathbb{R}^3)$ by points $\lambda=(\lambda_1,\dots,\lambda_N)\in\mathbb{R}^N$, such that the annihilation operators $a_n := a\left(\varphi_n\right)$ are given by $a_n=\lambda_n+\frac{1}{2\alpha^2}\partial_{\lambda_n}$, where λ_n is the multiplication operator by the function $\lambda\mapsto\lambda_n$ on $L^2\left(\mathbb{R}^N\right)$, see also Eq. (3.4.2), where Π is the projection from Eq. (3.4.1) and $\{\varphi_1,\dots,\varphi_N\}$ is the orthonormal basis of $\Pi L^2(\mathbb{R}^3)$ constructed around Eq. (3.5.11). Let us also use for functions $\varphi\mapsto g(\varphi)$ depending on elements $\varphi\in\Pi L^2(\mathbb{R}^3)$ the convenient notation $g(\lambda) := g\left(\sum_{n=1}^N\lambda_n\varphi_n\right)$, where $\lambda\in\mathbb{R}^N$.

Lemma 3.6.1. *Let $C>0$ and $0<\sigma\leqslant\frac{1}{4}$, and assume s,h and σ satisfy $2s<h$ and $\sigma<\frac{1-5s}{4}$. Furthermore let us define $\Lambda := \alpha^{\frac{4}{5}(1+\sigma)}$ and $L := \alpha^{1+\sigma}$. Then we obtain for any state Ψ satisfying $\langle\Psi|\mathbb{H}_\Lambda|\Psi\rangle\leqslant C$, $\operatorname{supp}(\Psi)\subset B_{4L}(0)$ and*

$$\chi\left(W^{-1}_{\varphi^{\mathrm{Pek}}}\mathcal{N}W_{\varphi^{\mathrm{Pek}}}\leqslant\alpha^{-h}\right)\Psi=\Psi, \qquad (3.6.1)$$

that

$$\begin{aligned}
\langle\Psi|\mathbb{H}_\Lambda|\Psi\rangle \geqslant e^{\mathrm{Pek}} &+ \left\langle\Psi\middle|-\frac{1}{4\alpha^4}\sum_{n=1}^N\partial^2_{\lambda_n}+J_{t^\lambda,\alpha^{-s}}\big[\tau(\lambda)\big]+\mathcal{N}-\sum_{n=1}^N a^\dagger_n a_n\middle|\Psi\right\rangle-\frac{N}{2\alpha^2} \\
&+O\left(\alpha^{s-\frac{12}{5}(1+\sigma)}+\alpha^{-2(1+\sigma)}\right), \qquad (3.6.2)
\end{aligned}$$

where t^φ and $\tau(\varphi)$ are defined in Lemma 3.5.3 and $J_{t,\epsilon}$ is defined in Eq. (3.5.13). Furthermore, there exists a $\beta>0$, such that $\langle\Psi|1-\mathbb{B}|\Psi\rangle\leqslant e^{-\beta\alpha^{2(1-s)}}$, where $\mathbb{B}$ is the multiplication operator by the function $\lambda\mapsto\chi\left(|t^\lambda|<\alpha^{-s}\right)$.

Proof. Applying Eq. (3.2.3) with Λ and ℓ as in the definition of Π, see Eq. (3.4.1), and $K := \Lambda$, and utilizing Eq. (3.2.5), we obtain for a suitable C'

$$\langle\Psi|\mathbb{H}_\Lambda|\Psi\rangle \geqslant \langle\Psi|\mathbb{H}^0_{\Lambda,\ell}|\Psi\rangle - C'\alpha^{-2(1+\sigma)}. \tag{3.6.3}$$

Making use of $\sum_{n=1}^N a_n^\dagger a_n = \sum_{n=1}^N \left(-\frac{1}{4\alpha^4}\partial^2_{\lambda_n} + \lambda_n^2\right) - \frac{N}{2\alpha^2}$ and $a_n + a_n^\dagger = 2\lambda_n$, we further have the identity

$$\begin{aligned}\mathbb{H}^0_{\Lambda,\ell} &= -\Delta_x - 2\sum_{n=1}^N \langle\varphi_n|w_x\rangle\lambda_n + \sum_{n=1}^N\left(-\frac{1}{4\alpha^4}\partial^2_{\lambda_n} + \lambda_n^2\right) - \frac{N}{2\alpha^2} + \mathcal{N} - \sum_{n=1}^N a_n^\dagger a_n \\ &= -\Delta_x + V_\lambda(x) + \sum_{n=1}^N\left(-\frac{1}{4\alpha^4}\partial^2_{\lambda_n} + \lambda_n^2\right) - \frac{N}{2\alpha^2} + \mathcal{N} - \sum_{n=1}^N a_n^\dagger a_n,\end{aligned}$$

with V_φ defined in Eq. (3.5.1). Clearly $-\Delta_x + V_\lambda \geqslant \inf\sigma\left(-\Delta_x + V_\lambda\right) = \mathcal{F}^{\text{Pek}}(\lambda) - \sum_{n=1}^N \lambda_n^2$, which yields the inequality $\mathbb{H}^0_{\Lambda,\ell} \geqslant \mathbb{K} + \mathcal{N} - \sum_{n=1}^N a_n^\dagger a_n$ with

$$\mathbb{K} := -\frac{1}{4\alpha^4}\sum_{n=1}^N \partial^2_{\lambda_n} + \mathcal{F}^{\text{Pek}}(\lambda) - \frac{N}{2\alpha^2}. \tag{3.6.4}$$

Combining Eqs. (3.6.3) and (3.6.4), we obtain

$$\left\langle\Psi\middle|\mathbb{H}_\Lambda - \mathcal{N} + \sum_{n=1}^N a_n^\dagger a_n\middle|\Psi\right\rangle + C'\alpha^{-2(1+\sigma)} \geqslant \langle\Psi|\mathbb{K}|\Psi\rangle = \langle\mathbb{K}\rangle_\gamma, \tag{3.6.5}$$

where γ is the reduced density matrix on the Hilbert space $\mathcal{F}\left(\Pi L^2(\mathbb{R}^3)\right) \cong L^2\big(\mathbb{R}^N\big)$ corresponding to the state Ψ, i.e. we trace out the electron component as well as all the modes in the orthogonal complement of $\Pi L^2(\mathbb{R}^3)$,

$$\gamma := \operatorname{Tr}_{L^2(\mathbb{R}^3)\otimes\mathcal{F}(L^2(\mathbb{R}^3))\to\mathcal{F}(\Pi L^2(\mathbb{R}^3))}\left[\,|\Psi\rangle\langle\Psi|\,\right].$$

Note that we have the inequality $W^{-1}_{\Pi\varphi^{\text{Pek}}}\left(\sum_{n=1}^N a_n^\dagger a_n\right)W_{\Pi\varphi^{\text{Pek}}} \leqslant W^{-1}_{\varphi^{\text{Pek}}}\mathcal{N}W_{\varphi^{\text{Pek}}}$. The operators on the left and right hand side commute, and consequently (3.6.1) implies that $\chi\left(W^{-1}_{\Pi\varphi^{\text{Pek}}}\left(\sum_{n=1}^N a_n^\dagger a_n\right)W_{\Pi\varphi^{\text{Pek}}} \leqslant \alpha^{-h}\right)\Psi = \Psi$. This in particular means that the transformed reduced density matrix $\widetilde{\gamma} := W_{\Pi\varphi^{\text{Pek}}}\gamma W^{-1}_{\Pi\varphi^{\text{Pek}}}$ satisfies

$$\chi\left(\sum_{n=1}^N a_n^\dagger a_n \leqslant \alpha^{-h}\right)\widetilde{\gamma} = \widetilde{\gamma}. \tag{3.6.6}$$

Using the identification $\varphi = \sum_{n=1}^N \lambda_n\varphi_n$ as before, the Weyl operator $W_{\Pi\varphi^{\text{Pek}}}$ acts as $\left(W_{\Pi\varphi^{\text{Pek}}}\Psi\right)(\lambda) = \Psi\left(\lambda + \lambda^{\text{Pek}}\right)$ with $\lambda^{\text{Pek}} := \left(\langle\varphi_1|\varphi^{\text{Pek}}\rangle, \dots, \langle\varphi_N|\varphi^{\text{Pek}}\rangle\right)$. Due to Eq. (3.6.6), and the fact that $2s < h$ and $\sigma < \frac{1-5s}{4}$, the assumptions of Proposition 3.4.2 are satisfied, and therefore we obtain for any $D > 0$ the existence of a constant $\beta > 0$ such that for α

large enough

$$\int_{|\lambda-\lambda^{\mathrm{Pek}}|_\diamond \geqslant \alpha^{-s}D} \left(1+|\lambda-\lambda^{\mathrm{Pek}}|^2\right)\rho(\lambda)\mathrm{d}\lambda = \int_{|\lambda|_\diamond \geqslant \alpha^{-s}D} \left(1+|\lambda|^2\right)\widetilde{\rho}(\lambda)\mathrm{d}\lambda \leqslant e^{-\beta\alpha^{2(1-s)}}, \tag{3.6.7}$$

$$\begin{aligned}\int_{|t^\lambda|\geqslant \alpha^{-s}D} \left(1+|\lambda-\lambda^{\mathrm{Pek}}|^2\right)\rho(\lambda)\mathrm{d}\lambda &\leqslant \sum_{n=1}^{3}\int_{|\lambda_n|\geqslant \frac{\alpha^{-s}}{\sqrt{3}}D} \left(1+|\lambda-\lambda^{\mathrm{Pek}}|^2\right)\rho(\lambda)\mathrm{d}\lambda \\ &= \sum_{n=1}^{3}\int_{|\lambda_n|\geqslant \frac{\alpha^{-s}}{\sqrt{3}}D} \left(1+|\lambda|^2\right)\widetilde{\rho}(\lambda)\mathrm{d}\lambda \leqslant e^{-\beta\alpha^{2(1-s)}},\end{aligned} \tag{3.6.8}$$

where ρ and $\widetilde{\rho}$ are the density functions corresponding to γ and $\widetilde{\gamma}$, respectively, and where we have used $t^\lambda = (\lambda_1,\lambda_2,\lambda_3) \in \mathbb{R}^3$. For the concrete choice $D := 1$, Eq. (3.6.8) immediately yields the claim $\langle \Psi | 1-\mathbb{B} | \Psi\rangle = \int_{|t^\lambda|\geqslant \alpha^{-s}} \rho(\lambda)\mathrm{d}\lambda \leqslant e^{-\beta\alpha^{2(1-s)}}$.

In order to verify Eq. (3.6.2), we need to find a sufficient lower bound for the expectation value $\langle \mathbb{K}\rangle_\gamma$, where $\mathbb{K}$ is the operator from Eq. (3.6.4). Recall the definition of the transformation $\tau : \Pi L^2(\mathbb{R}^3) \longrightarrow \Pi L^2(\mathbb{R}^3)$ from Definition 3.5.3 and the operator $J_{t,\epsilon}$ from Eq. (3.5.13). As a first step we will provide a lower bound on $\langle \mathcal{F}^{\mathrm{Pek}}(\lambda)\rangle_\gamma$, using Eq. (3.5.14) and the fact that $\sup_{|t|\leqslant t_0} \left\|(1-\Pi)\,\varphi^{\mathrm{Pek}}_{x_t}\right\|^2 \lesssim \alpha^{-\frac{12}{5}(1+\sigma)}$ for t_0 small enough, which follows from Lemma 3.8.1 together with $x_t \underset{t\to 0}{\longrightarrow} 0$. We define the operator $\mathbb{A} := \chi\left(|\lambda-\lambda^{\mathrm{Pek}}|_\diamond < \alpha^{-s}D\right)\chi\left(\left|t^\lambda\right| < \alpha^{-s}D\right)$, where D is as in Theorem 3.5.4, and estimate

$$\begin{aligned}\langle \mathcal{F}^{\mathrm{Pek}}(\lambda)\rangle_\gamma &= \langle \mathcal{F}^{\mathrm{Pek}}(\lambda)\,\mathbb{A}\rangle_\gamma + \langle \mathcal{F}^{\mathrm{Pek}}(\lambda)\,(1-\mathbb{A})\rangle_\gamma \\ &\geqslant \left\langle \left(e^{\mathrm{Pek}} + J_{t^\lambda,\alpha^{-s}}\!\left[\tau(\lambda)\right]\right)\mathbb{A}\right\rangle_\gamma + \langle \mathcal{F}^{\mathrm{Pek}}(\lambda)\,(1-\mathbb{A})\rangle_\gamma + O\left(\alpha^{s-\frac{12}{5}(1+\sigma)}\right) \\ &= \left\langle e^{\mathrm{Pek}} + J_{t^\lambda,\alpha^{-s}}\!\left[\tau(\lambda)\right]\right\rangle_\gamma + \left\langle X\right\rangle_\gamma + O\left(\alpha^{s-\frac{12}{5}(1+\sigma)}\right)\end{aligned} \tag{3.6.9}$$

with $X := \left(\mathcal{F}^{\mathrm{Pek}}(\lambda) - e^{\mathrm{Pek}} - J_{t^\lambda,\alpha^{-s}}\!\left[\tau(\lambda)\right]\right)(1-\mathbb{A})$. Using Eqs. (3.6.7) and (3.6.8) as well as the fact that $1-\mathbb{A} \leqslant \chi\left(|\lambda-\lambda^{\mathrm{Pek}}|_\diamond \geqslant D\alpha^{-s}\right) + \chi\left(\left|t^\lambda\right| \geqslant D\alpha^{-s}\right)$, we obtain $\left\langle X\right\rangle_\gamma \lesssim e^{-\beta\alpha^{2(1-s)}}$, where we have used that $\mathcal{F}^{\mathrm{Pek}}(\lambda)$ and $J_{t^\lambda,\alpha^{-s}}\!\left[\tau(\lambda)\right]$ are bounded by $C(1+|\lambda|^2)$ for suitable $C>0$. By Eq. (3.6.9) we therefore have the estimate $\langle \mathcal{F}^{\mathrm{Pek}}(\lambda)\rangle_\gamma \geqslant \left\langle e^{\mathrm{Pek}} + J_{t^\lambda,\alpha^{-s}}\!\left[\tau(\lambda)\right]\right\rangle_\gamma + O\left(\alpha^{s-\frac{12}{5}(1+\sigma)}\right)$, and consequently

$$\langle \mathbb{K}\rangle_\gamma \geqslant e^{\mathrm{Pek}} + \left\langle -\frac{1}{4\alpha^4}\sum_{n=1}^{N}\partial^2_{\lambda_n} + J_{t^\lambda,\alpha^{-s}}\!\left[\tau(\lambda)\right]\right\rangle_\gamma - \frac{N}{2\alpha^2} + O\left(\alpha^{s-\frac{12}{5}(1+\sigma)}\right). \tag{3.6.10}$$

Since $\left\langle -\frac{1}{4\alpha^4}\sum_{n=4}^{N}\partial^2_{\lambda_n} + J_{t^\lambda,\alpha^{-s}}\!\left[\tau(\lambda)\right]\right\rangle_\gamma = \left\langle \Psi\middle| -\frac{1}{4\alpha^4}\sum_{n=4}^{N}\partial^2_{\lambda_n} + J_{t^\lambda,\alpha^{-s}}\!\left[\tau(\lambda)\right]\middle|\Psi\right\rangle$, this concludes the proof together with Eq. (3.6.5). ∎

In the following, let Ψ_α be the sequence of states constructed in Theorem 3.3.13, satisfying $\langle \Psi_\alpha | \mathbb{H}_\Lambda | \Psi_\alpha\rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$, $\mathrm{supp}\,(\Psi_\alpha) \subset B_{4L}(0)$ with $L = \alpha^{1+\sigma}$ and strong condensation with respect to φ^{Pek}, i.e. $\chi\left(W^{-1}_{\varphi^{\mathrm{Pek}}}\mathcal{N}W_{\varphi^{\mathrm{Pek}}} \leqslant \alpha^{-h}\right)\Psi_\alpha = \Psi_\alpha$, and furthermore let $s < \frac{1}{29}$ be a given constant and let us choose σ and h such that $2s < h < \frac{2}{29}$ and $\frac{s}{2} \leqslant \sigma < \frac{1-5s}{4}$.

Note that $h < \frac{2}{29}$ makes sure that the assumption of Theorem 3.3.13 is satisfied, while $2s < h$ and $\sigma < \frac{1-5s}{4}$ are necessary in order to apply Lemma 3.6.1. The final assumption $\frac{s}{2} \leqslant \sigma$ will be useful later in Eq. (3.6.15) in order to make sure that $\alpha^{-2(1+\sigma)} \leqslant \alpha^{-(2+s)}$. Making use of $-\frac{1}{4\alpha^4}\sum_{n=1}^{3} \partial_{\lambda_n}^2 \geqslant 0$ and $\mathcal{N} \geqslant \sum_{n=1}^{N} a_n^\dagger a_n$, we obtain by Lemma 3.6.1 that

$$E_\alpha \geqslant e^{\mathrm{Pek}} + \left\langle \Psi_\alpha \middle| -\frac{1}{4\alpha^4}\sum_{n=4}^{N} \partial_{\lambda_n}^2 + J_{t^\lambda,\alpha^{-s}}\big[\tau(\lambda)\big] \middle| \Psi_\alpha \right\rangle - \frac{N}{2\alpha^2} + O\left(\alpha^{-2(1+\sigma)}\right) \tag{3.6.11}$$

for a suitable C', where we have used $\alpha^{s-\frac{12}{5}(1+\sigma)} \leqslant \alpha^{-2(1+\sigma)}$ and $E_\alpha - \langle \Psi_\alpha | \mathbb{H}_\Lambda | \Psi_\alpha \rangle \gtrsim -\alpha^{-2(1+\sigma)}$. In order to further estimate the expectation value in Eq. (3.6.11), let us define the unitary transformation $(\mathcal{U}\Psi)(\lambda) := \Psi(\tau'(\lambda))$ with $\tau'(\lambda) := \Big(\big\langle \varphi_n | \tau(\lambda) \big\rangle\Big)_{n=1}^{N} \in \mathbb{R}^N$. Since τ' acts as a shift operator on each of the planes $X_t := \{\lambda : (\lambda_1, \lambda_2, \lambda_3) = t\}$ for $t \in \mathbb{R}^3$, it is clear that $\det \mathrm{D}|_\lambda \tau' = 1$, which in particular means that the operator $\mathcal{U}$ is indeed unitary, and we have $\partial_{\lambda_n} = \mathcal{U}^{-1}\partial_{\lambda_n}\mathcal{U}$ for $n \geqslant 4$. Furthermore we define the operator

$$\mathbb{Q}_{t,\epsilon} := -\frac{1}{4\alpha^4}\sum_{n=4}^{N} \partial_{\lambda_n}^2 + \sum_{n,m=1}^{N} \left(J_{t,\epsilon}\right)_{n,m} \lambda_n \lambda_m$$

with $\left(J_{t,\epsilon}\right)_{n,m} := \langle \varphi_n | J_{t,\epsilon} | \varphi_m \rangle$. Note that $\left(J_{t,\epsilon}\right)_{n,m} = \left(J_{t,\epsilon}\right)_{m,n} = 0$ in case $n \in \{1,2,3\}$, i.e. the operator $\mathbb{Q}_{t,\epsilon}$ depends only on the variables λ_n for $n \geqslant 4$ and not on $t^\lambda = (\lambda_1, \lambda_2, \lambda_3)$, hence it acts on the Fock space $\mathcal{F}\big(\mathrm{span}\{\varphi_4, \ldots, \varphi_N\}\big) \cong L^2\big(\mathbb{R}^{N-3}\big)$ only. Utilizing the fact that $\mathcal{U}^{-1} J_{t^\lambda,\alpha^{-s}}\big[\tau(\lambda)\big]\mathcal{U} = J_{t^\lambda,\alpha^{-s}}\big[\lambda\big] = \sum_{n,m=1}^{N} \left(J_{t^\lambda,\alpha^{-s}}\right)_{n,m} \lambda_n \lambda_m$, where we used that $\mathcal{U}^{-1} t^\lambda \mathcal{U} = t^\lambda$, we obtain

$$\mathcal{U}^{-1}\left(-\frac{1}{4\alpha^4}\sum_{n=4}^{N} \partial_{\lambda_n}^2 + J_{t^\lambda,\alpha^{-s}}\big[\tau(\lambda)\big]\right)\mathcal{U} = \mathbb{Q}_{t^\lambda,\alpha^{-s}} \geqslant \mathbb{Q}_{t^\lambda,\alpha^{-s}}\mathbb{B} \geqslant \inf_{|t|<\alpha^{-s}} \inf \sigma\left(\mathbb{Q}_{t,\alpha^{-s}}\right)\mathbb{B},$$

where $\mathbb{B}$ is as in Lemma 3.6.1. Here we have used $\mathbb{Q}_{t^\lambda,\alpha^{-s}} \geqslant 0$, which follows from Lemma 3.9.5, as well as the fact that $1 - \mathbb{B}$ is non-negative and commutes with $\mathbb{Q}_{t^\lambda,\alpha^{-s}}$. Applying this inequality with respect to the state $\widetilde{\Psi}_\alpha := \mathcal{U}^{-1}\Psi_\alpha$ yields

$$\begin{aligned} \left\langle \Psi_\alpha \middle| -\frac{1}{4\alpha^4}\sum_{n=4}^{N} \partial_{\lambda_n}^2 + J_{t^\lambda,\alpha^{-s}}\big[\tau(\lambda)\big] \middle| \Psi_\alpha \right\rangle &\geqslant \inf_{|t|<\alpha^{-s}} \inf \sigma\left(\mathbb{Q}_{t,\alpha^{-s}}\right) \big\langle \widetilde{\Psi}_\alpha \big| \mathbb{B} \big| \widetilde{\Psi}_\alpha \big\rangle \\ &\geqslant \inf_{|t|<\alpha^{-s}} \inf \sigma\left(\mathbb{Q}_{t,\alpha^{-s}}\right) - \frac{N}{2\alpha^2}\big\langle \widetilde{\Psi}_\alpha \big| 1 - \mathbb{B} \big| \widetilde{\Psi}_\alpha \big\rangle \end{aligned} \tag{3.6.12}$$

where we have used $J_{t,\epsilon} \leqslant 1$, and therefore $\inf \sigma\left(\mathbb{Q}_{t,\epsilon}\right) \leqslant \frac{N}{2\alpha^2}$. By Lemma 3.6.1, we know that $\big\langle \widetilde{\Psi}_\alpha \big| 1 - \mathbb{B} \big| \widetilde{\Psi}_\alpha \big\rangle = \big\langle \Psi_\alpha \big| 1 - \mathbb{B} \big| \Psi_\alpha \big\rangle \leqslant e^{-\beta\alpha^{2-2s}}$. Combining Eqs. (3.6.11) and (3.6.12), and making use of the fact that $N \lesssim \alpha^p$ for some $p > 0$, yields

$$E_\alpha \geqslant e^{\mathrm{Pek}} + \inf_{|t|<\alpha^{-s}} \inf \sigma\left(\mathbb{Q}_{t,\alpha^{-s}}\right) - \frac{N}{2\alpha^2} + O\left(\alpha^{-2(1+\sigma)}\right). \tag{3.6.13}$$

Since the operator $\mathbb{Q}_{t,\alpha^{-s}}$ is quadratic in ∂_{λ_n} and λ_n, we have an explicit formula for its ground state energy, given by

$$\inf \sigma\left(\mathbb{Q}_{t,\alpha^{-s}}\right) - \frac{N}{2\alpha^2} = -\frac{\mathrm{Tr}_{\Pi L^2(\mathbb{R}^3)}\big[1 - \sqrt{J_{t,\alpha^{-s}}}\big]}{2\alpha^2}, \tag{3.6.14}$$

where we used the fact that $J_{t,\alpha^{-s}} \geqslant 0$ for α large enough, as shown in Lemma 3.9.5. Using Eq. (3.9.7), we can approximate this quantity by

$$\sup_{|t|<\alpha^{-s}} \left|\mathrm{Tr}_{\Pi L^2(\mathbb{R}^3)}[1 - \sqrt{J_{t,\alpha^{-s}}}\,] - \mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right]\right| \lesssim \alpha^{-s} + \alpha^{-\frac{1}{5}},$$

where H^{Pek} is defined in Eq. (3.1.4). Consequently Eq. (3.6.13) yields

$$E_\alpha - e^{\mathrm{Pek}} + \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] \gtrsim -\alpha^{-2(1+\sigma)} - \alpha^{-(2+s)} - \alpha^{-\left(2+\frac{1}{5}\right)}, \tag{3.6.15}$$

which concludes the proof, since all the terms on the right side are of order $\alpha^{-(2+s)}$.

3.7 Approximation by Coherent States

This section is devoted to the proof of Theorem 3.3.2, which states that asymptotically the phonon part of any low energy state is a convex combination of the coherent states $\Omega_{\varphi_x^{\mathrm{Pek}}}$ with $x \in \mathbb{R}^3$, where the convex combination is taken on the level of density matrices. As a central tool we will verify in Lemma 3.7.2 an asymptotic formula for the expectation value $\langle \Psi | \widehat{F} | \Psi \rangle$ in terms of the lower symbol $\mathbb{P}_y$ corresponding to the state Ψ, see Eq. (3.7.6). Furthermore we will make use of the inequality

$$\inf_{x\in\mathbb{R}^3} \|\varphi - \varphi_x^{\mathrm{Pek}}\|^2 \lesssim \mathcal{F}^{\mathrm{Pek}}(\varphi) - e^{\mathrm{Pek}} \tag{3.7.1}$$

derived in [38, Lemma 7], which implies that the only coherent states Ω_φ with a low energy have their point of condensation φ close to the manifold of Pekar minimizers $\{\varphi_x^{\mathrm{Pek}} : x \in \mathbb{R}^3\}$. We start with the subsequent Lemma 3.7.1, which provides an asymptotic formula for $\widehat{F}$ operators in terms of creation and annihilation operators.

Lemma 3.7.1. *Let $m \in \mathbb{N}$ and $C > 0$ be given constants, $\{g_n : n \in \mathbb{N}\}$ an orthonormal basis of $L^2(\mathbb{R}^3)$ and let us denote $a_n := a(g_n)$. Then there exists a constant $T > 0$ such that for all functions F of the form*

$$F(\rho) = \int \dots \int f(x_1, \dots, x_m)\, \mathrm{d}\rho(x_1) \dots \mathrm{d}\rho(x_m), \tag{3.7.2}$$

with $f : \mathbb{R}^{3\times m} \longrightarrow \mathbb{R}$ bounded, and states Ψ satisfying $\chi(\mathcal{N} \leqslant C)\,\Psi = \Psi$, we can approximate the operator $\widehat{F}$ from Definition 3.3.1 by

$$\left| \langle \Psi | \widehat{F} | \Psi \rangle - \sum_{I,J\in\mathbb{N}^m} f_{I,J} \langle \Psi | a_{I_1}^\dagger \dots a_{I_m}^\dagger a_{J_1} \dots a_{J_m} | \Psi \rangle \right| \leqslant T \|f\|_\infty \alpha^{-2}, \tag{3.7.3}$$

where we interpret f as a multiplication operator on $L^2(\mathbb{R}^3)^{\otimes^m} \cong L^2(\mathbb{R}^{3\times m})$ and denote the matrix elements $f_{I,J} := \langle g_{I_1} \otimes \dots \otimes g_{I_m} | f | g_{J_1} \otimes \dots \otimes g_{J_m} \rangle$.

Proof. By the assumption $\chi(\mathcal{N} \leqslant C)\,\Psi = \Psi$, we can represent the state Ψ as $\Psi = \bigoplus_{n \leqslant C\alpha^2} \Psi_n$ where $\Psi_n(y, x^1, \dots, x^n)$ is a function of the electron variable y and the n phonon coordinates $x^k \in \mathbb{R}^3$. As in the proof of Lemma 3.3.3, we will suppress the dependence on the electron variable y in our notation. Using the definition of $\widehat{F}$ in Definition 3.3.1, as well as the notation $X = (x^1, \dots, x^n)$, we can write

$$\big\langle \Psi \big| \widehat{F} \big| \Psi \big\rangle = \sum_{n \leqslant C\alpha^2} \int_{\mathbb{R}^{3n}} F\left(\alpha^{-2} \sum_{k=1}^{n} \delta_{x^k}\right) |\Psi_n(X)|^2 \mathrm{d}X$$
$$= \alpha^{-2m} \sum_{n \leqslant C\alpha^2} \sum_{k \in \{1,\dots,n\}^m} \int_{\mathbb{R}^{3n}} f(x^{k_1}, \dots, x^{k_m}) |\Psi_n(X)|^2 \mathrm{d}X.$$

Defining $\mathcal{K}$ as the set of all $k \in \{1, \dots, n\}^m$ satisfying $k_i \neq k_j$ for all $i \neq j$, we can further express the operator $\sum_{I,J \in \mathbb{N}^m} f_{I,J}\, a^\dagger_{I_1} \dots a^\dagger_{I_m} a_{J_1} \dots a_{J_m}$ as

$$\sum_{I,J \in \mathbb{N}^m} f_{I,J} \big\langle \Psi \big| a^\dagger_{I_1} \dots a^\dagger_{I_m} a_{J_1} \dots a_{J_m} \big| \Psi \big\rangle = \alpha^{-2m} \sum_{n \leqslant C\alpha^2} \sum_{k \in \mathcal{K}} \int_{\mathbb{R}^{3n}} f(x^{k_1}, \dots, x^{k_m}) |\Psi_n(X)|^2 \mathrm{d}X.$$

Consequently we can identify the left hand side of Eq. (3.7.3) as

$$\left| \alpha^{-2m} \sum_{n \leqslant C\alpha^2} \sum_{k \in \{1,\dots,n\}^m \setminus \mathcal{K}} \int_{\mathbb{R}^{3n}} f(x^{k_1}, \dots, x^{k_m}) |\Psi_n(X)|^2 \mathrm{d}X \right|$$
$$\leqslant \|f\|_\infty \sum_{n \leqslant C\alpha^2} \left(\sum_{k \in \{1,\dots,n\}^m \setminus \mathcal{K}} \alpha^{-2m} \right) \int_{\mathbb{R}^{3n}} |\Psi_n(X)|^2 \mathrm{d}X.$$

Since $\sum_{k \in \{1,\dots,n\}^m \setminus \mathcal{K}} \alpha^{-2m} = \left(n^m - \frac{n!}{(n-m)!}\right) \alpha^{-2m} \leqslant m 2^m n^{m-1} \alpha^{-2m} \lesssim \alpha^{-2}$ for $n \leqslant C\alpha^2$ and since $\sum_{n \leqslant C\alpha^2} \int_{\mathbb{R}^{3n}} |\Psi_n(X)|^2 \mathrm{d}X = \|\Psi\|^2 = 1$, this concludes the proof. ■

In the following we are going to define the lower symbol $\mathbb{P}_y$ corresponding to a state $\Psi \in L^2\Big(\mathbb{R}^3, \mathcal{F}\big(L^2(\mathbb{R}^3)\big)\Big)$. Since we consider the Fock space over the infinite dimensional Hilbert space $L^2(\mathbb{R}^3)$, we need to modify the usual definition of the lower symbol by introducing suitable localizations. For $0 < s \leqslant \frac{4}{27}$ and $y \in \mathbb{R}^3$, let us define $\ell_* := \alpha^{-\frac{5}{2}s}$ and $\Lambda_* := \alpha^{2s}$, and the projection

$$\Pi_y := \Pi^y_{\Lambda_*, \ell_*}, \tag{3.7.4}$$

see Definition 3.2.1. We have $N_* := \dim \Pi_y L^2(\mathbb{R}^3) \lesssim (\Lambda_*/\ell_*)^3 \leqslant \alpha^2$ by our assumption $s \leqslant \frac{4}{27}$. Using the notation $\{e_{y,1}, \dots, e_{y,N_*}\}$ for the orthonormal basis of $\Pi_y L^2(\mathbb{R}^3)$ from Definition 3.2.1, we introduce for $\xi \in \mathbb{C}^{N_*}$ the coherent states $\Omega_{y,\xi} := e^{\alpha^2 a^\dagger(\varphi_{y,\xi}) - \alpha^2 a(\varphi_{y,\xi})}\Omega$, where Ω is the vacuum in $\mathcal{F}\left(\Pi_y L^2(\mathbb{R}^3)\right)$ and $\varphi_{y,\xi} := \sum_{n=1}^{N_*} \xi_n e_{y,n} \in \Pi_y L^2(\mathbb{R}^3)$. Furthermore we define wave-functions Ψ_y localized in the electron coordinates x as

$$\Psi_y(x) := L_*^{-\frac{3}{2}} \chi\left(\frac{x-y}{L_*}\right) \Psi(x), \tag{3.7.5}$$

where $y \in \mathbb{R}^3$ and $L_* := \alpha^{\frac{s}{2}}$, and χ is a smooth non-negative function with $\mathrm{supp}\,(\chi) \subset B_1(0)$ and $\int \chi(y)^2 \,\mathrm{d}y = 1$. For the following construction, note that we can identify $L^2\Big(\mathbb{R}^3, \mathcal{F}\big(L^2(\mathbb{R}^3)\big)\Big) \cong \mathcal{F}\left(\Pi_y L^2(\mathbb{R}^3)\right) \otimes L^2\Big(\mathbb{R}^3, \mathcal{F}\Big(\Pi_y L^2(\mathbb{R}^3)^\perp\Big)\Big)$. Let us now define measures $\mathbb{P}_y$ on $\mathbb{C}^{N_*} \cong \mathbb{R}^{2N_*}$ corresponding to the state Ψ_y as

$$\frac{\mathrm{d}\mathbb{P}_y}{\mathrm{d}\xi} := \frac{1}{\pi^{N_*}} \left\| \Theta_{y,\xi} \Psi_y \right\|^2, \tag{3.7.6}$$

where $\Theta_{y,\xi}$ is the orthogonal projection onto the set spanned by elements of the form $\Omega_{y,\xi} \otimes \widetilde{\Psi}$ with $\widetilde{\Psi} \in L^2\Big(\mathbb{R}^3, \mathcal{F}\Big(\Pi_y L^2(\mathbb{R}^3)^\perp\Big)\Big)$. Note that the coherent states $\Omega_{y,\xi}$ provide a resolution of the identity $\frac{1}{\pi^{N_*}} \int_{\mathbb{C}^{N_*}} |\Omega_{y,\xi}\rangle\langle\Omega_{y,\xi}| \, \mathrm{d}\xi = 1_{\mathcal{F}(\Pi_y L^2(\mathbb{R}^3))}$, see for example [79], and consequently the projections $\Theta_{y,\xi}$ satisfy $\frac{1}{\pi^{N_*}} \int_{\mathbb{C}^{N_*}} \Theta_{y,\xi} \, \mathrm{d}\xi = 1$. In particular we see that the total mass of the measure $\mathbb{P}_y$ is $\int \mathrm{d}\mathbb{P}_y = \|\Psi_y\|^2$ and therefore

$$\iint \mathrm{d}\mathbb{P}_y \mathrm{d}y = \int \|\Psi_y\|^2 \mathrm{d}y = \|\Psi\|^2 = 1.$$

In the following Lemma 3.7.2 and Corollary 3.7.3 we will provide an asymptotic formula for the expectation value $\big\langle \Psi_y \big| \widehat{F} \big| \Psi_y \big\rangle$, respectively $\big\langle \Psi \big| \widehat{F} \big| \Psi \big\rangle$, in terms of the measures $\mathbb{P}_y$.

Lemma 3.7.2. *Given $m \in \mathbb{N}$, $C > 0$ and $g \in L^2(\mathbb{R}^3)$, there exists a $T > 0$ such that for all F of the form (3.7.2), $y \in \mathbb{R}^3$ and $\epsilon > 0$, and states Ψ satisfying $\chi(\mathcal{N} \leqslant C)\, \Psi = \Psi$*

$$\frac{1}{T\|f\|_\infty} \left| \big\langle \Psi_y \big| \widehat{F} \, \big| \Psi_y \big\rangle - \int F\left(|\varphi_{y,\xi}|^2\right) \mathrm{d}\mathbb{P}_y(\xi) \right| \leqslant \left(\frac{N_*}{\alpha^2} + \epsilon\right) \|\Psi_y\|^2 + \epsilon^{-1} \big\langle \Psi_y \big| \mathcal{N}^y_{>N_*} \big| \Psi_y \big\rangle, \tag{3.7.7}$$

with $\mathcal{N}^y_{>N_*} := \mathcal{N} - \sum_{n=1}^{N_*} a^\dagger_{y,n} a_{y,n}$ and $a_{y,n} := a\left(e_{y,n}\right)$, and furthermore

$$\frac{1}{T} \left| \big\langle \Psi_y \big| W_g^{-1} \mathcal{N} W_g \big| \Psi_y \big\rangle - \int \|\varphi_{y,\xi} - g\|^2 \mathrm{d}\mathbb{P}_y(\xi) \right| \leqslant \left(\frac{N_*}{\alpha^2} + \epsilon\right) \|\Psi_y\|^2 + \epsilon^{-1} \big\langle \Psi_y \big| \mathcal{N}^y_{>N_*} \big| \Psi_y \big\rangle, \tag{3.7.8}$$

where W_g is the corresponding Weyl transformation.

Proof. Let $\{g_n : n \in \mathbb{N}\}$ be a completion of $\{e_{y,1}, \dots, e_{y,N_*}\}$ to an orthonormal basis of $L^2(\mathbb{R}^3)$ and let us define $a_n := a\left(g_n\right)$. We further introduce an operator $\widetilde{F}$ as

$$\widetilde{F} := \sum_{I,J \in \{1,\dots,N_*\}^m} f_{I,J} \, a^\dagger_{I_1} \dots a^\dagger_{I_m} a_{J_1} \dots a_{J_m} = \sum_{I,J \in \mathbb{N}^m} \left(\Pi_y^{\otimes m} f \Pi_y^{\otimes m}\right)_{I,J} a^\dagger_{I_1} \dots a^\dagger_{I_m} a_{J_1} \dots a_{J_m}. \tag{3.7.9}$$

In the following we want to verify that both $\|f\|_\infty^{-1} \left| \big\langle \Psi_y \big| \widehat{F} \, \big| \Psi_y \big\rangle - \big\langle \Psi_y \big| \widetilde{F} \, \big| \Psi_y \big\rangle \right|$ and $\|f\|_\infty^{-1} \left| \big\langle \Psi_y \big| \widetilde{F} \, \big| \Psi_y \big\rangle - \int F\left(|\varphi_{y,\xi}|^2\right) \, \mathrm{d}\mathbb{P}_y\left(\xi\right) \right|$ are, up to a multiplicative constant, bounded by the right hand side of Eq. (3.7.7). Applying the Cauchy–Schwarz inequality, we obtain for all $\epsilon > 0$

$$\begin{aligned} \pm\left(f - \Pi_y^{\otimes m} f \, \Pi_y^{\otimes m}\right) &= \pm f\left(1 - \Pi_y^{\otimes m}\right) \pm \left(1 - \Pi_y^{\otimes m}\right) f \, \Pi_y^{\otimes m} \leqslant \epsilon\|f\|_\infty + \epsilon^{-1}\|f\|_\infty \left(1 - \Pi_y^{\otimes m}\right) \\ &\leqslant \epsilon\|f\|_\infty + \epsilon^{-1}\|f\|_\infty \left((1 - \Pi_y)_1 + \dots + (1 - \Pi_y)_m\right), \end{aligned}$$

where $(1 - \Pi_y)_j$ means that the operator $1 - \Pi_y$ acts on the j-th factor in the tensor product. Consequently we have the operator inequality

$$\pm\left(\sum_{I,J \in \mathbb{N}^m} f_{I,J} \, a^\dagger_{I_1} \dots a^\dagger_{I_m} a_{J_1} \dots a_{J_m} - \widetilde{F}\right) \leqslant \epsilon\|f\|_\infty \mathcal{N}^m + \epsilon^{-1}\|f\|_\infty m \, \mathcal{N}^y_{>N_*} \mathcal{N}^{m-1}.$$

Making use of Eq. (3.7.3) and the fact that $\chi\left(\mathcal{N} \leqslant C\right)\Psi_y = \Psi_y$ further yields

$$\left|\left\langle \Psi_y|\widehat{F}|\Psi_y\right\rangle - \sum_{I,J\in\mathbb{N}^m} f_{I,J}\left\langle \Psi_y|a_{I_1}^\dagger \dots a_{I_m}^\dagger a_{J_1}\dots a_{J_m}|\Psi_y\right\rangle\right| \leqslant d\alpha^{-2}\|f\|_\infty \|\Psi_y\|^2$$

for a suitable constant $d > 0$. We have thus shown the bound

$$\frac{1}{\|f\|_\infty}\left|\left\langle \Psi_y|\widehat{F}\,|\Psi_y\right\rangle - \left\langle \Psi_y|\widetilde{F}\,|\Psi_y\right\rangle\right| \leqslant \left(d\alpha^{-2} + \epsilon C^m\right)\|\Psi_y\|^2 + \epsilon^{-1} m C^{m-1}\left\langle \Psi_y|\mathcal{N}^y_{>N_*}|\Psi_y\right\rangle \tag{3.7.10}$$

which is of the desired form.

In order to verify that $\frac{1}{\|f\|_\infty}\left|\left\langle \Psi_y\middle|\widetilde{F}\,\middle|\Psi_y\right\rangle - \int F\left(|\varphi_{y,\xi}|^2\right)\,\mathrm{d}\mathbb{P}_y\left(\xi\right)\right|$ is of the same order as the right hand side of Eq. (3.7.7) as well, we will first compute $\widetilde{F}$ with reversed operator ordering, i.e. we compute

$$\sum_{I,J\in\{1,\dots,N_*\}^m} f_{I,J}\, a_{J_1}\dots a_{J_m} a_{I_1}^\dagger \dots a_{I_m}^\dagger = \sum_{I,J\in\{1,\dots,N_*\}^m} f_{I,J}\, a_{I_1}^\dagger \dots a_{I_m}^\dagger a_{J_1}\dots a_{J_m} \tag{3.7.11}$$
$$+ \sum_{n=1}^m \frac{1}{\alpha^{2n} n!}\sum_{\sigma,\tau\in\mathcal{S}^{m,n}}\left(\sum_{I',J'} f^{\sigma,\tau}_{I',J'} \prod_{k\notin\{\sigma_1,\dots,\sigma_n\}} a^\dagger_{I'_k} \prod_{\ell\notin\{\tau_1,\dots,\tau_n\}} a_{J'_\ell}\right)$$

where $\mathcal{S}^{m,n}$ is the set of all sequences $\sigma = (\sigma_1,\dots,\sigma_n)$ without repetitions having values $\sigma_k \in \{1,\dots,m\}$ and the coordinate matrices $f^{\sigma,\tau}$ are defined as

$$f^{\sigma,\tau}_{I',J'} := \sum_{I,J\in\{1,\dots,N_*\}^m} f_{I,J}\,\delta_{I_{\sigma_1},J_{\tau_1}}\dots\delta_{I_{\sigma_n},J_{\tau_n}} \prod_{k\notin\{\sigma_1,\dots,\sigma_n\}} \delta_{I_k,I'_k} \prod_{\ell\notin\{\tau_1,\dots,\tau_n\}} \delta_{J_\ell,J'_\ell}$$

for $I' \in \{1,\dots,N_*\}^{\{1,\dots,m\}\setminus\{\sigma_1,\dots,\sigma_n\}}$ and $J' \in \{1,\dots,N_*\}^{\{1,\dots,m\}\setminus\{\tau_1,\dots,\tau_n\}}$. One can verify Eq. (3.7.11) either by iteratively applying the (rescaled) canonical commutation relations $[a_i, a_j^\dagger] = \alpha^{-2}\delta_{i,j}$, or by using the fact that the operator $e^{\alpha^{-2}\nabla_{\bar{\xi}}\nabla_\xi}$, which is well defined on polynomials in ξ and $\bar{\xi}$, transforms the upper symbol into the lower symbol (see e.g. [107]), and computing its action on $P(\xi) := \sum_{I,J\in\{1,\dots,N_*\}^m} f_{I,J}\overline{\xi_{I_1}\dots\xi_{I_m}}\xi_{J_1}\dots\xi_{J_m}$ as

$$e^{\alpha^{-2}\nabla_{\bar{\xi}}\nabla_\xi}\left(P\right)\left(\xi\right) = P(\xi) + \sum_{n=1}^m \frac{1}{\alpha^{2n} n!}\sum_{\sigma,\tau\in\mathcal{S}^{m,n}}\left(\sum_{I',J'} f^{\sigma,\tau}_{I',J'} \prod_{k\notin\{\sigma_1,\dots,\sigma_n\}} \overline{\xi_{I'_k}} \prod_{\ell\notin\{\tau_1,\dots,\tau_n\}} \xi_{J'_\ell}\right).$$

In order to identify the left hand side of Eq. (3.7.11), we will make use of the resolution of identity $\frac{1}{\pi^{N_*}}\int_{\mathbb{C}^{N_*}} \Theta_{y,\xi}\,\mathrm{d}\xi = 1$, where $\Theta_{y,\xi}$ is defined below Eq. (3.7.6), which allows us to rewrite the anti-wick ordered term $a_{J_1}\dots a_{J_m} a_{I_1}^\dagger \dots a_{I_m}^\dagger$ as

$$\frac{1}{\pi^{N_*}}\int_{\mathbb{C}^{N_*}} a_{J_1}\dots a_{J_m}\Theta_{y,\xi} a_{I_1}^\dagger\dots a_{I_m}^\dagger\,\mathrm{d}\xi = \frac{1}{\pi^{N_*}}\int_{\mathbb{C}^{N_*}} \xi_{J_1}\dots\xi_{J_m}\overline{\xi_{I_1}\dots\xi_{I_m}}\Theta_{y,\xi}\,\mathrm{d}\xi.$$

Here we have used that $a_i\Theta_{y,\xi} = \xi_i\Theta_{y,\xi}$ for all $i \in \{1,\dots,N_*\}$. By the definition of $\mathbb{P}_y$ in Eq. (3.7.6) we can therefore rewrite the expectation value of the first term on the left hand side of Eq. (3.7.11) with respect to the state Ψ_y as

$$\sum_{I,J\in\{1,\dots,N_*\}^m} f_{I,J}\left\langle \Psi_y|a_{J_1}\dots a_{J_m}a_{I_1}^\dagger\dots a_{I_m}^\dagger|\Psi_y\right\rangle = \sum_{I,J\in\{1,\dots,N_*\}^m} f_{I,J}\int \xi_{J_1}\dots\xi_{J_m}\overline{\xi_{I_1}\dots\xi_{I_m}}\mathrm{d}\mathbb{P}_y(\xi)$$
$$= \int\left\langle \varphi_{y,\xi}^{\otimes m}|f|\varphi_{y,\xi}^{\otimes m}\right\rangle \mathrm{d}\mathbb{P}_y(\xi) = \int F\left(|\varphi_{y,\xi}|^2\right)\,\mathrm{d}\mathbb{P}_y\left(\xi\right). \tag{3.7.12}$$

In order to control the terms in the second line of Eq. (3.7.11), we can estimate the norm $\|f^{\sigma,\tau}\|_{\mathrm{op}} \leqslant \|f\|_\infty N_*^n$ for all $\sigma,\tau \in \mathcal{S}^{m,n}$, which follow from

$$\begin{aligned}\langle v|f^{\sigma,\tau}|w\rangle &= \sum_{I,J\in\{1,\ldots,N_*\}^m} f_{I,J}\delta_{I_{\sigma_1},J_{\tau_1}}\ldots\delta_{I_{\sigma_n},J_{\tau_n}}\overline{v_{I'}}w_{J'} = \sum_{k\in\{1,\ldots,N_*\}^n}\left\langle v^k\middle|f\middle|w^k\right\rangle\\ &\leqslant \|f\|_\infty \sum_{k\in\{1,\ldots,N_*\}^n}\|v^k\|\|w^k\| \leqslant \|f\|_\infty N_*^n\|v\|\|w\|,\end{aligned}$$

where I' denotes the restriction of I to $\{1,\ldots,m\}\backslash\{\sigma_1,\ldots,\sigma_n\}$ and v^k is defined as $\left(v^k\right)_I := \delta_{I_{\sigma_1},k_1}\ldots\delta_{I_{\sigma_n},k_n}v_{I'}$, and J' and w^k are defined analogue. Hence we obtain

$$\left|\frac{1}{\alpha^{2n}}\sum_{I',J'} f^{\sigma,\tau}_{I',J'}\langle\Psi_y|\prod_{k\notin\{\sigma_1,\ldots,\sigma_n\}}a^\dagger_{I'_k}\prod_{\ell\notin\{\tau_1,\ldots,\tau_n\}}a_{J'_\ell}|\Psi_y\rangle\right| \leqslant \|f\|_\infty\left(\frac{N_*}{\alpha^2}\right)^n\langle\Psi_y|\mathcal{N}^{m-n}|\Psi_y\rangle$$

for $n \geqslant 1$. Since $\chi\left(\mathcal{N}\leqslant C\right)\Psi_y = \Psi_y$ and $N_* \lesssim \alpha^2$, see the comment below Eq. (3.7.4), this is a quantity of order $\|f\|_\infty\frac{N_*}{\alpha^2}\|\Psi_y\|^2$. Combing this estimate with Eq. (3.7.11) and Eq. (3.7.12) yields that $\frac{1}{\|f\|_\infty}\left|\left\langle\Psi_y\middle|\widetilde{F}\middle|\Psi_y\right\rangle - \int F\left(|\varphi_{y,\xi}|^2\right)\mathrm{d}\mathbb{P}_y(\xi)\right|$ is, up to a multiplicative factor, bounded by the right hand side of Eq. (3.7.7). Together with Eq. (3.7.10), this concludes the proof of Eq. (3.7.7).

In order to verify Eq. (3.7.8), let us define $G(\rho) := \int\mathrm{d}\rho$. Note that $W_g^{-1}\mathcal{N}W_g = \mathcal{N} - a(g) - a^\dagger(g) + \|g\|^2 = \widehat{G} - a(g) - a^\dagger(g) + \|g\|^2$. Furthermore we have $\left\langle\Psi_y\middle|a(\Pi_y g) + a^\dagger(\Pi_y g)\middle|\Psi_y\right\rangle = \int\left(\langle g|\varphi_{y,\xi}\rangle + \langle\varphi_{y,\xi}|g\rangle\right)\mathrm{d}\mathbb{P}_y(\xi)$, where we used that $a(g)+a^\dagger(g)$ is anti-Wick ordered, and

$$\left|\left\langle\Psi_y\middle|a(g)+a^\dagger(g)-a(\Pi_y g)-a^\dagger(\Pi_y g)\middle|\Psi_y\right\rangle\right| \leqslant \epsilon^{-1}\langle\Psi_y|\mathcal{N}^y_{>N_*}|\Psi_y\rangle + \epsilon\|g\|^2\|\Psi_y\|^2.$$

Hence, applying Eq. (3.7.7) with respect to the function G and using that $\int\|\varphi_{y,\xi}-g\|^2\mathrm{d}\mathbb{P}_y = \int\left(G\left(|\varphi_{y,\xi}|^2\right) + \langle g|\varphi_{y,\xi}\rangle + \langle\varphi_{y,\xi}|g\rangle\right)\mathrm{d}\mathbb{P}_y(\xi) + \|g\|^2\|\Psi_y\|^2$ concludes the proof of Eq. (3.7.8). ∎

Corollary 3.7.3. *Given constants $m\in\mathbb{N}, C>0$ and $g\in L^2(\mathbb{R}^3)$, there exists a constant $T>0$ such that for all F of the form (3.7.2) and states Ψ satisfying $\chi\left(\mathcal{N}\leqslant C\right)\Psi = \Psi$ and $\langle\Psi|\mathbb{H}_K|\Psi\rangle \leqslant e^{\mathrm{Pek}} + \delta e$, with $\delta e \geqslant 0$ and $K \geqslant \Lambda_* = \alpha^{2s}$,*

$$\frac{1}{T\|f\|_\infty}\left|\left\langle\Psi\middle|\widehat{F}\middle|\Psi\right\rangle - \iint F\left(|\varphi_{y,\xi}|^2\right)\mathrm{d}\mathbb{P}_y(\xi)\,\mathrm{d}y\right| \leqslant \sqrt{\delta e} + \alpha^{-\frac{s}{2}} + \alpha^{\frac{27}{2}s-2}, \tag{3.7.13}$$

and furthermore

$$\frac{1}{T}\left|\left\langle\Psi\middle|W_g^{-1}\mathcal{N}W_g\middle|\Psi\right\rangle - \iint\|\varphi_{y,\xi}-g\|^2\mathrm{d}\mathbb{P}_y(\xi)\,\mathrm{d}y\right| \leqslant \sqrt{\delta e} + \alpha^{-\frac{s}{2}} + \alpha^{\frac{27}{2}s-2}. \tag{3.7.14}$$

Proof. Using the fact that we have $\left\langle\Psi\middle|\widehat{F}\middle|\Psi\right\rangle = \int\left\langle\Psi_y\middle|\widehat{F}\middle|\Psi_y\right\rangle\mathrm{d}y$ and $\left\langle\Psi\middle|W_g^{-1}\mathcal{N}W_g\middle|\Psi\right\rangle = \int\left\langle\Psi_y\middle|W_g^{-1}\mathcal{N}W_g\middle|\Psi_y\right\rangle\mathrm{d}y$, and applying Eq. (3.7.7), respectively Eq. (3.7.8), immediately yields that the left hand sides of Eqs. (3.7.13) and (3.7.14) are bounded by

$$\frac{N_*}{\alpha^2} + \epsilon + \epsilon^{-1}\int\langle\Psi_y|\mathcal{N}^y_{>N_*}|\Psi_y\rangle\,\mathrm{d}y \tag{3.7.15}$$

for any $\epsilon > 0$. In order to bound $\int \langle \Psi_y | \mathcal{N}^y_{>N_*} | \Psi_y \rangle \mathrm{d}y$ from above, let us first apply Eq. (3.2.3) together with Eq. (3.2.5), which provides the auxiliary estimate

$$\int |\langle \Psi_y | \mathbb{H}^y_{\Lambda_*,\ell_*} | \Psi_y \rangle - \langle \Psi_y | \mathbb{H}_K | \Psi_y \rangle | \mathrm{d}y \lesssim \alpha^{-s} \int \langle \Psi_y | -\Delta_x + \mathcal{N} + 1 | \Psi_y \rangle \mathrm{d}y$$
$$\leqslant \alpha^{-s} \int \langle \Psi_y | 2\mathbb{H}_K + d + 1 | \Psi_y \rangle \mathrm{d}y.$$

Note that the assumptions of Eq. (3.2.3) are indeed satisfied, since $K \geqslant \Lambda_*$ and $\mathrm{supp}\,(\Psi_y) \subset B_{L_*}(y)$. In combination with the IMS identity $\int \langle \Psi_y | \mathbb{H}_K | \Psi_y \rangle \mathrm{d}y = \langle \Psi | \mathbb{H}_K | \Psi \rangle + L_*^{-2} \|\nabla \chi\|^2$, where χ is the function from Eq. (3.7.5), this furthermore yields

$$\left| \int \langle \Psi_y | \mathbb{H}^y_{\Lambda_*,\ell_*} | \Psi_y \rangle \mathrm{d}y - \langle \Psi | \mathbb{H}_K | \Psi \rangle \right| \lesssim \alpha^{-s} \left(\langle \Psi | \mathbb{H}_K | \Psi \rangle + d + 1 \right), \tag{3.7.16}$$

where we have used $L_*^{-2} = \alpha^{-s}$. Furthermore $\langle \Psi | \mathbb{H}_K | \Psi \rangle \leqslant e^{\mathrm{Pek}} + \delta e$ by assumption, and consequently $|\int \langle \Psi_y | \mathbb{H}^y_{\Lambda_*,\ell_*} | \Psi_y \rangle \mathrm{d}y - \langle \Psi | \mathbb{H}_K | \Psi \rangle| \leqslant D\alpha^{-s}(\delta e + 1)$ for a suitable D. Consequently

$$\langle \Psi | \mathbb{H}_K | \Psi \rangle \geqslant \int \langle \Psi_y | \mathbb{H}^y_{\Lambda_*,\ell_*} | \Psi_y \rangle \mathrm{d}y - D\alpha^{-s}(\delta e + 1)$$
$$\geqslant E_\alpha + \int \langle \Psi_y | \mathcal{N}^y_{>N_*} | \Psi_y \rangle \mathrm{d}y - D\alpha^{-s}(\delta e + 1). \tag{3.7.17}$$

where we have used that $\mathbb{H}^y_{\Lambda_*,\ell_*} \geqslant E_\alpha + \mathcal{N}^y_{>N_*}$ in the second inequality. Using Eq. (3.7.17) as well as the fact that $E_\alpha - e^{\mathrm{Pek}} \gtrsim -\alpha^{-\frac{1}{5}} \geqslant -\alpha^{-s}$, see [79], we obtain the upper bound

$$\int \langle \Psi_y | \mathcal{N}^y_{>N_*} | \Psi_y \rangle \mathrm{d}y \lesssim \langle \Psi | \mathbb{H}_K | \Psi \rangle - e^{\mathrm{Pek}} + \alpha^{-s}(\delta e + 1) \lesssim \delta e + \alpha^{-s}. \tag{3.7.18}$$

Choosing $\epsilon := \sqrt{\delta e + \alpha^{-s}}$ in Eq. (3.7.15) therefore concludes the proof together with the observation that $\frac{N_*}{\alpha^2} \lesssim \alpha^{\frac{27}{2}s-2}$. ■

In the following Lemma 3.7.4 we are investigating the support properties of the lower symbol $\mathbb{P}_y$. In particular we derive bounds on the associated moments and verify that $\varphi_{y,\xi}$ is typically close to the manifold of minimizers $\{\varphi_x^{\mathrm{Pek}} : x \in \mathbb{R}^3\}$.

Lemma 3.7.4. *Given constants $m \in \mathbb{N}$ and $C > 0$, there exists a $T > 0$, such that $\iint |\xi|^{2m} \mathrm{d}\mathbb{P}_y(\xi)\,\mathrm{d}y \leqslant T$ for all Ψ satisfying $\chi(\mathcal{N} \leqslant C)\Psi = \Psi$, and furthermore we have for all $K \geqslant \Lambda_*$, where Λ_* is as in the definition of Π^y in Eq. (3.7.4),*

$$\frac{1}{T} \iint \inf_{x \in \mathbb{R}^3} \|\varphi_{y,\xi} - \varphi_x^{\mathrm{Pek}}\|^2 \mathrm{d}\mathbb{P}_y(\xi)\,\mathrm{d}y \leqslant \langle \Psi | \mathbb{H}_K | \Psi \rangle - e^{\mathrm{Pek}} + \alpha^{-s} + \alpha^{\frac{27}{2}s-2}. \tag{3.7.19}$$

Proof. For $m \in \mathbb{N}$, let us define the function $G(\rho) := \left(\int \mathrm{d}\rho(x)\right)^m = \int \dots \int \mathrm{d}\rho(x_1) \dots \mathrm{d}\rho(x_m)$, which is clearly of the form given in Eq. (3.7.2). Consequently by Lemma 3.7.2

$$\int |\xi|^{2m} \mathrm{d}\mathbb{P}_y(\xi) = \int G\left(|\varphi_{y,\xi}|^2\right) \mathrm{d}\mathbb{P}_y(\xi) \lesssim \langle \Psi_y | \widehat{G} | \Psi_y \rangle + \left(\frac{N_*}{\alpha^2} + 1 \right) \|\Psi_y\|^2 + \langle \Psi_y | \mathcal{N}^y_{>N_*} | \Psi_y \rangle$$
$$= \langle \Psi_y | \mathcal{N}^{2m} | \Psi_y \rangle + \left(\frac{N_*}{\alpha^2} + 1 \right) \|\Psi_y\|^2 + \langle \Psi_y | \mathcal{N}^y_{>N_*} | \Psi_y \rangle \leqslant \left(C^{2m} + \frac{N_*}{\alpha^2} + 1 + C \right) \|\Psi_y\|^2,$$

which concludes the proof of the first part, since $N_* \lesssim \alpha^2$ and $\int \|\Psi_y\|^2 \mathrm{d}y = \|\Psi\|^2 = 1$.

Regarding the proof of Eq. (3.7.19), we have the simple bound

$$\begin{aligned}\mathbb{H}^y_{\Lambda_*,\ell_*} &= -\Delta_x - a\left(\Pi_y w_x\right) - a^\dagger\left(\Pi_y w_x\right) + \mathcal{N} \geqslant -\Delta_x - a\left(\Pi_y w_x\right) - a^\dagger\left(\Pi_y w_x\right) + \sum_{n=1}^{N_*} a^\dagger_{y,n} a_{y,n} \\ &= -\Delta_x - a\left(\Pi_y w_x\right) - a^\dagger\left(\Pi_y w_x\right) + \sum_{n=1}^{N_*} a_{y,n} a^\dagger_{y,n} - \frac{N_*}{\alpha^2}. \end{aligned} \tag{3.7.20}$$

Since all terms in Eq. (3.7.20) are represented in anti-Wick ordering, we can follow [79] and express, similar as in the proof of Lemma 3.7.2, their expectation value as

$$\begin{aligned}\left\langle \Psi_y \middle| -\Delta_x - a\left(\Pi_y w_x\right) - a^\dagger\left(\Pi_y w_x\right) + \sum_{n=1}^{N_*} a_{y,n} a^\dagger_{y,n} \middle| \Psi_y \right\rangle &= \int \left(\langle \psi^\xi_y | -\Delta_x + V_{\varphi_{y,\xi}} | \psi^\xi_y \rangle + \|\varphi_{y,\xi}\|^2 \right) \mathrm{d}\mathbb{P}_y(\xi) \\ \geqslant \int \left(\inf \sigma\left(-\Delta_x + V_{\varphi_{y,\xi}}\right) + \|\varphi_{y,\xi}\|^2 \right) \mathrm{d}\mathbb{P}_y\left(\xi\right) &= \int \mathcal{F}^{\mathrm{Pek}}(\varphi_{y,\xi})\, \mathrm{d}\mathbb{P}_y\left(\xi\right), \end{aligned} \tag{3.7.21}$$

with $\psi^\xi_y := \frac{\Theta_{y,\xi}\Psi_y}{\|\Theta_{y,\xi}\Psi_y\|}$ where $\Theta_{y,\xi}$ is defined below Eq. (3.7.6), $\mathcal{F}^{\mathrm{Pek}}$ is the Pekar functional and V_φ is defined in Eq. (3.5.1). Making use of Eq. (3.7.1) we obtain together with Eqs. (3.7.16), (3.7.20) and (3.7.21)

$$\begin{aligned}\int\int \inf_{x\in\mathbb{R}^3} \|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\|^2 \mathrm{d}\mathbb{P}_y\left(\xi\right) \mathrm{d}y &\lesssim \int \langle \Psi_y | \mathbb{H}^y_{\Lambda_*,\ell_*} | \Psi_y \rangle \,\mathrm{d}y - e^{\mathrm{Pek}} + \frac{N_*}{\alpha^2} \\ &\lesssim \langle \Psi | \mathbb{H}_K | \Psi \rangle - e^{\mathrm{Pek}} + \frac{N_*}{\alpha^2} + D\alpha^{-s}\left(\langle \Psi | \mathbb{H}_K | \Psi \rangle + d + 1 \right), \end{aligned}$$

for a suitable $D > 0$. This concludes the proof, since we have $N_* \lesssim \alpha^{\frac{27}{2}s}$. ∎

The bound in Eq. (3.7.19) suggests that $\varphi_{y,\xi}$ is close to $\varphi^{\mathrm{Pek}}_{x^{y,\xi}}$ with a high probability, where $x^{y,\xi}$ is the minimizer of $x \mapsto \|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\|$. Motivated by this observation we expect $\iint F\left(|\varphi_{y,\xi}|^2\right) \mathrm{d}\mathbb{P}_y \mathrm{d}y \approx \iint F\left(\left|\varphi^{\mathrm{Pek}}_{x^{y,\xi}}\right|^2\right) \mathrm{d}\mathbb{P}_y \mathrm{d}y$ for measures $\mathbb{P}_y$ for low energy states Ψ, and therefore it seems natural to define the measure μ in Theorem 3.3.2 as $\int f \mathrm{d}\mu := \iint f\left(x^{y,\xi}\right) \mathrm{d}\mathbb{P}_y \mathrm{d}y$, allowing us to identify $\iint F\left(\left|\varphi^{\mathrm{Pek}}_{x^{y,\xi}}\right|^2\right) \mathrm{d}\mathbb{P}_y \mathrm{d}y = \int F\left(\left|\varphi^{\mathrm{Pek}}_x\right|^2\right) \mathrm{d}\mu$. This expression is however ill-defined, since the infimum $\inf_{x\in\mathbb{R}^3} \|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\|$ is not necessarily attained and it is not necessarily unique. In order to avoid these difficulties, we will slightly modify the definition of the measure μ in the proof of Lemma 3.7.5.

Lemma 3.7.5. *Given $m \in \mathbb{N}, C > 0$ and $g \in L^2(\mathbb{R}^3)$ we can find a constant $T > 0$, such that for all states Ψ satisfying $\chi\left(\mathcal{N} \leqslant C\right)\Psi = \Psi$ and $\langle \Psi | \mathbb{H}_K | \Psi \rangle \leqslant e^{\mathrm{Pek}} + \delta e$, with $\delta e \geqslant 0$ and $K \geqslant \Lambda_*$, there exists a probability measure μ on $\mathbb{R}^3$ with the property*

$$\frac{1}{T\|f\|_\infty} \left| \iint F\left(|\varphi_{y,\xi}|^2\right) \mathrm{d}\mathbb{P}_y(\xi)\, \mathrm{d}y - \int F\left(\left|\varphi^{\mathrm{Pek}}_x\right|^2\right) \mathrm{d}\mu(x) \right| \leqslant \sqrt{\delta e} + \alpha^{-\frac{s}{2}} + \alpha^{\frac{27}{4}s - 1}, \tag{3.7.22}$$

for all F of the form (3.7.2), and furthermore

$$\frac{1}{T} \left| \iint \|\varphi_{y,\xi} - g\|^2 \mathrm{d}\mathbb{P}_y(\xi)\, \mathrm{d}y - \int \|\varphi^{\mathrm{Pek}}_x - g\|^2 \mathrm{d}\mu(x) \right| \leqslant \sqrt{\delta e} + \alpha^{-\frac{s}{2}} + \alpha^{\frac{27}{4}s - 1}. \tag{3.7.23}$$

Proof. For $\epsilon > 0$, let $\bigcup_{n=1}^{\infty} A_{\epsilon,n} = \mathbb{C}^{N*}$ be a partition of $\mathbb{C}^{N*}$ consisting of non-empty measurable sets $A_{\epsilon,n}$ having a diameter bounded by $d(A_{\epsilon,n}) \leqslant \epsilon$. Furthermore choose $\xi_{\epsilon,n} \in A_{\epsilon,n}$ and $x_{\epsilon,n} \in \mathbb{R}^3$ satisfying $\|\varphi_{0,\xi_{\epsilon,n}} - \varphi^{\mathrm{Pek}}_{x_{\epsilon,n}}\| \leqslant \inf_{x\in\mathbb{R}^3} \|\varphi_{0,\xi_{\epsilon,n}} - \varphi^{\mathrm{Pek}}_{x}\| + \epsilon$. Then

$$\|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}}\| = \|\varphi_{0,\xi} - \varphi^{\mathrm{Pek}}_{x_{\epsilon,n}}\| \leqslant \|\varphi_{0,\xi_{\epsilon,n}} - \varphi^{\mathrm{Pek}}_{x_{\epsilon,n}}\| + \|\varphi_{0,\xi} - \varphi_{0,\xi_{\epsilon,n}}\| \leqslant \|\varphi_{0,\xi_{\epsilon,n}} - \varphi^{\mathrm{Pek}}_{x_{\epsilon,n}}\| + \epsilon$$
$$\leqslant \inf_{x\in\mathbb{R}^3} \|\varphi_{0,\xi_{\epsilon,n}} - \varphi^{\mathrm{Pek}}_{x}\| + 2\epsilon \leqslant \inf_{x\in\mathbb{R}^3} \|\varphi_{0,\xi} - \varphi^{\mathrm{Pek}}_{x}\| + 3\epsilon = \inf_{x\in\mathbb{R}^3} \|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_{x}\| + 3\epsilon. \quad (3.7.24)$$

Let us now define the probability measure μ on $\mathbb{R}^3$ by specifying its action on functions $f \in C(\mathbb{R}^3)$ as

$$\int f \mathrm{d}\mu := \sum_{n=1}^{\infty} \int f(y + x_{\epsilon,n}) \mathbb{P}_y(A_{\epsilon,n})\, \mathrm{d}y = \sum_{n=1}^{\infty} \int\int_{A_{\epsilon,n}} f(y + x_{\epsilon,n})\, \mathrm{d}\mathbb{P}_y \mathrm{d}y.$$

Since $\int F(|\varphi_{y,\xi}|^2) \mathrm{d}\mathbb{P}_y(\xi) = \sum_{n=1}^{\infty} \int_{A_{\epsilon,n}} F(|\varphi_{y,\xi}|^2) \mathrm{d}\mathbb{P}_y(\xi)$, we can estimate the left hand side of Eq. (3.7.22) with the aid of the triangle inequality by

$$\sum_{n=1}^{\infty} \int\int_{A_{\epsilon,n}} \left| F(|\varphi_{y,\xi}|^2) - F\left(\left|\varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}}\right|^2\right) \right| \mathrm{d}\mathbb{P}_y(\xi)\, \mathrm{d}y. \quad (3.7.25)$$

From the concrete form of the function F given in Eq. (3.7.2), as well as the facts that $\|\varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}}\| = \|\varphi^{\mathrm{Pek}}_0\|$ is finite and $\|\varphi_{y,\xi}\| = |\xi|$, one readily concludes that

$$\left| F(|\varphi_{y,\xi}|^2) - F\left(\left|\varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}}\right|^2\right) \right| \lesssim \|f\|_\infty \left\| \varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}} \right\| (1 + |\xi|)^{2m-1}.$$

Using Eq. (3.7.24) we further obtain for any $\kappa > 0$ and $\xi \in A_{\epsilon,n}$

$$\left\| \varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}} \right\| (1 + |\xi|)^{2m-1} \leqslant \left(\inf_{x\in\mathbb{R}^3} \|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\| + 3\epsilon \right) (1 + |\xi|)^{2m-1}$$
$$\leqslant \kappa^{-1} \inf_{x\in\mathbb{R}^3} \|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\|^2 + \frac{\kappa}{4} (1 + |\xi|)^{4m-2} + 3\epsilon (1 + |\xi|)^{2m-1},$$

and therefore the expression in Eq. (3.7.25) can be bounded from above by

$$\|f\|_\infty \Bigg(\kappa^{-1} \iint \inf_{x\in\mathbb{R}^3} \|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\|^2 \mathrm{d}\mathbb{P}_y(\xi)\, \mathrm{d}y + \frac{\kappa}{4} \iint (1 + |\xi|)^{4m-2} \mathrm{d}\mathbb{P}_y(\xi)\, \mathrm{d}y$$
$$+ 3\epsilon \iint (1 + |\xi|)^{2m-1} \mathrm{d}\mathbb{P}_y(\xi)\, \mathrm{d}y \Bigg).$$

By Lemma 3.7.4 this concludes the proof of (3.7.22) with $\epsilon := \kappa := \sqrt{\delta e + \alpha^{-s} + \alpha^{\frac{27}{2}s-2}}$. Eq. (3.7.23) can be proven analogously, using the estimate

$$\left| \|\varphi_{y,\xi} - g\|^2 - \|\varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}} - g\|^2 \right| \lesssim \left\| \varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}} \right\| (1 + |\xi|)$$

for $\xi \in A_{\epsilon,n}$. ■

Combining Eq. (3.7.13), respectively Eq. (3.7.14), with Eq. (3.7.22), respectively Eq. (3.7.23), immediately yields that the left hand side of Eq. (3.3.2), respectively Eq. (3.3.3), is of the order $\sqrt{\delta e} + \alpha^{-\frac{s}{2}} + \alpha^{\frac{27}{4}s-1}$. Optimizing in the parameter $0 < s \leqslant \frac{4}{27}$ concludes the proof of Theorem 3.3.2 with the concrete choice $s := \frac{4}{29}$.

3.8 Properties of the Pekar Minimizer

In the following section we derive certain useful properties concerning the minimizer φ^{Pek} of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$ in (3.5.4). We start with Lemma 3.8.1, where we quantify the error of applying the cut-off Π to a minimizer, where Π is the projection defined in Eq. (3.4.1) for a given parameter $0 < \sigma < \frac{1}{4}$. The subsequent Lemmas 3.8.2 and 3.8.3 then concern the concentration of the density $\left|\varphi^{\mathrm{Pek}}\right|^2$ around the origin.

Lemma 3.8.1. *For all* $r > 0$ *we have the estimates* $\sup_{|x|\leqslant r} \left\|(1-\Pi)\,\varphi_x^{\mathrm{Pek}}\right\| \lesssim \alpha^{-\frac{6}{5}(1+\sigma)}$. *Moreover,* $\left\|(1-\Pi)\,\partial_{x_n}\varphi^{\mathrm{Pek}}\right\| \lesssim \alpha^{-\frac{2}{5}(1+\sigma)}$ *for* $n \in \{1,2,3\}$.

Proof. We can write $\varphi^{\mathrm{Pek}} = 4\sqrt{\pi}\,(-\Delta)^{-\frac{1}{2}}\left|\psi^{\mathrm{Pek}}\right|^2$ where ψ^{Pek} is the ground state of the operator $H_{V^{\mathrm{Pek}}}$. Consequently $\varphi_x^{\mathrm{Pek}} = 4\sqrt{\pi}\,(f_x + g_x)$ with the definitions $\widehat{f}_x(k) = \mathbb{1}_{B_\Lambda}(k)\frac{\widehat{|\psi^{\mathrm{Pek}}|^2}(k)}{|k|}e^{ik\cdot x}$ and $\widehat{g}_x(k) = \mathbb{1}_{\mathbb{R}^3\setminus B_\Lambda}(k)\frac{\widehat{|\psi^{\mathrm{Pek}}|^2}(k)}{|k|}e^{ik\cdot x}$, where $\widehat{\cdot}$ denotes the Fourier transform. In the first step we are going to estimate $\|\,(1-\Pi)\,g_x\| = \|g_x\|$ by

$$\|g_x\|^2 = \int_{|k|\geqslant\Lambda} \frac{\left|\widehat{|\psi^{\mathrm{Pek}}|^2}\,(k)\right|^2}{|k|^2}\mathrm{d}k \leqslant \left\||k|^2\,\widehat{|\psi^{\mathrm{Pek}}|^2}\,(k)\right\|_\infty^2 \int_{|k|\geqslant\Lambda}\frac{1}{|k|^6}\mathrm{d}k \lesssim \frac{1}{\Lambda^3} = \alpha^{-\frac{12}{5}(1+\sigma)}, \tag{3.8.1}$$

where we have used that $\psi^{\mathrm{Pek}} \in H^2(\mathbb{R}^3)$, see [76, 95], and therefore $\left\||k|^2\,\widehat{|\psi^{\mathrm{Pek}}|^2}\,(k)\right\|_\infty < \infty$. In order to estimate the remaining part $\|\,(1-\Pi)\,f_x\|$, let us first compute

$$\begin{aligned} f_x(y) &= \frac{1}{\sqrt{(2\pi)^3}}\int_{|k|\leqslant\Lambda}\frac{\widehat{|\psi^{\mathrm{Pek}}|^2}\,(k)}{|k|}e^{ik\cdot(x-y)}\mathrm{d}k = \frac{1}{(2\pi)^3}\int_{|k|\leqslant\Lambda}\frac{e^{ik\cdot(x-y)}}{|k|}\int_{\mathbb{R}^3}\left|\psi^{\mathrm{Pek}}(z)\right|^2 e^{ik\cdot z}\mathrm{d}z\mathrm{d}k \\ &= \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\left|\psi^{\mathrm{Pek}}(z)\right|^2\int_{|k|\leqslant\Lambda}\frac{e^{ik\cdot(x+z-y)}}{|k|}\mathrm{d}k\,\mathrm{d}z = \frac{1}{\sqrt{4\pi}}\int_{\mathbb{R}^3}\left|\psi^{\mathrm{Pek}}(z)\right|^2\Pi_\Lambda w_{x+z}(y)\,\mathrm{d}z \end{aligned}$$

using the projection Π_Λ from Definition 3.2.1 and the function w_x from Lemma 3.2.2. Consequently we obtain by Lemma 3.2.2

$$\begin{aligned} \|\,(1-\Pi)\,f_x\| &\leqslant \frac{1}{\sqrt{4\pi}}\int_{\mathbb{R}^3}\left|\psi^{\mathrm{Pek}}(z)\right|^2\|\Pi_\Lambda w_{x+z} - \Pi w_{x+z}\|\,\mathrm{d}z \\ &\lesssim \ell\sqrt{\Lambda}\int_{\mathbb{R}^3}|z|\left|\psi^{\mathrm{Pek}}(z)\right|^2\,\mathrm{d}z + \ell\sqrt{\Lambda}|x| + \sqrt{\ell}, \end{aligned}$$

where we have used $(1-\Pi)\,\Pi_\Lambda = \Pi_\Lambda - \Pi$ and $\int_{\mathbb{R}^3}\left|\psi^{\mathrm{Pek}}(z)\right|^2\,\mathrm{d}z = 1$. This concludes the proof of the first part, since the terms $\ell\sqrt{\Lambda}$ and $\sqrt{\ell}$ are all bounded by $\alpha^{-\frac{6}{5}(1+\sigma)}$, and the state ψ^{Pek} satisfies $\int_{\mathbb{R}^3}|z|^p\left|\psi^{\mathrm{Pek}}(z)\right|^2\,\mathrm{d}z < \infty$ for any $p \geqslant 0$, see [95].

In order to verify the second part, we write again $\partial_{x_n}\varphi^{\mathrm{Pek}} = 4\sqrt{\pi}\,(\partial_{x_n}f_0 + \partial_{x_n}g_0)$. In analogy to Eq. (3.8.1) we have $\|\partial_{x_n}g_0\|^2 \lesssim \frac{1}{\Lambda} = \alpha^{-\frac{4}{5}(1+\sigma)}$. Furthermore $\partial_{x_n}f_0(x) =$

$-\frac{1}{\sqrt{4\pi}}\int_{\mathbb{R}^3}\partial_{z_n}\left(\left|\psi^{\mathrm{Pek}}(z)\right|^2\right)\Pi_\Lambda w_z(x)\,\mathrm{d}z$, hence proceeding as above yields

$$\|(1-\Pi)\,\partial_{x_n}f_0\| \lesssim \ell\sqrt{\Lambda}\int_{\mathbb{R}^3}|z|\left|\partial_{z_n}\left(\left|\psi^{\mathrm{Pek}}(z)\right|^2\right)\right|\mathrm{d}z + \left(\ell\sqrt{\Lambda}|x|+\sqrt{\ell}\right)\int_{\mathbb{R}^3}\left|\partial_{z_n}\left(\left|\psi^{\mathrm{Pek}}(z)\right|^2\right)\right|\mathrm{d}z.$$

This concludes the proof, since

$$\int_{\mathbb{R}^3}|z|\left|\partial_{x_n}\left(\left|\psi^{\mathrm{Pek}}(z)\right|^2\right)\right|\mathrm{d}z = 2\int_{\mathbb{R}^3}|z||\psi^{\mathrm{Pek}}(z)||\partial_{z_n}\psi^{\mathrm{Pek}}(z)|\,\mathrm{d}z \leqslant \int_{\mathbb{R}^3}|z|^2|\psi^{\mathrm{Pek}}(z)|^2\,\mathrm{d}z + \int_{\mathbb{R}^3}|\nabla\psi^{\mathrm{Pek}}(z)|^2\,\mathrm{d}z < \infty$$

and similarly with $|z|$ replaced by 1. ■

Lemma 3.8.2. *There exists a constant C such that $\int_{t\leqslant x_i\leqslant t+\epsilon}\left|\varphi^{\mathrm{Pek}}(x)\right|^2\mathrm{d}x \leqslant C\,\epsilon$ for all $t\in\mathbb{R}$, $\epsilon>0$ and $i\in\{1,2,3\}$.*

Proof. By the reflection symmetry of the Pekar minimizer, it is enough to prove the statement for $i=1$. For this purpose, let us define the function $D:\mathbb{R}\to\mathbb{R}$ as

$$D(t) := \int_{\mathbb{R}^2}\left|\varphi^{\mathrm{Pek}}(t,x_2,x_3)\right|^2\mathrm{d}x_2\mathrm{d}x_3$$

In order to prove the Lemma, we are going to show that D is a bounded function. Since $D(t)\underset{t\to\pm\infty}{\longrightarrow}0$, we have $\|D\|_\infty\leqslant\int|D'(t)|\mathrm{d}t$ and furthermore

$$\int|D'(t)|\mathrm{d}t \leqslant \int\int_{\mathbb{R}^2}\left|\partial_t\left|\varphi^{\mathrm{Pek}}(t,x_2,x_3)\right|^2\right|\mathrm{d}x_2\mathrm{d}x_3\mathrm{d}t \leqslant \int_{\mathbb{R}^3}\left|\nabla_x\left|\varphi^{\mathrm{Pek}}\right|^2\right|\mathrm{d}x = 2\int_{\mathbb{R}^3}\varphi^{\mathrm{Pek}}(x)\left|\nabla_x\varphi^{\mathrm{Pek}}\right|\mathrm{d}x \leqslant \|\varphi^{\mathrm{Pek}}\|^2+\|\nabla\varphi^{\mathrm{Pek}}\|^2<\infty,$$

where we have used that $\varphi^{\mathrm{Pek}}\in H^1(\mathbb{R}^3)$. ■

Lemma 3.8.3. *The Pekar minimizers φ^{Pek}_x satisfy $\left\|\varphi^{\mathrm{Pek}}_x-\varphi^{\mathrm{Pek}}\right\|^2\lesssim\sum_{i=1}^3 P_i^\epsilon\left(\left|\varphi^{\mathrm{Pek}}_x\right|^2\right)+\alpha^{-u}$, where P_i^ϵ is defined in Eq. (3.3.18).*

Proof. Since $\left\|\varphi^{\mathrm{Pek}}_x-\varphi^{\mathrm{Pek}}\right\|\leqslant\left\|\varphi^{\mathrm{Pek}}_x\right\|+\left\|\varphi^{\mathrm{Pek}}\right\|=2\left\|\varphi^{\mathrm{Pek}}\right\|$ and $\left\|\varphi^{\mathrm{Pek}}_x-\varphi^{\mathrm{Pek}}\right\|^2\leqslant|x|^2\left\|\nabla\varphi^{\mathrm{Pek}}\right\|^2$, we have $\left\|\varphi^{\mathrm{Pek}}_x-\varphi^{\mathrm{Pek}}\right\|^2\lesssim\min\{|x|^2,1\}$. Therefore it is enough to show that we have $\min\{x_i^2,1\}\lesssim P_i^\epsilon\left(\left|\varphi^{\mathrm{Pek}}_x\right|^2\right)+\epsilon$. By the reflection symmetry of φ^{Pek}, we can assume w.l.o.g. that $i=1$. We identify $\frac{1}{\|\varphi^{\mathrm{Pek}}\|^4}P_1^\epsilon\left(\left|\varphi^{\mathrm{Pek}}_x\right|^2\right)$

$$\frac{1}{4}-\frac{1}{\|\varphi^{\mathrm{Pek}}\|^2}\int_{y_1\leqslant x_1+\epsilon}\left|\varphi^{\mathrm{Pek}}(y)\right|^2\mathrm{d}y\left(1-\frac{1}{\|\varphi^{\mathrm{Pek}}\|^2}\int_{y_1\leqslant x_1-\epsilon}\left|\varphi^{\mathrm{Pek}}(y)\right|^2\mathrm{d}y\right)$$
$$=\left(\frac{1}{2}-F(x_1)\right)^2+F(x_1)\big(F(x_1-\epsilon)-F(x_1)\big)+\big(F(x_1)-F(x_1+\epsilon)\big)\big(1-F(x_1-\epsilon)\big)$$
$$\geqslant\left(\frac{1}{2}-F(x_1)\right)^2+\big(F(x_1-\epsilon)-F(x_1)\big)+\big(F(x_1)-F(x_1+\epsilon)\big)\geqslant\left(\frac{1}{2}-F(x_1)\right)^2-2C\,\epsilon$$

with $F(t) := \frac{1}{\|\varphi^{\mathrm{Pek}}\|^2} \int_{y_1 \leqslant t} |\varphi^{\mathrm{Pek}}(y)|^2 \, \mathrm{d}y$, where C is the constant from Lemma 3.8.2. Since φ^{Pek} is radially decreasing, see [76], it is clear that $|\varphi^{\mathrm{Pek}}(x)|^2 \geqslant c > 0$ for all $x \in [-\delta, \delta]^3$ where $\delta, c > 0$ are suitable constants. Assuming $x_1 > 0$ w.l.o.g. we conclude that $\|\varphi^{\mathrm{Pek}}\|^2 \left(F(x_1) - \frac{1}{2}\right) \geqslant c \int_{0 \leqslant y_1 \leqslant x_1} \mathbb{1}_{[-\delta,\delta]^3}(y) \, \mathrm{d}y = 4c\delta^2 \min\{x_1, \delta\} \gtrsim \min\{x_1, 1\}$. ∎

3.9 Properties of the Projection Π

In the following section we discuss properties of the Projections Π defined in Eq. (3.4.1) and Π_K defined in Definition 3.2.1. The first two results in Lemma 3.9.1 and Corollary 3.9.2 concern the space confinement of elements in the range of Π, to be precise we show that the associated potentials V_φ defined in Eq. (3.5.1) are concentrated in a ball of radius α^q for a suitable $q > 0$. While Lemma 3.9.3 is an auxiliary result, we will show in the subsequent Lemmas 3.9.4 and 3.9.5 that the operator $J_{t,\epsilon}$ is an approximation of the Hessian $\mathrm{Hess}|_{\varphi^{\mathrm{Pek}}} \mathcal{F}^{\mathrm{Pek}}$, where $J_{t,\epsilon}$ is the operator defined in Eq. (3.5.14). Finally, we will show in Lemma 3.9.6 that the functions $\Pi_K w_x$, which appear in the definition of $\mathbb{H}_K$ in Eq. (3.2.2), are confined in space around the origin. We will then use this result in order to quantify the energy cost of having the electron and the phonon field localized in different regions of space, see Corollary 3.9.7.

The proof of the following auxiliary Lemma 3.9.1 is an easy analysis exercise and is left to the reader.

Lemma 3.9.1. *There exists a constant $C > 0$ such that for $f \in C^3(\mathbb{R}^3)$ and $K := (k_1, k_1') \times (k_2, k_2') \times (k_3, k_3') \subset \mathbb{R}^3$ with $k_i < k_i' < k_i + 2$*

$$\left| \widehat{(\mathbb{1}_K f)}(x) \right| \leqslant C \frac{\|f\|_{C^3(K)}}{(1 + |x_1|)(1 + |x_2|)(1 + |x_3|)}$$

for all $x = (x_1, x_2, x_3) \in \mathbb{R}^3$, where $\|f\|_{C^3(K)} := \max_{|\alpha| \leqslant 3} \sup_{x \in K} |\partial^\alpha f(x)|$ and $\widehat{\cdot}$ denotes the Fourier transform.

Corollary 3.9.2. *There exists a constant $v > 0$, such that for all $r > 0$ and $\varphi \in \Pi L^2(\mathbb{R}^3)$*

$$\left\| \mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} V_\varphi \right\| \lesssim \frac{\alpha^v \|\varphi\|}{\sqrt{r}}, \tag{3.9.1}$$

where Π is defined in Eq. (3.4.1) and V_φ is defined in Eq. (3.5.1).

Proof. Let e_n be the basis from Definition 3.2.1 corresponding to concrete choices of Λ and ℓ defined above Eq. (3.4.1). Given $\varphi = \sum_{n=1}^N \lambda_n e_n \in \Pi L^2(\mathbb{R}^3)$, $\lambda_n \in \mathbb{C}$, we have the rough estimate

$$\left\| \mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} V_\varphi \right\| \leqslant \sum_{n=1}^N |\lambda_n| \left\| \mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} V_{e_n} \right\| \leqslant \sqrt{N} \|\varphi\| \sup_{n \in \{1, \ldots, N\}} \left\| \mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} V_{e_n} \right\|.$$

Since $N \leqslant \alpha^p$ for a suitable constant p, it is enough to verify Eq. (3.9.1) for $\varphi = e_n$. Making use of $V_{e_n} = \widehat{\mathbb{1}_{K_n} f}$ with $K_n := (z_1^n - \ell, z_1^n + \ell) \times (z_2^n - \ell, z_2^n + \ell) \times (z_3^n - \ell, z_3^n + \ell)$ and

$f(k) = \frac{-2}{\sqrt{(2\pi)^3 \int_{K_n} \frac{1}{|k|^2} \mathrm{d}k}} \frac{1}{|k|^2}$, and the fact that $(z_k^n + \ell) - (z_k^n - \ell) = 2\ell \leqslant 2$, we obtain by Lemma 3.9.1

$$\left\| \mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} V_{e_n} \right\|^2 \lesssim \alpha^{2p'} \int_{|x|>r} \frac{1}{(1+|x_1|)^2(1+|x_3|)^2(1+|x_3|)^2} \mathrm{d}x \lesssim \alpha^{2p'} \frac{1}{r},$$

where we have used $K_n \subset \mathbb{R}^3 \setminus B_{2\ell}(0)$ and therefore $\|f\|_{C^3(K)} \lesssim \ell^{-\frac{3}{2}} \Lambda(\ell)^{-5} = \alpha^{p'}$ for a suitable $p' > 0$. ∎

Lemma 3.9.3. *For $\psi \in L^2(\mathbb{R}^3)$ and $T > 0$,*

$$\int\int_{|k'|\leqslant T} \frac{|\widehat{\psi}(k-k')|^2}{(1+|k|^2)\,|k'|^2} \mathrm{d}k' \mathrm{d}k \lesssim \|\psi\|^2 T, \tag{3.9.2}$$

$$\int\int_{|k'|>T} \frac{|\widehat{\psi}(k-k')|^2}{(1+|k|^2)\,|k'|^2} \mathrm{d}k' \mathrm{d}k \lesssim \frac{\|\psi\|^2}{\sqrt{T}}. \tag{3.9.3}$$

Furthermore, interpreting ψ as a multiplication operator we have

$$\left\| (1-\Delta)^{-\frac{1}{2}} \psi \, (-\Delta)^{-\frac{1}{2}} \right\|_{\mathrm{HS}} \lesssim \|\psi\|, \tag{3.9.4}$$

$$\left\| (1-\Delta)^{-\frac{1}{2}} (-\Delta)^{-\frac{1}{2}} \psi \right\|_{\mathrm{HS}} = \sqrt{2}\pi \|\psi\|. \tag{3.9.5}$$

Proof. Eq. (3.9.2) and Eq. (3.9.3) immediately follow from the estimates

$$\int\int_{|k'|\leqslant T} \frac{|\widehat{\psi}(k-k')|^2}{(1+|k|^2)\,|k'|^2} \mathrm{d}k' \mathrm{d}k \leqslant \int\int_{|k'|\leqslant T} \frac{|\widehat{\psi}(k-k')|^2}{|k'|^2} \mathrm{d}k' \mathrm{d}k = \|\psi\|^2 4\pi T,$$

$$\int\int_{|k'|>T} \frac{|\widehat{\psi}(k-k')|^2}{(1+|k|^2)\,|k'|^2} \mathrm{d}k' \mathrm{d}k \leqslant \frac{1}{2} \int\int_{|k'|>T} \left(\frac{1}{\sqrt{T}(1+|k|^2)^2} + \frac{\sqrt{T}}{|k'|^4} \right) |\widehat{\psi}(k-k')|^2 \mathrm{d}k' \mathrm{d}k$$
$$\leqslant \frac{1}{2} \left(\int \frac{1}{(1+|k|^2)^2} \mathrm{d}k + 4\pi \right) \frac{\|\psi\|^2}{\sqrt{T}}.$$

By making use of the fact that the integral kernel of $(1-\Delta)^{-\frac{1}{2}} \psi \, (-\Delta)^{-\frac{1}{2}}$ in Fourier space is given as $\frac{\widehat{\psi}(k-k')}{\sqrt{1+|k|^2|k'|}}$, Eq. (3.9.4) immediately follows from Eq. (3.9.3) and Eq. (3.9.2) with the concrete choice $T = 1$. Finally Eq. (3.9.5) follows from the fact that the corresponding integral kernel is given by $\frac{\widehat{\psi}(k-k')}{\sqrt{1+|k|^2|k|}}$ and the identity $\int\int \frac{|\widehat{\psi}(k-k')|^2}{|k|^2(1+|k|^2)} \mathrm{d}k' \mathrm{d}k = \int \frac{1}{|k|^2(1+|k|^2)} \mathrm{d}k \, \|\psi\|^2 = 2\pi^2 \|\psi\|^2$. ∎

Lemma 3.9.4. *We have $\mathrm{Tr}\left[(1-\Pi) \, L_x^{\mathrm{Pek}} \, (1-\Pi)\right] \lesssim \alpha^{-\frac{2}{5}}$ for $|x| \lesssim 1$, where L_x^{Pek} is the operator defined above Eq. (3.5.13).*

Proof. With the definition $\psi_x^{\mathrm{Pek}}(y) := \psi^{\mathrm{Pek}}(y-x)$, we can express the operator L_x^{Pek} as $L_x^{\mathrm{Pek}} = 2 \left| (1-\Delta)^{-\frac{1}{2}} \psi_x^{\mathrm{Pek}} \, (-\Delta)^{-\frac{1}{2}} \right|^2$. Since the integral kernel of $(1-\Delta)^{-\frac{1}{2}} \psi_x^{\mathrm{Pek}} \, (-\Delta)^{-\frac{1}{2}}$ is given by $\frac{\widehat{\psi}_x^{\mathrm{Pek}}(k-k')}{\sqrt{1+|k|^2|k'|}}$ in Fourier space and since the one of Π reads $\sum_{n=1}^N \frac{\mathbb{1}_{C_{z^n}}(k) \mathbb{1}_{C_{z^n}}(k')}{\int_{C_{z^n}} \frac{1}{|q|^2} \mathrm{d}q \, |k| \, |k'|}$, where C_{z^n} is as in Definition 3.2.1, we can further express the integral kernel of the operator $(1-\Delta)^{-\frac{1}{2}}\,\psi_x^{\mathrm{Pek}}\,(-\Delta)^{-\frac{1}{2}}\,(1-\Pi)$ as

$$\sum_{n=1}^{N}\frac{\int_{C_{z^n}}\frac{\widehat{\psi}_x^{\mathrm{Pek}}(k-k')-\widehat{\psi}_x^{\mathrm{Pek}}(k-q)}{\sqrt{1+|k|^2}|k'|}\frac{1}{|q|^2}\mathrm{d}q}{\int_{C_{z^n}}\frac{1}{|q'|^2}\mathrm{d}q}\mathbb{1}_{C_{z^n}}(k')+\frac{\widehat{\psi}_x^{\mathrm{Pek}}(k-k')}{\sqrt{1+|k|^2}|k'|}\mathbb{1}_{\mathbb{R}^3\setminus\left(\bigcup_n C_{z^n}\right)}(k'). \tag{3.9.6}$$

In the following we need to show that the $L^2(\mathbb{R}^3\times\mathbb{R}^3)$ norm of the expression in Eq. (3.9.6) is of order $\alpha^{-\frac{1}{5}}$. As in the proof of Lemma 3.2.2, we will use $\mathbb{R}^3\setminus\left(\bigcup_n C_{z^n}\right)\subset B_{2\ell}\cup(\mathbb{R}^3\setminus B_{\Lambda-4\ell})$, where Λ and ℓ are defined above Eq. (3.4.1). Applying Eq. (3.9.2) with $T=2\ell$ and Eq. (3.9.3) with $T=\Lambda-4\ell$ yields

$$\int\int_{\mathbb{R}^3\setminus\left(\bigcup_n C_{z^n}\right)}\frac{|\widehat{\psi}_x^{\mathrm{Pek}}(k-k')|^2}{(1+|k|^2)|k'|^2}\,\mathrm{d}k'\mathrm{d}k\lesssim 2\ell+\frac{1}{\sqrt{\Lambda-4\ell}}\lesssim\alpha^{-\frac{2}{5}}.$$

In order to estimate the L^2 norm of $f(k,k'):=\sum_{n=1}^{N}\frac{\int_{C_{z^n}}\frac{\widehat{\psi}_x^{\mathrm{Pek}}(k-k')-\widehat{\psi}_x^{\mathrm{Pek}}(k-q)}{\sqrt{1+|k|^2}|k'|}\frac{1}{|q|^2}\mathrm{d}q}{\int_{C_{z^n}}\frac{1}{|q|^2}\mathrm{d}q}\mathbb{1}_{C_{z^n}}(k')$, let us define $\psi_{x,s,\eta}(y):=\frac{\eta}{|\eta|}\cdot ye^{is\eta\cdot y}\psi_x^{\mathrm{Pek}}(y)$ for $s\in\mathbb{R},\eta\in\mathbb{R}^3$ and $\xi:=q-k'$, and compute

$$\widehat{\psi}_x^{\mathrm{Pek}}(k-k')-\widehat{\psi}_x^{\mathrm{Pek}}(k-q)=\int_0^1\xi\cdot\nabla\widehat{\psi}_x^{\mathrm{Pek}}(k-k'+s\xi)\mathrm{d}s=|\xi|\int_0^1\widehat{\psi}_{x,s,\xi}(k-k')\mathrm{d}s.$$

Making use of the inequality $\frac{\frac{1}{|q|^2}}{\int_{C_{z^n}}\frac{1}{|q'|^2}\mathrm{d}q'}\lesssim\ell^{-3}$ for $q\in C_{z^n}$ and the fact that $\xi=q-k'\in K:=(-2\ell,2\ell)^3$ for all $k',q\in C_{z^n}$, yields

$$|f(k,k')|^2\lesssim\sum_{n=1}^{N}\mathbb{1}_{C_{z^n}}(k')\ell^{-4}\left|\int_K\int_0^1\frac{|\widehat{\psi}_{x,s,\xi}(k-k')|}{\sqrt{1+|k|^2}|k'|}\mathrm{d}s\mathrm{d}\xi\right|^2$$
$$\leqslant\sum_{n=1}^{N}\mathbb{1}_{C_{z^n}}(k')8\ell^{-1}\int_K\int_0^1\frac{\left|\widehat{\psi}_{x,s,\xi}(k-k')\right|^2}{(1+|k|^2)|k'|^2}\mathrm{d}s\mathrm{d}\xi\leqslant 8\ell^{-1}\int_K\int_0^1\frac{\left|\widehat{\psi}_{x,s,\xi}(k-k')\right|^2}{(1+|k|^2)|k'|^2}\mathrm{d}s\mathrm{d}\xi,$$

where we have applied the Cauchy–Schwarz inequality. An application of Lemma 3.9.3 with $T=1$ then yields

$$\iint|f(k,k')|^2\,\mathrm{d}k'\mathrm{d}k\lesssim\ell^{-1}\int_K\int_0^1\|\psi_{x,s,\xi}\|^2\mathrm{d}s\mathrm{d}\xi\leqslant C\ell^2\lesssim\alpha^{-8},$$

where we used that $\|\psi_{x,s,\eta}\|\leqslant C$ for all $|x|\lesssim 1$ and a suitable constant $C<\infty$. ■

Lemma 3.9.5. *Recall the operator H^{Pek} from Eq. (3.1.4). Then there exists a constant $c>0$ such that $J_{t,\epsilon}\geqslant c\,\pi$ for ϵ small enough and α large enough. Furthermore*

$$\left|\mathrm{Tr}_{\Pi L^2(\mathbb{R}^3)}\left[1-\sqrt{J_{t,\epsilon}}\right]-\mathrm{Tr}\left[1-\sqrt{H^{\mathrm{Pek}}}\right]\right|\lesssim\epsilon+\alpha^{-\frac{1}{5}} \tag{3.9.7}$$

for $|t|<\epsilon$, ϵ small enough and α large enough.

Proof. Recall the definition of π and $J_{t,\epsilon}$ in, respectively below, Eq. (3.5.13) for $|t|<\epsilon<\delta_*$, where δ_* is defined before Definition 3.5.3. In the following we are going to verify that $\|(1+\epsilon)\pi\left(K^{\mathrm{Pek}}_{x_t}+\epsilon L^{\mathrm{Pek}}_{x_t}\right)\pi\|_{\mathrm{op}}\leqslant 1-c$ for a suitable constant $c>0$, small ϵ and $|t|<\epsilon$, which immediately implies $J_{t,\epsilon}\geqslant c\pi$. Let π_x be the orthogonal projection onto $\{\partial_{x_1}\varphi^{\mathrm{Pek}}_x,\partial_{x_2}\varphi^{\mathrm{Pek}}_x,\partial_{x_3}\varphi^{\mathrm{Pek}}_x\}^{\perp}$ and let φ_n be defined in Eq. (3.5.11). Then we estimate

$$\begin{aligned}\mathrm{Tr}\left[|\pi_0-\pi_x|\right]&\leqslant 2\sum_{n=1}^{3}\left\|\varphi_n-\frac{\partial_{x_n}\varphi^{\mathrm{Pek}}_x}{\|\partial_{x_n}\varphi^{\mathrm{Pek}}_x\|}\right\| \\ &\leqslant 2\sum_{n=1}^{3}\left\|\frac{\partial_{x_n}\varphi^{\mathrm{Pek}}}{\|\partial_{x_n}\varphi^{\mathrm{Pek}}\|}-\frac{\partial_{x_n}\varphi^{\mathrm{Pek}}_x}{\|\partial_{x_n}\varphi^{\mathrm{Pek}}_x\|}\right\|+2\sum_{n=1}^{3}\left\|\varphi_n-\frac{\partial_{x_n}\varphi^{\mathrm{Pek}}}{\|\partial_{x_n}\varphi^{\mathrm{Pek}}\|}\right\|\lesssim|x|+\alpha^{-\frac{2}{5}},\end{aligned}\tag{3.9.8}$$

where we have used Lemma 3.8.1 in order to obtain $\|\partial_{x_n}\varphi^{\mathrm{Pek}}-\Pi\partial_{x_n}\varphi^{\mathrm{Pek}}\|\lesssim\alpha^{-\frac{2}{5}}$ and the fact that $\varphi^{\mathrm{Pek}}\in H^2(\mathbb{R}^3)$, which yields $\|\partial_{x_n}\varphi^{\mathrm{Pek}}_x-\partial_{x_n}\varphi^{\mathrm{Pek}}\|\leqslant|x|\left\|\nabla\partial_{x_n}\varphi^{\mathrm{Pek}}\right\|\lesssim|x|$. Hence $\mathrm{Tr}\left[|\pi_0-\pi_{\pm x_t}|\right]\lesssim|t|+\alpha^{-\frac{2}{5}}$ for t small enough. It is a straightforward consequence of (3.7.1) that the operator norm of $\pi_0K^{\mathrm{Pek}}\pi_0$ is bounded by $\|\pi_0K^{\mathrm{Pek}}\pi_0\|_{\mathrm{op}}<1$ (see also [91, Lemma 1.1]). Therefore we obtain, using $\pi=\Pi\pi_0=\pi_0\Pi$,

$$\begin{aligned}\left\|(1+\epsilon)\pi\big(K^{\mathrm{Pek}}_{x_t}+\epsilon L^{\mathrm{Pek}}_{x_t}\big)\pi\right\|_{\mathrm{op}}&\leqslant\left\|(1+\epsilon)\pi_0\big(K^{\mathrm{Pek}}_{x_t}+\epsilon L^{\mathrm{Pek}}_{x_t}\big)\pi_0\right\|_{\mathrm{op}}=\left\|\pi_0K^{\mathrm{Pek}}_{x_t}\pi_0\right\|_{\mathrm{op}}+O(\epsilon)\\&=\left\|\pi_{-x_t}K^{\mathrm{Pek}}\pi_{-x_t}\right\|_{\mathrm{op}}+O(\epsilon)=\left\|\pi_0K^{\mathrm{Pek}}\pi_0\right\|_{\mathrm{op}}+O(\epsilon)+O\big(\alpha^{-2/5}\big)\leqslant 1-c\end{aligned}\tag{3.9.9}$$

for a suitable constant $c>0$, ϵ small enough, $|t|<\epsilon$ and α large enough.

In order to verify Eq. (3.9.7), let $|t|<\epsilon$ and ϵ be small enough such that $J_{t,\epsilon}\geqslant 0$, and let us compute

$$\mathrm{Tr}_{\Pi L^2(\mathbb{R}^3)}\Big[1-\sqrt{J_{t,\epsilon}}\Big]=\mathrm{Tr}\left[1+\pi_0^{\perp}-\sqrt{1-(1+\epsilon)\pi\left(K^{\mathrm{Pek}}_{x_t}+\epsilon L^{\mathrm{Pek}}_{x_t}\right)\pi}\right],$$

Furthermore we have the identity $\mathrm{Tr}\left[1-\sqrt{1-K^{\mathrm{Pek}}}\right]=\mathrm{Tr}\left[1+\pi_0^{\perp}-\sqrt{1-\pi_0K^{\mathrm{Pek}}\pi_0}\right]=\mathrm{Tr}\left[1-\sqrt{1-\pi_{x_t}K^{\mathrm{Pek}}_{x_t}\pi_{x_t}}\,\right]+\mathrm{Tr}\left[\pi_0^{\perp}\right]$. Using the definition of K^{Pek} in Eq. (3.5.6), we can express $\mathrm{Tr}_{\Pi L^2(\mathbb{R}^3)}\Big[1-\sqrt{J_{t,\epsilon}}\,\Big]-\mathrm{Tr}\left[1-\sqrt{H^{\mathrm{Pek}}}\,\right]$ as

$$\mathrm{Tr}\left[1-\sqrt{1-(1+\epsilon)\pi\left(K^{\mathrm{Pek}}_{x_t}+\epsilon L^{\mathrm{Pek}}_{x_t}\right)\pi}\right]-\mathrm{Tr}\left[1-\sqrt{1-\pi_{x_t}K^{\mathrm{Pek}}_{x_t}\pi_{x_t}}\right].\tag{3.9.10}$$

In the following let f be a smooth function with compact support satisfying $f(x)=1-\sqrt{1-x}$ for $0\leqslant x\leqslant 1-c$, where c is as in Eq. (3.9.9), and let us define the operators $A:=(1+\epsilon)\pi\left(K^{\mathrm{Pek}}_{x_t}+\epsilon L^{\mathrm{Pek}}_{x_t}\right)\pi$ and $B:=\pi_{x_t}K^{\mathrm{Pek}}_{x_t}\pi_{x_t}$. Using Eq. (3.9.10) and $\left\|(1+\epsilon)\pi\left(K^{\mathrm{Pek}}_{x_t}+\epsilon L^{\mathrm{Pek}}_{x_t}\right)\pi\right\|_{\mathrm{op}}\leqslant 1-c$ for t and ϵ small enough, we obtain

$$\begin{aligned}\left|\mathrm{Tr}_{\Pi L^2(\mathbb{R}^3)}\Big[1-\sqrt{J_{t,\epsilon}}\,\Big]-\mathrm{Tr}\left[1-\sqrt{H^{\mathrm{Pek}}}\,\right]\right|&=\left|\mathrm{Tr}\left[f(A)-f(B)\right]\right|\\&\leqslant\|f(A)-f(B)\|_1\leqslant\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}|t\widehat{f}(t)|\,\mathrm{d}t\,\|A-B\|_1,\end{aligned}\tag{3.9.11}$$

where $\|\cdot\|_1$ is the trace norm and $\widehat{f}$ is the Fourier transformation of f. In order to estimate the right hand side of Eq. (3.9.11), we write $A-B=T_1+\pi_0T_2\pi_0+\pi T_3\pi$ with $T_1:=(\pi_0-\pi_{x_t})K^{\mathrm{Pek}}_{x_t}\pi_0+\pi_{x_t}K^{\mathrm{Pek}}_{x_t}(\pi_0-\pi_{x_t})$, $T_2:=(\Pi-1)K^{\mathrm{Pek}}_{x_t}\Pi+K^{\mathrm{Pek}}_{x_t}(\Pi-1)$ and $T_3:=\epsilon\left(K^{\mathrm{Pek}}_{x_t}+(1+\epsilon)L^{\mathrm{Pek}}_{x_t}\right)$. Clearly we have the estimates $\|\pi T_3\pi\|_1\leqslant\|T_3\|_1\lesssim\epsilon$ and $\|T_1\|_1\lesssim\|\pi_0-\pi_{x_t}\|_1\lesssim t+\alpha^{-\frac{2}{5}}$ by Eq. (3.9.8), using the fact that $K^{\mathrm{Pek}}_{x_t}$ is trace-class, which follows from $K_{x_t}^{\mathrm{Pek}} \lesssim L_{x_t}^{\mathrm{Pek}}$ and the fact that $L_{x_t}^{\mathrm{Pek}}$ is trace-class, see Eq. (3.9.4) with $\psi := \psi^{\mathrm{Pek}}$. Using Lemma 3.9.4 together with a Cauchy–Schwarz estimate for the trace norm, we can bound the final contribution $\pi_0 T_2 \pi_0$ by

$$\|\pi_0 T_2 \pi_0\|_1 \leqslant \|T_2\|_1 \leqslant 2\mathrm{Tr}\left[\Pi K_{x_t}^{\mathrm{Pek}} \Pi\right]^{\frac{1}{2}} \mathrm{Tr}\left[(1-\Pi) K_{x_t}^{\mathrm{Pek}} (1-\Pi)\right]^{\frac{1}{2}} \lesssim \alpha^{-\frac{1}{5}}.$$

∎

The following Lemma 3.9.6 is an auxiliary result, which we will use to quantify the energy cost of having the electron and the phonon field localized in different regions of space, see Corollary 3.9.7.

Lemma 3.9.6. *Let $w_0(y) = \pi^{-\frac{3}{2}} \frac{1}{|y|^2}$ and let Π_K be the projection defined in Definition 3.2.1. Then there exist a constant D such that*

$$\|\mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} \Pi_K w_0\| \leqslant \frac{D}{\sqrt{r}}$$

for all $K, r > 0$.

Proof. The Fourier transform of $\Pi_K w_0$ is given by $\frac{\chi(|k| \leqslant K)}{\sqrt{2\pi^2}|k|}$. Defining the function u via its Fourier transform as $\widehat{u}(k) := \frac{\chi^\epsilon(2\epsilon \leqslant |k| \leqslant K)}{\sqrt{2\pi^2}|k|}$, where $\epsilon > 0$ and χ^ϵ is defined in Eq. (3.3.1), we have

$$\|\Pi_K w_0 - u\|^2 \leqslant \frac{1}{2\pi^2} \int_{|k| \leqslant 3\epsilon} \frac{1}{|k|^2} \mathrm{d}k + \frac{1}{2\pi^2} \int_{K-\epsilon \leqslant |k| \leqslant K+\epsilon} \frac{1}{|k|^2} \mathrm{d}k = \frac{6\epsilon}{\pi},$$

and consequently $\|\mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} \Pi_K w_0\| \leqslant \sqrt{\frac{6\epsilon}{\pi}} + \|\mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} u\|$. Making use of the observation that $\frac{1}{|y|} \mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)}(y) \leqslant \frac{1}{r}$ yields

$$\|\mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} u\|^2 \leqslant \frac{1}{r^2} \int_{\mathbb{R}^3} |y|^2 |u(y)|^2 \mathrm{d}y = \frac{1}{r^2} \|\nabla_k \hat{u}\|^2 = \frac{1}{2\pi^2 r^2} \|f_1 - f_2\|^2$$

with $f_1(k) := \frac{\chi^\epsilon(2\epsilon \leqslant |k| \leqslant K)}{|k|^2}$ and $f_2(k) := \frac{\nabla_k \chi^\epsilon(2\epsilon \leqslant |k| \leqslant K)}{|k|}$. Clearly we can bound $\|f_1\|^2 \leqslant \int_{|k| \geqslant \epsilon} \frac{1}{|k|^4} \mathrm{d}k = \frac{4\pi}{\epsilon}$. Furthermore we obtain, using $\|\nabla_k \chi^\epsilon(2\epsilon \leqslant |k| \leqslant K)\|_\infty \lesssim \frac{1}{\epsilon}$,

$$\|f_2\|^2 \lesssim \frac{1}{\epsilon^2} \left(\int_{\epsilon \leqslant |k| \leqslant 3\epsilon} \frac{1}{|k|^2} \mathrm{d}k + \int_{K-\epsilon \leqslant |k| \leqslant K+\epsilon} \frac{1}{|k|^2} \mathrm{d}k \right) = \frac{4}{\epsilon}.$$

In combination this yields $\|\mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} \Pi_K w_0\|^2 \lesssim \epsilon + \frac{1}{r^2 \epsilon}$, which concludes the proof with the concrete choice $\epsilon := \frac{1}{r}$. ∎

Corollary 3.9.7. *Given $A \subset \mathbb{R}^3$, let us define the operator $\mathcal{N}_A := \widehat{D_A}$ with $D_A(\rho) := \int_A \mathrm{d}\rho(y)$, using the notation of Definition 3.3.1, i.e. $\alpha^2 \mathcal{N}_A$ counts the number of particles in the region A. Furthermore let $A' \subset \mathbb{R}^3$. Then given a constant $C > 0$, there exists a constant $D > 0$ such that for all states Ψ with $\mathrm{supp}(\Psi) \subset A'$ and $\chi(\mathcal{N} \leqslant C)\Psi = \Psi$*

$$\langle \Psi | \mathbb{H}_K | \Psi \rangle \geqslant E_\alpha + \langle \Psi | \mathcal{N}_A | \Psi \rangle - \sqrt{\frac{D}{\mathrm{dist}(A, A')}},$$

where $K > 0$.

Proof. Let us define the function $v_x := \mathbb{1}_A \Pi_K w_x$ and rewrite $\mathbb{H}_K - \mathcal{N}_A$ as

$$\mathbb{H}_K - \mathcal{N}_A = -\Delta_x - a\left(\Pi_K w_x - v_x\right) - a^\dagger\left(\Pi_K w_x - v_x\right) + \mathcal{N} - \mathcal{N}_A - a\left(v_x\right) - a^\dagger\left(v_x\right).$$

Identifying $L^2\Big(\mathbb{R}^3, \mathcal{F}\big(L^2(\mathbb{R}^3)\big)\Big) \cong L^2\Big(\mathbb{R}^3, \mathcal{F}\Big(L^2(\mathbb{R}^3 \backslash A)\Big)\Big) \otimes \mathcal{F}\Big(L^2(A)\Big)$, we observe that $-\Delta_x - a\left(\Pi_K w_x - v_x\right) - a^\dagger\left(\Pi_K w_x - v_x\right) + \mathcal{N} - \mathcal{N}_A$ is the restriction (in the sense of quadratic forms) of $\mathbb{H}_K$ to states of the form $\Psi' \otimes \Omega$, where Ω is the vacuum in $\mathcal{F}\Big(L^2(A)\Big)$, and therefore we have the operator inequality $-\Delta_x - a\left(\Pi_K w_x - v_x\right) - a^\dagger\left(\Pi_K w_x - v_x\right) + \mathcal{N} - \mathcal{N}_A \geqslant E_\alpha$. Consequently

$$\langle \Psi | \mathbb{H}_K - \mathcal{N}_A | \Psi \rangle \geqslant E_\alpha - \langle \Psi | a\left(v_x\right) + a^\dagger\left(v_x\right) | \Psi \rangle \geqslant E_\alpha - \sup_{x \in A'} \|v_x\| \left(1 + C\right),$$

where we have used the operator inequality $a\left(v_x\right) + a^\dagger\left(v_x\right) \geqslant -\|v_x\|\left(1 + \mathcal{N}\right)$, as well as the assumptions $\operatorname{supp}(\Psi) \subset A'$ and $\chi\left(\mathcal{N} \leqslant C\right)\Psi = \Psi$, in the second inequality. This concludes the proof, since $\|v_x\|^2 = \int_A \left|\Pi_K w_0(y - x)\right|^2 \mathrm{d}y \leqslant \int_{|y| \geqslant \mathrm{dist}(A, A')} \left|\Pi_K w_0(y)\right|^2 \mathrm{d}y$ for all $x \in A'$ and $\int_{|y| \geqslant \mathrm{dist}(A, A')} \left|\Pi_K w_0(y)\right|^2 \mathrm{d}y \lesssim \frac{1}{\mathrm{dist}(A, A')}$, see Lemma 3.9.6. ∎

CHAPTER 4

The Fröhlich Polaron at Strong Coupling – Part II: Energy-Momentum Relation and effective Mass

ABSTRACT. We study the Fröhlich polaron model in $\mathbb{R}^3$, and prove a lower bound on its ground state energy as a function of the total momentum. The bound is asymptotically sharp at large coupling. In combination with a corresponding upper bound proved earlier [91], it shows that the energy is approximately parabolic below the continuum threshold, and that the polaron's effective mass (defined as the semi-latus rectum of the parabola) is given by the celebrated Landau–Pekar formula. In particular, it diverges as α^4 for large coupling constant α.

4.1 Introduction and Main Results

This is the second part of a study of the Fröhlich polaron [44] in the regime of strong coupling between the electron and the phonons, which are the optical modes of a polar crystal. Our goal is to quantify the heuristic picture that the mass of an electron in a polarizable medium effectively increases due to an emerging phonon cloud attached to it. We are going to verify that the energy-momentum relation of a polaron is asymptotically given by the semi-classical formula $E(P) - E(0) = \frac{|P|^2}{2\alpha^4 m}$, which agrees with the energy-momentum relation of a particle having mass $\alpha^4 m$, where $\alpha^4 m$ is the asymptotic formula conjectured by Landau and Pekar [63] for the mass of a polaron in the regime where the coupling parameter α goes to infinity.

Following the notation of the first part [17], where a second order expansion for the absolute ground state energy of a polaron was verified, we are going to use creation and annihilation operators satisfying the semi-classical rescaled canonical commutation relations $[a(f), a^\dagger(g)] = \alpha^{-2} \langle f|g\rangle$ for $f, g \in L^2(\mathbb{R}^3)$, in order to introduce the Fröhlich Hamiltonian acting on the Fock space $L^2(\mathbb{R}^3) \otimes \mathcal{F}(L^2(\mathbb{R}^3))$ as

$$\mathbb{H} := -\Delta_x - a(w_x) - a^\dagger(w_x) + \mathcal{N},$$

where $w_x(x') := \pi^{-\frac{3}{2}}|x' - x|^{-2}$ and the (rescaled) particle number operator $\mathcal{N}$ equals $\mathcal{N} := \sum_{n=1}^{\infty} a^\dagger(\varphi_n)a(\varphi_n)$ for an orthonormal basis $\{\varphi_n : n \in \mathbb{N}\}$ of $L^2(\mathbb{R}^3)$. The Fröhlich

Hamiltonian $\mathbb{H}$ commutes with the components $(\mathbb{P}_1, \mathbb{P}_2, \mathbb{P}_3)$ of the total momentum operator

$$\mathbb{P} := \frac{1}{i}\nabla + \alpha^2 \int_{\mathbb{R}^3} k\, a_k^\dagger a_k \mathrm{d}k\,,$$

where we use the standard notation $\int_{\mathbb{R}^3} f(k) a_k^\dagger a_k \mathrm{d}k$ as a symbolic expression for the operator $\sum_{n,m=1}^{\infty} \left\langle \varphi_n \middle| f\left(\frac{1}{i}\nabla\right) \middle| \varphi_m \right\rangle a^\dagger(\varphi_n) a(\varphi_m)$. Hence we can study their joint spectrum $\sigma(\mathbb{P}, \mathbb{H}) \subseteq \mathbb{R}^4$, and define the ground state energy $E_\alpha(P)$ of $\mathbb{H}$ at total momentum P as $E_\alpha(P) := \inf\left\{ E : (P, E) \in \sigma(\mathbb{P}, \mathbb{H}) \right\}$. Our main result below is the proof of the asymptotic energy-momentum relation

$$E_\alpha(P) = E_\alpha(0) + \min\left\{ \frac{|P|^2}{2\alpha^4 m}, \alpha^{-2} \right\} + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right), \tag{4.1.1}$$

where $w > 0$ is a suitable constant and m is the conjectured constant by Landau and Pekar. In order to provide an explicit expression for m, let us first define the Pekar functional $\mathcal{F}^{\mathrm{Pek}}(\varphi) := \|\varphi\|^2 + \inf \sigma(-\Delta + V_\varphi)$ for $\varphi \in L^2(\mathbb{R}^3)$, where we define the potential $V_\varphi := -2(-\Delta)^{-\frac{1}{2}} \mathfrak{Re}\, \varphi$. If follows from the analysis in [76] that there exists a unique radial minimizer φ^{Pek} of the functional $\mathcal{F}^{\mathrm{Pek}}$. With this minimizer at hand, we can introduce the constant $m := \frac{2}{3}\left\|\nabla \varphi^{\mathrm{Pek}}\right\|^2$ in Eq. (4.1.1).

In order to formulate our main Theorem 4.1.1, let us further introduce the minimal Pekar energy $e^{\mathrm{Pek}} := \inf_\varphi \mathcal{F}^{\mathrm{Pek}}(\varphi)$ as well as the Hessian H^{Pek} of $\mathcal{F}^{\mathrm{Pek}}$ at the minimizer φ^{Pek} restricted to real-valued functions $\varphi \in L^2_{\mathbb{R}}(\mathbb{R}^3)$, i.e. we define H^{Pek} as the unique self-adjoint operator on $L^2(\mathbb{R}^3)$ satisfying

$$\langle \varphi | H^{\mathrm{Pek}} | \varphi \rangle = \lim_{\epsilon \to 0} \frac{1}{\epsilon^2}\left(\mathcal{F}^{\mathrm{Pek}}\left(\varphi^{\mathrm{Pek}} + \epsilon\varphi\right) - e^{\mathrm{Pek}} \right)$$

for all $\varphi \in L^2_{\mathbb{R}}(\mathbb{R}^3)$. With this notation at hand, we can state our main new result in Theorem 4.1.1. It provides a sharp asymptotic lower bound on the ground state energy $E_\alpha(P)$ of the operator $\mathbb{H}$ as a function of the total momentum $\mathbb{P}$.

Theorem 4.1.1. *There exists a constant $w > 0$ such that*

$$E_\alpha(P) \geqslant e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \min\left\{ \frac{|P|^2}{2\alpha^4 m}, \alpha^{-2} \right\} - \alpha^{-(2+w)} \tag{4.1.2}$$

for all $P \in \mathbb{R}^3$ and for all $\alpha \geqslant \alpha_0$, where α_0 is a suitable constant.

That the lower bound in Eq. (4.1.2) is indeed sharp follows from the corresponding asymptotic upper bound established in [91], given by

$$E_\alpha(P) \leqslant e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \min\left\{ \frac{|P|^2}{2\alpha^4 m}, \alpha^{-2} \right\} + C_\epsilon \alpha^{-\frac{5}{2}+\epsilon}, \tag{4.1.3}$$

where $\epsilon > 0$ is arbitrary and C_ϵ a suitable constant. In combination with Eq. (4.1.2) this shows that

$$E_\alpha(P) = e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \min\left\{ \frac{|P|^2}{2\alpha^4 m}, \alpha^{-2} \right\} + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right)$$

for all $P \in \mathbb{R}^3$, which in particular proves Eq. (4.1.1). Note that α^{-2} corresponds to the continuum threshold; i.e., $\sigma(\mathbb{P},\mathbb{H}) \supset \mathbb{R}^3 \times [E_\alpha(0)+\alpha^{-2},\infty)$, the latter corresponding to states describing free phonons on top of the polaron ground state [93**?**].

In particular, $E_\alpha(P)$ has an approximate parabolic shape below the continuum threshold, i.e., for $|P| < \sqrt{2m}\alpha$. The Landau–Pekar formula for the effective mass appears in the limit $\alpha \to \infty$ as the semi-latus rectum of the parabola, in the sense that for any $0 < |P| < \sqrt{2m}$

$$m = \lim_{\alpha\to\infty} \alpha^{-4} \frac{|\alpha P|^2}{2\left(E_\alpha(\alpha P) - E_\alpha(0)\right)} . \tag{4.1.4}$$

It is common the define the polaron's effective mass for fixed α as

$$M_{\text{eff}}(\alpha) := \lim_{P\to 0} \frac{|P|^2}{2\left(E_\alpha(P) - E_\alpha(0)\right)} .$$

The quantity on the right hand side of Eq. (4.1.4) is clearly related to the large α limit of $\alpha^{-4}M_{\text{eff}}(\alpha)$, with the difference being that the limit $P \to 0$ is taken before the limit $\alpha \to \infty$. While it is not clear at this point how to obtain the lower bound $\lim_{\alpha\to\infty}\alpha^{-4}M_{\text{eff}}(\alpha) \geqslant m$, we can make use of the inequality $E_\alpha(P) \leqslant E_\alpha(0) + \frac{|P|^2}{2M_{\text{eff}}(\alpha)}$ recently proved in [110] in order to verify the upper bound $\lim_{\alpha\to\infty}\alpha^{-4}M_{\text{eff}}(\alpha) \leqslant m$. In fact, by applying Eq. (4.1.1) in the special case of P satisfying $|P| = \sqrt{2m}\alpha$ we have

$$E_\alpha(0) + \frac{1}{\alpha^2} + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right) = E_\alpha(P) \leqslant E_\alpha(0) + \frac{m\alpha^2}{M_{\text{eff}}(\alpha)},$$

which yields the claimed upper bound on $M_{\text{eff}}(\alpha)$. We formulate it as the subsequent Corollary.

Corollary 4.1.2. *There exists a constant $w > 0$ such that $M_{\text{eff}}(\alpha) \leqslant \alpha^4 m + O_{\alpha\to\infty}(\alpha^{4-w})$.*

The remainder of this paper contains the proof of Theorem 4.1.1. In order to guide the reader, we start with a short explanation of the main strategy.

Proof strategy of Theorem 4.1.1. Since $(P, E_\alpha(P))$ is an element of the joint spectrum of the operator pair $(\mathbb{P},\mathbb{H})$, there clearly exist states Ψ_α satisfying $\mathbb{P}\Psi_\alpha \approx P\Psi_\alpha$ and $\mathbb{H}\Psi_\alpha \approx E_\alpha(P)\Psi_\alpha$. In order to verify Theorem 4.1.1, it is therefore enough to show that $\langle\Psi_\alpha|\mathbb{H}|\Psi_\alpha\rangle$ is bounded from below by the right hand side of Eq. (4.1.2). For this to hold it is crucial to use the additional information $\mathbb{P}\Psi_\alpha \approx P\Psi_\alpha$ on the momentum, since in general $\mathbb{H}$, as an operator, is not bounded from below by the right hand side of Eq. (4.1.2). It is not possible to transform the constrained minimization problem to a global one by the usual method of Lagrange multipliers, since the operators $\mathbb{P}$ are not bounded relative to $\mathbb{H}$. More precisely, while clearly

$$E_\alpha(P) \geqslant \inf \sigma(\mathbb{H} + \lambda(P - \mathbb{P})) \tag{4.1.5}$$

for any $\lambda \in \mathbb{R}^3$, such a bound is insufficient as the right hand side is $-\infty$ for $\lambda \neq 0$, which follows easily from the fact that $E_\alpha(P)$ is bounded uniformly in P (compare with Eq. (4.1.1)).

In order to improve the lower bound in Eq. (4.1.5), we introduce a wavenumber cut-off Λ in the Hamiltonian $\mathbb{H}$ as well as in the momentum operator $\mathbb{P}$, leading to the study of the ground state energy $E_{\alpha,\Lambda}(P)$ of the truncated Hamiltonian $\mathbb{H}_\Lambda$ as a function of the truncated momentum $\mathbb{P}_\Lambda$. As we will show in the subsequent Section 4.2, it is enough to prove Eq. (4.1.2) for the modified energy $E_{\alpha,\Lambda}(P)$ in order to verify our main Theorem 4.1.1. By introducing the cut-off we manually exclude the radiative regime where a single phonon carries the total momentum, which is responsible for the (approximately) flat energy-momentum relation $E_\alpha(P)$ above the threshold $|P| = \sqrt{2m}\alpha$ and the resulting collapse of the quadratic approximation $E_\alpha(P) - E_\alpha(0) \approx \frac{|P|^2}{2\alpha^4 m}$ above this threshold.

In contrast, in the presence of the cut-off, it turns out that we can apply the method of Lagrange multiplies. We shall follow the strategy developed in the first part [17], and construct approximate eigenstates Ψ_α to the joint eigenvalue $(P, E_{\alpha,\Lambda}(P))$ of the operator pair $(\mathbb{P}_\Lambda, \mathbb{H}_\Lambda)$, which in addition satisfy (complete) Bose–Einstein condensation with respect to the minimizer φ^{Pek} of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$. In this context we call Ψ_α an approximate eigenstate in case $\langle \Psi_\alpha | (\mathbb{P}_\Lambda - P)^2 | \Psi_\alpha \rangle = O_{\alpha\to\infty}(\alpha^{2-r})$ and $E_{\alpha,\Lambda}(P) \geqslant \langle \Psi_\alpha | \mathbb{H}_\Lambda | \Psi_\alpha \rangle + O_{\alpha\to\infty}\big(\alpha^{-(2+r)}\big)$ for some $r > 0$. In order to verify that $E_{\alpha,\Lambda}(P)$ is bounded from below by the right hand side of Eq. (4.1.2), it is consequently enough to show that

$$\left\langle \Psi \middle| \mathbb{H}_\Lambda + \lambda\Big(P - \mathbb{P}_\Lambda\Big) \middle| \Psi \right\rangle \geqslant e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \lambda P - \frac{\alpha^4 m |\lambda|^2}{2} - \alpha^{-(2+w)} \tag{4.1.6}$$

for all states Ψ satisfying (complete) Bose–Einstein condensation with respect to the minimizer φ^{Pek}, providing the desired lower bound for the optimal choice $\lambda = \frac{P}{m\alpha^4}$, with the term $\frac{\alpha^4 m|\lambda|^2}{2}$ in Eq. (4.1.6) arising naturally as the Legendre transformation of the quadratic approximation $\frac{|P|^2}{2\alpha^4 m}$.

Since Eq. (4.1.6) claims a global lower bound, i.e. there is no constraint on the momentum of Ψ, we can utilize the methods developed in the first part [17], where a lower bound on the total minimum $E_\alpha = \inf \sigma(\mathbb{H})$ was established. The basic idea is that we can find, up to a unitary transformation, a lower bound on the operator $\mathbb{H}_\Lambda + \frac{P}{m\alpha^4}\Big(P - \mathbb{P}_\Lambda\Big)$ of the form $e^{\mathrm{Pek}} + \frac{|P|^2}{2\alpha^4 m} + \mathbb{Q} + O_{\alpha\to\infty}\big(\alpha^{-(2+r)}\big)$, where $\mathbb{Q}$ is a system of harmonic oscillators, which holds when tested against states satisfying (complete) Bose–Einstein condensation. The ground state energy of $\mathbb{Q}$ can then be computed explicitly, giving rise to the quantum correction $-\frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right]$ in Eq. (4.1.2).

Outline. The paper is structured as follows. In Section 4.2 we shall show that it is sufficient to prove Eq. (4.1.2) for a model including a suitable ultraviolet wavenumber cut-off in order to verify our main Theorem 4.1.1. In the subsequent Section 4.3, we will construct approximate eigenstates for the truncated model defined in Section 4.2, which in addition satisfy (complete) Bose–Einstein condensation with respect to the state φ^{Pek}. Section 4.4 is then devoted to the proof of our main technical Theorem 4.2.1, where we use the method of Lagrange multipliers in order to get rid of the momentum constraint. Finally, Appendix 4.5 contains auxiliary results on commutator estimates as well as properties of the Pekar minimizer φ^{Pek}, which get used in the proof.

4.2 Reduction to Bounded Wavenumbers

In this section we shall introduce the truncated Hamiltonian $\mathbb{H}_\Lambda$, which includes a wavenumber restriction $|k| \leqslant \Lambda$, and we are going to state our main technical Theorem 4.2.1, which provides an analogue of Theorem 4.1.1 for the truncated model. While the proof of Theorem 4.2.1 is the content of Sections 4.3 and 4.4, we will verify in this Section that Theorem 4.1.1 is a consequence of Theorem 4.2.1, i.e. we will explain why it is enough to prove Eq. (4.1.2) for a model including a wavenumber regularization. The quantum nature of our system, and in particular the discrete spectrum $\sigma(\mathcal{N}) = \left\{0, \frac{1}{\alpha^2}, \frac{2}{\alpha^2}, \dots\right\}$ of the number operator $\mathcal{N}$, is essential for this argument to work. In contrast, in the classical case the effective mass is infinite since there nothing prevents a priori the wavenumber from escaping to infinity without an energy penalty, and one has to introduce a suitable regularization in order to observe the expected asymptotics $M_{\text{eff}} = \alpha^4 m + o_{\alpha\to\infty}(\alpha^4)$, see [39].

Before formulating Theorem 4.2.1, we shall introduce some useful notation. Following [17], we define for a function $f : X \longrightarrow \mathbb{R}$, $\epsilon \geqslant 0$ and $-\infty \leqslant a \leqslant b \leqslant \infty$, the function $\chi^\epsilon(a \leqslant f \leqslant b) : X \longrightarrow [0,1]$ as

$$\chi^\epsilon(a \leqslant f(x) \leqslant b) := \begin{cases} \alpha\left(\frac{f(x)-b}{\epsilon}\right)\beta\left(\frac{f(x)-a}{\epsilon}\right), & \text{for } \epsilon > 0 \\ \mathbb{1}_{[a,b]}(f(x)), & \text{for } \epsilon = 0, \end{cases} \tag{4.2.1}$$

where $\alpha, \beta : \mathbb{R} \longrightarrow [0,1]$ are given C^∞ functions such that $\alpha^2 + \beta^2 = 1$, $\operatorname{supp}(\alpha) \subset (-\infty, 1)$ and $\operatorname{supp}(\beta) \subset (-1, \infty)$. Similarly we define the operator $\chi^\epsilon(a \leqslant T \leqslant b) := \int \chi^\epsilon(a \leqslant t \leqslant b)\,\mathrm{d}E$, where T is a self-adjoint operator and E the corresponding spectral measure. Furthermore let us write $\chi(a \leqslant f \leqslant b)$ in case $\epsilon = 0$ and $\chi^\epsilon(\cdot \leqslant b)$, respectively $\chi^\epsilon(a \leqslant \cdot)$, in case $a = -\infty$ or $b = \infty$, respectively. With this notation at hand, we define the Hamiltonian $\mathbb{H}_\Lambda$ with wavenumber cut-off $\Lambda \geqslant 0$ as

$$\mathbb{H}_\Lambda := -\Delta_x - a(\chi(|\nabla| \leqslant \Lambda)\, w_x) - a^\dagger(\chi(|\nabla| \leqslant \Lambda)\, w_x) + \mathcal{N}. \tag{4.2.2}$$

Theorem 4.2.1. *Let $E_{\alpha,\Lambda}(P)$ be the ground state energy of the operator $\mathbb{H}_\Lambda$ as a function of the (one-component of the) truncated total momentum*

$$\mathbb{P}_\Lambda := \frac{1}{i}\nabla_{x_1} + \alpha^2 \int \chi^1(\Lambda^{-1}|k_1| \leqslant 2) k_1\, a_k^\dagger a_k \mathrm{d}k$$

and let $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ with $0 < \sigma < \frac{1}{9}$. Then there exists a constant $w > 0$ such that for all $C > 0$, $|P| \leqslant C\alpha$ and $\alpha_0 \geqslant \alpha(\sigma, C)$

$$E_{\alpha,\Lambda}(P) \geqslant e^{\text{Pek}} - \frac{1}{2\alpha^2}\operatorname{Tr}\left[1 - \sqrt{H^{\text{Pek}}}\right] + \frac{|P|^2}{2\alpha^4 m} - \alpha^{-(2+w)}, \tag{4.2.3}$$

where $\alpha_0(\sigma, C)$ is a suitable constant.

For technical reasons we use here the smooth cut-off $\chi^1(\Lambda^{-1}|k_1| \leqslant 2)$ instead of the sharp cut-off $\chi(\Lambda^{-1}|k_1| \leqslant 1)$ in the definition of the momentum operator $\mathbb{P}_\Lambda$. Note also that the momentum cut-off appears in (4.2.2) only in the interaction term, and not in the field energy $\mathcal{N}$. In the following we shall argue that, as a consequence of Theorem 4.2.1, Eq. (4.2.3) is also valid with $\mathbb{P}_\Lambda$ replaced by $\mathbb{P}_1' := \frac{1}{i}\nabla_{x_1} + \alpha^2 \int_{|k|\leqslant\Lambda} k_j\, a_k^\dagger a_k \mathrm{d}k$ having the sharp cut-off, and with H_Λ replaced by the fully restricted Hamiltonian $\mathbb{H}_\Lambda' := \mathbb{H}_\Lambda - \int_{|k|>\Lambda} a_k^\dagger a_k \mathrm{d}k$. In order to see this, observe that $\mathbb{P}_1'$ and $\mathbb{H}_\Lambda'$ are the restrictions (in the sense of operators) of $\mathbb{P}_\Lambda$ and $\mathbb{H}_\Lambda$ to states of the form $\Psi' \otimes \Omega$, where $\Psi' \in L^2\Big(\mathbb{R}^3, \mathcal{F}\big(\operatorname{ran}\chi(|\nabla| \leqslant \Lambda)\big)\Big)$ and Ω is the vacuum in $\mathcal{F}\Big(\mathrm{ran}\chi\big(|\nabla| > \Lambda\big)\Big)$. Hence

$$\sigma\left(\mathbb{P}_1', \mathbb{H}_\Lambda'\right) \subseteq \sigma\left(\mathbb{P}_\Lambda, \mathbb{H}_\Lambda\right),$$

and therefore we obtain as an immediate consequence of the previous Theorem 4.2.1 that

$$E \geqslant e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \frac{|P|^2}{2\alpha^4 m} - \alpha^{-(2+w)} \tag{4.2.4}$$

for all $(P, E) \in \sigma\left(\mathbb{P}_1', \mathbb{H}_\Lambda'\right)$ with $|P| \leqslant C\alpha$ and $\alpha \geqslant \alpha_0(\sigma, C)$. In the proof of Theorem 4.1.1 below it will be useful to have Eq. (4.2.4) for $\mathbb{P}_1'$ and $\mathbb{H}_\Lambda'$, instead of Eq. (4.2.3) for $\mathbb{P}_\Lambda$ and $\mathbb{H}_\Lambda$.

In order to verify Theorem 4.1.1, it is convenient to introduce the ground state energy $E^*_{\alpha,\Lambda}(P)$ of the operator $\mathbb{H}_\Lambda$ as a function of $\mathbb{P}$. Note that in contrast to $E_{\alpha,\Lambda}(P)$, we do not use a wavenumber cut-off in the momentum operator here, while we still have the cut-off in the Hamiltonian $\mathbb{H}_\Lambda$. In the following Lemma 4.2.2 we are going to utilize the results in [40, 97], where the energy cost of introducing a wavenumber cut-off in the Hamiltonian is quantified, in order to compare $E^*_{\alpha,\Lambda}(P)$ with $E_\alpha(P)$.

Lemma 4.2.2. *Let $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ for $\sigma > 0$. Then there exists a constant $C' > 0$, such that for all $P \in \mathbb{R}^3$ and α large enough*

$$E_\alpha(P) \geqslant E^*_{\alpha,\Lambda}(P) - C'\alpha^{-2(1+\sigma)}.$$

Proof. By the results in [40, 97], there exists a $C > 0$ such that for α large enough

$$\mathbb{H}_\Lambda \leqslant \mathbb{H} + C\alpha^{-2(1+\sigma)}\left(\mathbb{H}^2 + 1\right). \tag{4.2.5}$$

This was first shown in [40] for a confined polaron model on a bounded domain, but the method extends in a straightforward way to the model on $\mathbb{R}^3$, as shown in [97] (see also [37] for the corresponding result for a polaron model on a torus). In the following, let Ψ_ϵ be a state satisfying $\chi\left(\sum_{j=1}^3 (\mathbb{P}_j - P_j)^2 \leqslant \epsilon^2\right)\Psi_\epsilon = \Psi_\epsilon$ and $\langle\Psi_\epsilon|\big(\mathbb{H} - E_\alpha(P)\big)^2|\Psi_\epsilon\rangle \leqslant \epsilon^2$, where $\epsilon > 0$. By Eq. (4.2.5) we therefore have

$$\begin{aligned}\langle\Psi_\epsilon|\mathbb{H}_\Lambda|\Psi_\epsilon\rangle &\leqslant E_\alpha(P) + C\alpha^{-2(1+\sigma)}\left(\langle\Psi_\epsilon|\mathbb{H}^2|\Psi_\epsilon\rangle + 1\right) + \epsilon \\ &\leqslant E_\alpha(P) + C\alpha^{-2(1+\sigma)}\left(2E_\alpha(P)^2 + 2\epsilon^2 + 1\right) + \epsilon \leqslant E_\alpha(P) + C'\alpha^{-2(1+\sigma)} + \epsilon\end{aligned}$$

for $0 < \epsilon \leqslant 1$ and a suitable C', where we used that $E_\alpha(P)$ is uniformly bounded for $P \in \mathbb{R}^3$ and $\alpha \geqslant 1$ in the last inequality. Hence $\chi\left(\mathbb{H}_\Lambda \leqslant E_\alpha(P) + C'\alpha^{-2(1+\sigma)} + \epsilon\right)\Psi_\epsilon \neq 0$. Using $\chi\left(\sum_{j=1}^3 (\mathbb{P}_j - P_j)^2 \leqslant \epsilon^2\right)\Psi_\epsilon = \Psi_\epsilon$, we obtain

$$A_\epsilon := \sigma\left(\mathbb{P}, \mathbb{H}_\Lambda\right) \cap \left(B_\epsilon(P) \times \left(-\infty, E_\alpha(P) + C'\alpha^{-2(1+\sigma)} + \epsilon\right]\right) \neq \varnothing.$$

Since $\mathbb{H}_\Lambda$ is bounded from below, $(A_\epsilon)_{0<\epsilon\leqslant 1}$ is a monotone sequence of non-empty compact sets, i.e. $A_{\epsilon_1} \subseteq A_{\epsilon_2}$ for $\epsilon_1 \leqslant \epsilon_2$, and consequently

$$\sigma\left(\mathbb{P}, \mathbb{H}_\Lambda\right) \cap \left(\{P\} \times \left(-\infty, E_\alpha(P) + C'\alpha^{-2(1+\sigma)}\right]\right) = \bigcap_{0<\epsilon\leqslant 1} A_\epsilon \neq \varnothing,$$

which is equivalent to $E^*_{\alpha,\Lambda}(P) \leqslant E_\alpha(P) + C'\alpha^{-2(1+\sigma)}$. ∎

Given Theorem 4.2.1 we can now give a proof of Theorem 4.1.1.

Proof of Theorem 4.1.1. In the first step of the proof, we are going to verify Eq. (4.1.2) for $|P| \leqslant \sqrt{2m}\alpha$. Due to the rotational symmetry, we can assume w.l.o.g. that $P = (P_1, 0, 0)$, and by Lemma 4.2.2 we know that

$$E_\alpha(P) + C'\alpha^{-2(1+\sigma)} \geqslant \inf\{E : (P_1, 0, 0, E) \in \sigma(\mathbb{P}_1, \mathbb{P}_2, \mathbb{P}_3, \mathbb{H}_\Lambda)\} \\ \geqslant \inf\{E : (P_1, E) \in \sigma(\mathbb{P}_1, \mathbb{H}_\Lambda)\}. \tag{4.2.6}$$

Making use of the fact that the operators $\mathbb{P}_1', \mathbb{H}_\Lambda', \mathbb{P}_1 - \mathbb{P}_1'$ and $\mathbb{H}_\Lambda - \mathbb{H}_\Lambda'$ are pairwise commuting and that $\mathbb{P}_1', \mathbb{H}_\Lambda'$ and $\mathbb{P}_1 - \mathbb{P}_1', \mathbb{H}_\Lambda - \mathbb{H}_\Lambda'$ act on different factors in the tensor product $L^2\Big(\mathbb{R}^3, \mathcal{F}\big(\mathrm{ran}\chi(|\nabla| \leqslant \Lambda)\big)\Big) \otimes \mathcal{F}\big(\mathrm{ran}\chi(|\nabla| > \Lambda)\big)$, their joint spectrum is well-defined and satisfies $\sigma(\mathbb{P}_1', \mathbb{H}_\Lambda', \mathbb{P}_1 - \mathbb{P}_1', \mathbb{H}_\Lambda - \mathbb{H}_\Lambda') = \sigma(\mathbb{P}_1', \mathbb{H}_\Lambda') \times \sigma(\mathbb{P}_1 - \mathbb{P}_1', \mathbb{H}_\Lambda - \mathbb{H}_\Lambda')$. Hence we can rewrite the right hand side of Eq. (4.2.6) as

$$\inf_{P_1' + \widetilde{P}_1 = P_1} \Big\{E' + \widetilde{E} : (P_1', E') \in \sigma(\mathbb{P}_1', \mathbb{H}_\Lambda'),\ (\widetilde{P}_1, \widetilde{E}) \in \sigma(\mathbb{P}_1 - \mathbb{P}_1', \mathbb{H}_\Lambda - \mathbb{H}_\Lambda')\Big\}.$$

In order to verify that $E' + \widetilde{E}$ is bounded from below by the right hand side of Eq. (4.1.2) for a suitable $w > 0$ and $|P_1| \leqslant \sqrt{2m}\alpha$, let us first consider the case $\widetilde{E} \geqslant \alpha^{-2}$. Since $E' \in \sigma(\mathbb{H}_\Lambda')$, we have $E' \geqslant \inf \sigma(\mathbb{H}_\Lambda') \geqslant \inf \sigma(\mathbb{H}) = E_\alpha$ and therefore

$$E' + \widetilde{E} \geqslant E_\alpha + \alpha^{-2} \geqslant e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \alpha^{-2} - \alpha^{-(2+w')}$$

for a suitable $w' > 0$, where we have used [17, Theorem 1.1]. Regarding the other case $\widetilde{E} < \alpha^{-2}$, note that we have $(\widetilde{P}_1, \widetilde{E}) \in \sigma(\mathbb{P}_1 - \mathbb{P}_1', \mathbb{H}_\Lambda - \mathbb{H}_\Lambda') = \{(0,0)\} \cup \bigcup_{\ell=1}^\infty \mathbb{R} \times \{\frac{\ell}{\alpha^2}\}$, and therefore $\widetilde{E} = 0$ and $\widetilde{P}_1 = 0$. Hence $|P_1'| = |P_1| \leqslant \sqrt{2m}\alpha$ and consequently

$$E' + \widetilde{E} = E' \geqslant e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \frac{|P_1'|^2}{2\alpha^4 m} - \alpha^{-(2+w)} \\ = e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \frac{|P_1|^2}{2\alpha^4 m} - \alpha^{-(2+w)},$$

where we have used $(P_1', E') \in \sigma(\mathbb{P}_1', \mathbb{H}_\Lambda')$ together with Eq. (4.2.4). This concludes the proof of Eq. (4.1.2) for $|P| \leqslant \sqrt{2m}\alpha$.

In order to verify Eq. (4.1.2) for $|P| > \sqrt{2m}\alpha$, we are going to use the fact that $P \mapsto E_\alpha(P)$ is a monotone radial function, as recently shown in [110], and consequently $E_\alpha(P) \geqslant E_\alpha\Big(\sqrt{2m}\frac{P}{|P|}\Big)$ for $|P| \geqslant \sqrt{2m}\alpha$. This reduces the problem to the previous case, and hence concludes the proof of Theorem 4.1.1. ■

4.3 Construction of a Condensate

This section is devoted to the construction of approximate p ground states Ψ_α satisfying complete condensation in φ^{Pek}, which we will utilize in order to prove Theorem 4.2.1 in Section 4.4. In this context, we call Ψ_α an approximate p ground state in case $\langle \Psi_\alpha | \mathbb{H}_\Lambda | \Psi_\alpha \rangle = E_{\alpha,\Lambda}(\alpha^2 p) + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right)$, where $E_{\alpha,\Lambda}(\alpha^2 p)$ and $\mathbb{H}_\Lambda$ are defined in, respectively above, Theorem 4.2.1, and $\langle \Psi_\alpha | (\Upsilon_\Lambda - p)^2 | \Psi_\alpha \rangle \lesssim \alpha^{-(2+w)}$, with $w > 0$, where we define the (rescaled and truncated) phonon momentum operator

$$\Upsilon_\Lambda := \int \chi^1 \big(\Lambda^{-1}|k_1| \leqslant 2\big) k_1 \, a_k^\dagger a_k \mathrm{d}k \,.$$

Similarly to $\mathbb{H}_\Lambda$, it also depends on α due to the rescaled canonical commutation relations $[a(f), a^\dagger(g)] = \alpha^{-2}\langle g|f\rangle$ but we suppress the α dependence for the sake of readability. Here and in the following, we write $X \lesssim Y$ in case there exist constants $C, \alpha_0 > 0$ such that $X \leqslant CY$ for all $\alpha \geqslant \alpha_0$. It is clear that there exist states Ψ_α that satisfy both $\langle \Psi_\alpha|\mathbb{H}_\Lambda|\Psi_\alpha\rangle - E_{\alpha,\Lambda}(\alpha^2 p) \lesssim \alpha^{-(2+w)}$ and $\langle \Psi_\alpha | (\alpha^{-2}\,\mathbb{P}_\Lambda - p)^2 | \Psi_\alpha \rangle \lesssim \alpha^{-(2+w)}$, since $(p, E_{\alpha,\Lambda}(\alpha^2 p))$ is a point in the joint spectrum of $(\alpha^{-2}\,\mathbb{P}_\Lambda, \mathbb{H}_\Lambda)$. As part of the subsequent Lemma 4.3.1 we are going to show that the contribution of $\frac{1}{i\alpha^2}\nabla_{x_1}$ in $\alpha^{-2}\,\mathbb{P}_\Lambda = \frac{1}{i\alpha^2}\nabla_{x_1} + \Upsilon_\Lambda$ is negligibly small, i.e., we shall show that it does not matter whether one uses Υ_Λ or $\alpha^{-2}\,\mathbb{P}_\Lambda$ in the definition of approximate ground states. In particular, this will imply the existence of approximate p ground states. We will choose Ψ_α such that $\mathrm{supp}\,(\Psi_\alpha) \subseteq B_L(0)$ for a suitable L, where we define the support using the identification $L^2(\mathbb{R}^3) \otimes \mathcal{F}(L^2(\mathbb{R}^3)) \cong L^2(\mathbb{R}^3, \mathcal{F}(L^2(\mathbb{R}^3)))$ in order to represent elements $\Psi \in L^2(\mathbb{R}^3) \otimes \mathcal{F}(L^2(\mathbb{R}^3))$ as functions $x \mapsto \Psi(x)$ with values in $\mathcal{F}(L^2(\mathbb{R}^3))$, i.e. $\mathrm{supp}\,(\Psi)$ refers to the support of the electron.

In the rest of this paper, we will always assume that $\alpha \geqslant 1$. Most of the results in this Section include $E_{\alpha,\Lambda}(\alpha^2 p) \leqslant E_\alpha + C|p|^2$ as an assumption for an arbitrary, but fixed, constant $C > 0$, where E_α denotes the ground state energy of $\mathbb{H}$. For the purpose of proving Theorem 4.2.1 this is not a restriction, since we can always pick $C \geqslant \frac{1}{2m}$ and therefore $E_{\alpha,\Lambda}(\alpha^2 p) > E_\alpha + C|p|^2$ immediately implies the statement of Theorem 4.2.1

$$E_{\alpha,\Lambda}\big(\alpha^2 p\big) > E_\alpha + C|p|^2 \geqslant e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \frac{|p|^2}{2m} - \alpha^{-(2+s)},$$

where we used $E_\alpha \geqslant e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] - \alpha^{-(2+s)}$ by [17, Theorem 1.1].

Lemma 4.3.1. *Given $0 < \sigma < \frac{1}{4}$, let $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ and $L = \alpha^{1+\sigma}$, and assume p satisfies $|p| \leqslant \frac{C}{\alpha}$ and $E_{\alpha,\Lambda}(\alpha^2 p) \leqslant E_\alpha + C|p|^2$ for a given $C > 0$, where E_α is the ground state energy of $\mathbb{H}$. Then there exist states $\Psi_\alpha^\bullet$ satisfying $\langle \Psi_\alpha^\bullet | (\Upsilon_\Lambda - p)^2 | \Psi_\alpha^\bullet \rangle \lesssim \alpha^{2\sigma-4}$ and $\langle \Psi_\alpha^\bullet|\mathbb{H}_\Lambda|\Psi_\alpha^\bullet\rangle - E_{\alpha,\Lambda}(\alpha^2 p) \lesssim \alpha^{-2(1+\sigma)}$, as well as $\mathrm{supp}\,(\Psi_\alpha^\bullet) \subseteq B_L(0)$.*

Proof. Since $(p, E_{\alpha,\Lambda}(\alpha^2 p))$ is an element of the joint spectrum $\sigma\left(\frac{1}{i\alpha^2}\nabla_{x_1} + \Upsilon_\Lambda, \mathbb{H}_\Lambda\right)$, there exist states Ψ_α^0 satisfying $\langle \Psi_\alpha^0 | \left(\frac{1}{i\alpha^2}\nabla_{x_1} + \Upsilon_\Lambda - p\right)^2 | \Psi_\alpha^0 \rangle \leqslant \alpha^{-4}$ and

$$\langle \Psi_\alpha^0|\mathbb{H}_\Lambda|\Psi_\alpha^0\rangle \leqslant E_{\alpha,\Lambda}\big(\alpha^2 p\big) + \frac{1}{2}\alpha^{-2(1+\sigma)}. \tag{4.3.1}$$

From [17, Lemma 2.4] we know that $\langle \Psi_\alpha^0| - \Delta_x|\Psi_\alpha^0\rangle \leqslant 2\langle \Psi_\alpha^0|\mathbb{H}_\Lambda|\Psi_\alpha^0\rangle + d$ for a suitable constant $d > 0$, which implies that $\langle \Psi_\alpha^0| - \Delta_x|\Psi_\alpha^0\rangle \lesssim 1$ due to Eq. (4.3.1) and our assumption $E_{\alpha,\Lambda}(\alpha^2 p) \leqslant E_\alpha + C|p|^2 \leqslant C|p|^2 \leqslant \frac{C^3}{\alpha^2}$, and hence

$$\langle \Psi_\alpha^0|(\Upsilon_\Lambda - p)^2|\Psi_\alpha^0\rangle \leqslant 2\left\langle \Psi_\alpha^0\middle|\left(\frac{1}{i\alpha^2}\nabla_{x_1} + \Upsilon_\Lambda - p\right)^2\middle|\Psi_\alpha^0\right\rangle - 2\alpha^{-4}\langle \Psi_\alpha^0|\Delta_x|\Psi_\alpha^0\rangle \leqslant c\alpha^{-4} \tag{4.3.2}$$

for a suitable $c > 0$.

Let $\eta : \mathbb{R}^3 \longrightarrow [0, \infty)$ be a smooth function that is supported on $B_1(0)$ and satisfies $\int \eta^2 = 1$. With this at hand we define $\Psi_y(x) := L^{-\frac{3}{2}}\eta\left(L^{-1}(x-y)\right)\Psi^0_\alpha(x)$ and $Z_y := \|\Psi_y\|$, as well as the set $S \subseteq \mathbb{R}^3$ containing all y satisfying
$\langle \Psi_y|\mathbb{H}_\Lambda|\Psi_y\rangle > Z_y^2\left(E_{\alpha,\Lambda}(\alpha^2 p) + (1+\|\nabla\eta\|^2)\,\alpha^{-2(1+\sigma)}\right)$. Making use of the IMS identity we obtain

$$\begin{aligned}\langle \Psi^0_\alpha|\mathbb{H}_\Lambda|\Psi^0_\alpha\rangle &= \int \langle \Psi_y|\mathbb{H}_\Lambda|\Psi_y\rangle \mathrm{d}y - L^{-2}\|\nabla\eta\|^2 \\ &\geqslant \int_S Z_y^2 \mathrm{d}y \left(E_{\alpha,\Lambda}\big(\alpha^2 p\big) + \left(1+\|\nabla\eta\|^2\right)\alpha^{-2(1+\sigma)}\right) + \left(1 - \int_S Z_y^2\,\mathrm{d}y\right) E_\alpha - L^{-2}\|\nabla\eta\|^2,\end{aligned}$$

where we have used $\langle \Psi_y|\mathbb{H}_\Lambda|\Psi_y\rangle \geqslant E_\alpha$ and $\int Z_y^2\,\mathrm{d}y = 1$. Using Eq. (4.3.1) and $L^{-2} = \alpha^{-2(1+\sigma)}$ therefore yields

$$\begin{aligned}\left(E_{\alpha,\Lambda}\big(\alpha^2 p\big) - E_\alpha + \left(1+\|\nabla\eta\|^2\right)\alpha^{-2(1+\sigma)}\right)\int_S Z_y^2\,\mathrm{d}y \\ \leqslant E_{\alpha,\Lambda}\big(\alpha^2 p\big) - E_\alpha + \left(\frac{1}{2} + \|\nabla\eta\|^2\right)\alpha^{-2(1+\sigma)},\end{aligned}$$

and consequently $\int_S Z_y^2\,\mathrm{d}y \leqslant 1-\gamma_\alpha$ with $\gamma_\alpha := \frac{1}{2}\frac{\alpha^{-2(1+\sigma)}}{E_{\alpha,\Lambda}(\alpha^2 p)-E_\alpha+(1+\|\nabla\eta\|^2)\alpha^{-2(1+\sigma)}}$. Let us further define $S' \subseteq \mathbb{R}^3$ as the set of all y satisfying $\left\langle \Psi_y\right|(\Upsilon_\Lambda - p)^2\left|\Psi_y\right\rangle > Z_y^2\frac{2c}{\gamma_\alpha}\alpha^{-4}$. Clearly we have, using Eq. (4.3.2),

$$\frac{2c}{\gamma_\alpha}\alpha^{-4}\int_{S'} Z_y^2\,\mathrm{d}y \leqslant \int \left\langle \Psi_y\right|(\Upsilon_\Lambda - p)^2\left|\Psi_y\right\rangle \mathrm{d}y = \left\langle \Psi^0_\alpha\right|(\Upsilon_\Lambda - p)^2\left|\Psi^0_\alpha\right\rangle \leqslant c\alpha^{-4},$$

and hence $\int_{S'} Z_y^2\,\mathrm{d}y \leqslant \frac{\gamma_\alpha}{2}$. Consequently $\int_{S\cup S'} Z_y^2\,\mathrm{d}y \leqslant \int_S Z_y^2\,\mathrm{d}y + \int_{S'} Z_y^2\,\mathrm{d}y \leqslant 1 - \frac{\gamma_\alpha}{2} < 1$. Since $\int Z_y^2\,\mathrm{d}y = 1$, this means in particular that there exists a $y \notin S \cup S'$ with $Z_y > 0$, i.e. $\Psi^\bullet_\alpha := Z_y^{-1}\Psi_y$ satisfies $\langle \Psi^\bullet_\alpha|\mathbb{H}_\Lambda|\Psi^\bullet_\alpha\rangle \leqslant E_{\alpha,\Lambda}(\alpha^2 p) + (1+\|\nabla\eta\|^2)\,\alpha^{-2(1+\sigma)}$ and $\left\langle \Psi^\bullet_\alpha\right|(\Upsilon_\Lambda - p)^2\left|\Psi^\bullet_\alpha\right\rangle \leqslant \frac{2c}{\gamma_\alpha}\alpha^{-4} \lesssim \alpha^{2\sigma-4}$, where we have used $E_{\alpha,\Lambda}(\alpha^2 p) - E_\alpha \lesssim |p|^2 \lesssim \alpha^{-2}$ in the last estimate. Moreover, we clearly have $\mathrm{supp}\,(\Psi^\bullet_\alpha) \subseteq B_L(y)$. By the translation invariance of $\mathbb{H}_\Lambda$ and Υ_Λ, we can assume w.l.o.g. that $y = 0$, which concludes the proof. ∎

In the following Lemmas 4.3.2 and 4.3.4, we will use localization methods in order to construct approximate p ground states with useful additional properties, which we will use in Lemma 3.3.12, together with an additional localization procedure, in order to show the existence of approximate p ground states satisfying complete condensation. In Theorem 4.3.7 we will then apply a final localization step in order to obtain complete condensation in a stronger sense, following the argument in [72].

In order to formulate our various localization results, we follow [17] and define for a function $F : \mathcal{M}(\mathbb{R}^3) \longrightarrow \mathbb{R}$, where $\mathcal{M}(\mathbb{R}^3)$ is the set of all finite (Borel) measures on $\mathbb{R}^3$, the operator $\widehat{F}$ acting on $\mathcal{F}(L^2(\mathbb{R}^3)) = \bigoplus_{n=0}^{\infty} L^2_{\mathrm{sym}}(\mathbb{R}^{3\times n})$ as $\widehat{F}\bigoplus_{n=0}^{\infty}\Psi_n := \bigoplus_{n=0}^{\infty}\Psi^*_n$ with $\Psi^*_n(x^1,\dots,x^n) := F^n(x^1,\dots,x^n)\Psi_n(x^1,\dots,x^n)$, where

$$F^n(x^1,\dots,x^n) := F\left(\alpha^{-2}\sum_{k=1}^{n}\delta_{x^k}\right) \tag{4.3.3}$$

and $\widehat{F}_0 := F(0)$, i.e. $\widehat{F}$ acts component-wise on $\bigoplus_{n=0}^{\infty} L^2_{\mathrm{sym}}(\mathbb{R}^{3\times n})$ by multiplication with the real-valued function $(x^1, \ldots, x^n) \mapsto F\left(\alpha^{-2}\sum_{k=1}^n \delta_{x^k}\right)$.

With this notation at hand, we define for given positive c_-, c_+ and ϵ' the function $F_*(\rho) := \chi^{\epsilon'}\left(c_- + \epsilon' \leqslant \int \mathrm{d}\rho \leqslant c_+ - \epsilon'\right)$ and the states

$$\Psi'_\alpha := Z_\alpha^{-1}\widehat{F}_*\Psi^\bullet_\alpha, \tag{4.3.4}$$

with normalization constants $Z_\alpha := \|\widehat{F}_*\Psi^\bullet_\alpha\|$, where $\Psi^\bullet_\alpha$ is the sequence constructed in Lemma 4.3.1. Since $\mathcal{N} = \widehat{G}$ with $G(\rho) := \int \mathrm{d}\rho$, it is clear that the states Ψ'_α are localized to a region where the (scaled) number operator $\mathcal{N}$ is between c_- and c_+, i.e. $\chi\left(c_- \leqslant \mathcal{N} \leqslant c_+\right)\Psi'_\alpha = \Psi'_\alpha$. The following Lemma 4.3.2 quantifies the energy and momentum error of this localization procedure. The subsequent results in Lemmas 4.3.2, 4.3.4 and 3.3.12 as well as Theorem 4.3.7, which quantify the energy and momentum error of specific localization procedures, are generalizations of the corresponding results in [17], where only the energy cost of such localization procedures is discussed. In the following we will usually refer to the respective results in [17] when it comes to quantifying the energy error, and only discuss the localization error of the momentum operator Υ_Λ.

Lemma 4.3.2. *Given $0 < \sigma < \frac{1}{4}$, let $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ and $L = \alpha^{1+\sigma}$, and assume p satisfies $|p| \leqslant \frac{C}{\alpha}$ and $E_{\alpha,\Lambda}(\alpha^2 p) \leqslant E_\alpha + C|p|^2$ for a given $C > 0$. Then there exist constants c_-, c_+ and ϵ', such that the states Ψ'_α defined in Eq. (4.3.4) satisfy $\left\langle \Psi'_\alpha\right| (\Upsilon_\Lambda - p)^2 \left|\Psi'_\alpha\right\rangle \lesssim \alpha^{2\sigma-4}$ and $\langle \Psi'_\alpha|\mathbb{H}_\Lambda|\Psi'_\alpha\rangle - E_{\alpha,\Lambda}(\alpha^2 p) \lesssim \alpha^{-2(1+\sigma)}$.*

Proof. By our assumptions we clearly have $\widetilde{E}_\alpha - E_\alpha \lesssim \alpha^{-\frac{4}{29}}$ with $\widetilde{E}_\alpha := \langle\Psi^\bullet_\alpha|\mathbb{H}_\Lambda|\Psi^\bullet_\alpha\rangle$, and therefore we can apply [17, Lemma 3.4], which tells us that we can choose c_-, c_+ and ϵ', such that $\langle\Psi'_\alpha|\mathbb{H}_\Lambda|\Psi'_\alpha\rangle - E_{\alpha,\Lambda}(\alpha^2 p) \lesssim \alpha^{-2(1+\sigma)}$, and furthermore $Z_\alpha \underset{\alpha\to\infty}{\longrightarrow} 1$. Since $\widehat{F}_*$ commutes with Υ_Λ, we obtain with $\widetilde{\Psi}_\alpha := \sqrt{\frac{1-\widehat{F}_*^2}{1-Z_\alpha^2}}\Psi^\bullet_\alpha$

$$Z_\alpha^2\left\langle\Psi'_\alpha\right| (\Upsilon_\Lambda - p)^2 \left|\Psi'_\alpha\right\rangle + (1 - Z_\alpha^2)\left\langle\widetilde{\Psi}_\alpha\right| (\Upsilon_\Lambda - p)^2 \left|\widetilde{\Psi}_\alpha\right\rangle = \left\langle\Psi^\bullet_\alpha\right| (\Upsilon_\Lambda - p)^2 \left|\Psi^\bullet_\alpha\right\rangle$$

Hence $\left\langle\Psi'_\alpha\right| (\Upsilon_\Lambda - p)^2 \left|\Psi'_\alpha\right\rangle \leqslant Z_\alpha^{-2}\left\langle\Psi^\bullet_\alpha\right| (\Upsilon_\Lambda - p)^2 \left|\Psi^\bullet_\alpha\right\rangle \lesssim \alpha^{2\sigma-4}$. ■

When it comes to localizations with respect to more complicated functions F compared to the one used in Eq. (4.3.4), we first need to introduce some tools in order to quantify the localization error of the momentum operator. Given a function $F : \mathcal{M}(\mathbb{R}^3) \longrightarrow \mathbb{R}$, $\Omega \subseteq \mathcal{M}(\mathbb{R}^3)$ and $\lambda > 0$, let us define

$$\|F\|^2_{\Omega,\lambda} := \sup_{1\leqslant n\leqslant\lambda\alpha^2}\sup_{x\in\Omega_n}\left\|(F^{n,\bar{x}})'\right\|^2 = \sup_{1\leqslant n\leqslant\lambda\alpha^2}\sup_{x\in\Omega_n}\int_{\mathbb{R}}\left|\frac{\mathrm{d}}{\mathrm{d}t}F^n(t,\bar{x})\right|^2\mathrm{d}t, \tag{4.3.5}$$

where $x = (x^1, \ldots, x^n) \in \mathbb{R}^{3\times n}$ with $x^k = (x^k_1, x^k_2, x^k_3)$ and $\bar{x} := (x^1_2, x^1_3, x^2, \ldots, x^n) \in \mathbb{R}^{3\times n-1}$, i.e. we define $\bar{x}$ such that $x = (x^1_1, \bar{x})$, Ω_n is the set of all x such that $\alpha^{-2}\sum_{j=1}^n \delta_{x^j} \in \Omega$ and $F^{n,y} : \mathbb{R} \longrightarrow \mathbb{R}$ is defined as $F^{n,y}(t) := F^n(t, y)$ for $y \in \mathbb{R}^{3\times n-1}$, where F^n is as in Eq. (4.3.3).

Lemma 4.3.3. *Given $\lambda > 0$, there exists a constant $T > 0$ such that we have for all quadratic partitions of unity $\mathcal{P} = \{F_j : \mathcal{M}(\mathbb{R}^3) \longrightarrow \mathbb{R} : j \in J\}$, i.e. families of functions satisfying $0 \leqslant F_j \leqslant 1$ and $\sum_{j\in J} F_j^2 = 1$, $\Lambda > 0$, $|p| \leqslant \Lambda$, $\Omega \subseteq \mathcal{M}(\mathbb{R}^3)$ and states Ψ satisfying $\chi(\mathcal{N} \leqslant \lambda)\Psi = \Psi$ and $\widehat{\mathbb{1}_\Omega}\Psi = \Psi$*

$$\left|\sum_{j\in J}\langle \Psi_j|\left(\Upsilon_\Lambda - p\right)^2|\Psi_j\rangle - \langle \Psi|\left(\Upsilon_\Lambda - p\right)^2|\Psi\rangle\right| \leqslant T\Lambda \sum_{j\in J}\|F_j\|^2_{\Omega,\lambda},$$

where we define $\Psi_j := \widehat{F}_j\Psi$.

Proof. Using the IMS identity we can write

$$\sum_{j\in J}\langle \Psi_j|\left(\Upsilon_\Lambda - p\right)^2|\Psi_j\rangle - \langle \Psi|\left(\Upsilon_\Lambda - p\right)^2|\Psi\rangle = -\frac{1}{2}\sum_{j\in J}\Big\langle \Psi\Big|\left[\left[\left(\Upsilon_\Lambda - p\right)^2, \widehat{F}_j\right], \widehat{F}_j\right]\Big|\Psi\Big\rangle.$$

Hence it suffices to show that $\pm\Big\langle \Psi\Big|\left[\left[\left(\Upsilon_\Lambda - p\right)^2, \widehat{F}\right], \widehat{F}\right]\Big|\Psi\Big\rangle \lesssim \Lambda\|F\|^2_{\Omega,\lambda}$ for any bounded $F : \mathcal{M}(\mathbb{R}^3) \longrightarrow \mathbb{R}$ and state satisfying $\chi(\mathcal{N} \leqslant \lambda)\Psi = \Psi$ and $\widehat{\mathbb{1}_\Omega}\Psi = \Psi$. Let us start by estimating

$$\begin{aligned}\pm\left[\left[\left(\Upsilon_\Lambda - p\right)^2, \widehat{F}\right], \widehat{F}\right] &= \pm 2\left[\Upsilon_\Lambda, \widehat{F}\right]^2 \pm \left\{\Upsilon_\Lambda - p, \left[\left[\Upsilon_\Lambda, \widehat{F}\right], \widehat{F}\right]\right\} \\ &\leqslant -2\left[\Upsilon_\Lambda, \widehat{F}\right]^2 + \frac{\|F\|^2_{\Omega,\lambda}}{\Lambda}\left(\Upsilon_\Lambda - p\right)^2 + \frac{\Lambda}{\|F\|^2_{\Omega,\lambda}}\left[\left[\Upsilon_\Lambda, \widehat{F}\right], \widehat{F}\right]^2,\end{aligned}$$

where $\{A, B\} := AB + BA$. By the definition of Υ_Λ it is clear that $\frac{\|F\|^2_{\Omega,\lambda}}{\Lambda}\left(\Upsilon_\Lambda - p\right)^2 \lesssim \Lambda\|F\|^2_{\Omega,\lambda}\left(\mathcal{N} + 1\right)^2$ for $|p| \leqslant \Lambda$, and consequently $\pm\Big\langle \Psi\Big|\frac{\|F\|^2_{\Omega,\lambda}}{\Lambda}\left(\Upsilon_\Lambda - p\right)^2\Big|\Psi\Big\rangle \lesssim \Lambda\|F\|^2_{\Omega,\lambda}$. Using that Ψ is a function with values in $\mathcal{F}_{\leqslant\lambda\alpha^2}\left(L^2(\mathbb{R}^3)\right) := \bigoplus_{n\leqslant\lambda\alpha^2} L^2_{\mathrm{sym}}(\mathbb{R}^{3\times n})$, we are going to represent it as $\Psi = \bigoplus_{n\leqslant\lambda\alpha^2}\Psi_n$ where $\Psi_n(z, x^1, \dots, x^n)$ is a function of the electron variable z and the n phonon coordinates $x^j \in \mathbb{R}^3$ satisfying $\Psi_n(z, x^1, \dots, x^n) = 0$ for all $(x^1, \dots, x^n) \notin \Omega_n$. In order to simplify the notation, we will suppress the dependence on the electron variable z. We have $\left[\Upsilon_\Lambda, \widehat{F}\right]\Psi = \bigoplus_{1\leqslant n\leqslant\lambda\alpha^2}\alpha^{-2}n\Psi_n^*$ with $\Psi_n^* := \frac{1}{n}\sum_{j=1}^n\left[g\left(\frac{1}{i}\nabla_{x_1^j}\right), F^n\right]\Psi_n$, where $g(k) := \chi^1(\Lambda^{-1}|k| \leqslant 2)k$ for $k \in \mathbb{R}$. Hence

$$\Big\langle \Psi\Big| - \left[\Upsilon_\Lambda, \widehat{F}\right]^2\Big|\Psi\Big\rangle = \left\|\left[\Upsilon_\Lambda, \widehat{F}\right]\Psi\right\|^2 = \sum_{1\leqslant n\leqslant\lambda\alpha^2}\alpha^{-4}n^2\|\Psi_n^*\|^2 \leqslant \lambda^2\sum_{1\leqslant n\leqslant\lambda\alpha^2}\|\Psi_n^*\|^2,$$

and $\|\Psi_n^*\| \leqslant \frac{1}{n}\sum_{j=1}^n\left\|\left[g\left(\frac{1}{i}\nabla_{x_1^j}\right), F^n\right]\Psi_n\right\| = \left\|\left[g\left(\frac{1}{i}\nabla_{x_1^1}\right), F^n\right]\Psi_n\right\|$, where we have used the permutation symmetry of Ψ_n. By Lemma 4.5.1 we know that

$$\left\|\left[g\left(\frac{1}{i}\nabla_{x_1^1}\right), F^n\right]\Psi_n\right\| \leqslant \sup_{x\in\mathrm{supp}(\Psi_n)}\left\|\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), F^{n,\bar{x}}\right]\right\|_{\mathrm{op}}\|\Psi_n\| \lesssim \sqrt{\Lambda}\sup_{x\in\Omega_n}\|(F^{n,\bar{x}})'\|\|\Psi_n\|,$$

and therefore

$$\Big\langle \Psi\Big| - \left[\Upsilon_\Lambda, \widehat{F}\right]^2\Big|\Psi\Big\rangle \leqslant \lambda^2\Lambda\sup_{1\leqslant n\leqslant\lambda\alpha^2, x\in\Omega_n}\|(F^{n,\bar{x}})'\|^2\sum_{n\leqslant\lambda\alpha^2}\|\Psi_n\|^2 = \lambda^2\Lambda\|F\|^2_{\Omega,\lambda}.$$

In order to estimate the expectation value of $\left[\left[\Upsilon_\Lambda, \widehat{F}\right], \widehat{F}\right]^2$ we proceed similarly, by writing $\left[\left[\Upsilon_\Lambda, \widehat{F}\right], \widehat{F}\right]\Psi = \bigoplus_{n\leqslant\lambda\alpha^2}\alpha^{-2}n\widetilde{\Psi}_n$ with $\widetilde{\Psi}_n = \frac{1}{n}\sum_{j=1}^n\left[\left[g\left(\frac{1}{i}\nabla_{x_1^j}\right), F^n\right], F^n\right]\Psi_n$, and estimating $\left\langle\Psi\right|\left[\left[\Upsilon_\Lambda, \widehat{F}\right], \widehat{F}\right]^2\left|\Psi\right\rangle \leqslant \lambda^2\sum_{n\leqslant\lambda\alpha^2}\left\|\widetilde{\Psi}_n\right\|^2$ as well as

$$\left\|\widetilde{\Psi}_n\right\| \leqslant \sup_{x\in\mathrm{supp}(\Psi_n)}\left\|\left[\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{dt}}\right), F^{n,\bar{x}}\right], F^{n,\bar{x}}\right]\right\|_{\mathrm{op}}\|\Psi_n\| \leqslant \sup_{x\in\Omega_n}\|(F^{n,\bar{x}})'\|^2\|\Psi_n\|,$$

where we have again applied Lemma 4.5.1. This concludes the proof. ∎

With the subsequent localization step in Eq. (3.3.10), we want to restrict the state Ψ'_α to phonon density configurations ρ which have a sharp concentration of their mass. To be precise, for given R and $\epsilon, \delta > 0$, let us define $K_R(\rho) := \iint \chi^\epsilon(R-\epsilon \leqslant |x-y|)\,\mathrm{d}\rho(x)\mathrm{d}\rho(y)$ as well as $F_R(\rho) := \chi^{\frac{\delta}{3}}\left(K_R(\rho) \leqslant \frac{2\delta}{3}\right)$ and

$$\Psi''_\alpha := Z_{R,\alpha}^{-1}\widehat{F}_R\Psi'_\alpha, \tag{4.3.6}$$

where Ψ'_α is as in Lemma 4.3.2 and $Z_{R,\alpha} := \|\widehat{F}_R\Psi'_\alpha\|$. Clearly $\widehat{\mathbb{1}_\Omega}\Psi''_\alpha = \Psi''_\alpha$ where Ω is the set of all ρ satisfying $\iint_{|x-y|\geqslant R}\mathrm{d}\rho(x)\mathrm{d}\rho(y) \leqslant \delta$. In the following Lemma 4.3.4 we are going to quantify the energy and momentum cost of this localization procedure.

Lemma 4.3.4. *Given $0 < \sigma < \frac{1}{4}$, let $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ and $L := \alpha^{1+\sigma}$, and assume p satisfies $|p| \leqslant \frac{C}{\alpha}$ and $E_{\alpha,\Lambda}(\alpha^2 p) \leqslant E_\alpha + C|p|^2$ for a given $C > 0$. Then for any $\epsilon, \delta > 0$, there exists a constant $R > 0$, such that the states Ψ''_α defined in Eq. (4.3.6) satisfy $\left\langle\Psi''_\alpha\right|(\Upsilon_\Lambda - p)^2\left|\Psi''_\alpha\right\rangle \lesssim \alpha^{\frac{4}{5}\sigma-\frac{16}{5}}$ and $\langle\Psi''_\alpha|\mathbb{H}_\Lambda|\Psi''_\alpha\rangle - E_{\alpha,\Lambda}(\alpha^2 p) \lesssim \alpha^{-2(1+\sigma)}$.*

Proof. By the results in [17, Lemma 3.5], there exists a constant $R > 0$ such that $\langle\Psi''_\alpha|\mathbb{H}_\Lambda|\Psi''_\alpha\rangle - E_{\alpha,\Lambda}(\alpha^2 p) \lesssim \alpha^{-2(1+\sigma)}$ and $Z_{R,\alpha} \underset{\alpha\to\infty}{\longrightarrow} 1$. Applying Lemma 4.3.3 yields

$$\begin{aligned}\langle\widehat{F}_R\Psi'_\alpha|(\Upsilon_\Lambda - p)^2|\widehat{F}_R\Psi'_\alpha\rangle + &\langle\widehat{G}_R\Psi'_\alpha|(\Upsilon_\Lambda - p)^2|\widehat{G}_R\Psi'_\alpha\rangle\\ &\lesssim \alpha^{2\sigma-4} + \alpha^{\frac{4}{5}(1+\sigma)}\left(\|F_R\|^2_{\mathcal{M}(\mathbb{R}^3),c_+} + \|G_R\|^2_{\mathcal{M}(\mathbb{R}^3),c_+}\right)\end{aligned} \tag{4.3.7}$$

with $G_R := \sqrt{1-F_R^2}$, where we used $\langle\Psi'_\alpha|(\Upsilon_\Lambda - p)^2|\Psi'_\alpha\rangle \lesssim \alpha^{2\sigma-4}$ and $\chi(\mathcal{N} \leqslant c_+)\Psi'_\alpha = \Psi'_\alpha$. In order to estimate $\|F_R\|_{\mathcal{M}(\mathbb{R}^3),c_+}$, let us define the functions $g(s) := \chi^{\frac{\delta}{3}}\left(s \leqslant \frac{2\delta}{3}\right)$ and $h(s) := \chi^\epsilon(R-\epsilon \leqslant \sqrt{s})$. Then $F_R^n(x) = g\left(\alpha^{-4}\sum_{i,j=1}^n h(|x^i - x^j|^2)\right)$ and therefore $F_R^{n,y}(t) = g\left(\alpha^{-4}\sum_{i=2}^n h\left((t-y_1^j)^2 + \delta_y^i\right) + \mu_y\right)$ with $\delta_y^i := (y_2^1 - y_2^i)^2 + (y_3^1 - y_3^i)^2$ and $\mu_y := \alpha^{-4}\sum_{i,j=2}^n h(|y^i - y^j|^2)$. Consequently

$$\|(F_R^{n,y})'\| \leqslant 4\alpha^{-4}\|g'\|_\infty\sum_{i=2}^n\sqrt{\int_{\mathbb{R}}|t|^2\left|h'\left(t^2+\delta_y^i\right)\right|^2\mathrm{d}t} \leqslant 4\alpha^{-4}\|g'\|_\infty(n-1)\|h'\|_\infty\sqrt{\frac{2R^3}{3}},$$

where we have used $\mathrm{supp}(h') \subseteq [0, R^2)$ in the second inequality. Hence $\|F_R\|_{\mathcal{M}(\mathbb{R}^3),c_+} = \sup_{1\leqslant n\leqslant c_+\alpha^2}\sup_{x\in\mathbb{R}^{3\times n}}\|(F_R^{n,\bar{x}})'\| \lesssim \alpha^{-2}$. Similarly we have $\|G_R\|_{\mathcal{M}(\mathbb{R}^3),c_+} \lesssim \alpha^{-2}$. In combination with Eq. (4.3.7) we therefore obtain

$$\left\langle\Psi''_\alpha\right|(\Upsilon_\Lambda - p)^2\left|\Psi''_\alpha\right\rangle \lesssim Z_{R,\alpha}^{-2}\left(\alpha^{2\sigma-4} + \alpha^{\frac{4}{5}(1+\sigma)}\left(\|F_R\|^2_{\mathcal{M}(\mathbb{R}^3),c_+} + \|G_R\|^2_{\mathcal{M}(\mathbb{R}^3),c_+}\right)\right) \lesssim \alpha^{\frac{4}{5}\sigma-\frac{16}{5}}.$$

∎

Before we come to our next localization step in Lemma 3.3.12, we need to define the regularized median of a measure $\nu \in \mathcal{M}(\mathbb{R})$, see also [17, Definition 3.8], and derive a useful estimate for it in the subsequent Lemma 4.3.5. In the following let $x^\kappa(\nu) := \sup\{t : \int_{-\infty}^t \mathrm{d}\nu \leqslant \kappa \int \mathrm{d}\nu\}$ denote the κ-quantile, where we use the convention that boundaries are included in the domain of integration $\int_a^b f \mathrm{d}\nu := \int_{[a,b]} f \mathrm{d}\nu$, and let us define for $0 < q < \frac{1}{2}$ and $\nu \neq 0$

$$m_q(\nu) := \frac{1}{\int_{K_q(\nu)} \mathrm{d}\nu} \int_{K_q(\nu)} h \, \mathrm{d}\nu(h), \tag{4.3.8}$$

where $K_q(\nu) := [x^{\frac{1}{2}-q}(\nu), x^{\frac{1}{2}+q}(\nu)]$, and $m_q(0) := 0$. Furthermore we will denote the marginal measures of $\rho \in \mathcal{M}(\mathbb{R}^3)$ as ρ_i, i.e. $\rho_i(A) := \rho([x_i \in A])$, where $A \subseteq \mathbb{R}$ is measurable and $i \in \{1, 2, 3\}$.

Lemma 4.3.5. *Let us define Ω_{reg} as the set of all $\rho \in \mathcal{M}(\mathbb{R}^3)$ satisfying $\int_{x_i = t} \mathrm{d}\rho(x) \leqslant \alpha^{-2}$ for $t \in \mathbb{R}$ and $i \in \{1, 2, 3\}$, and Ω as the set of all $\rho \in \Omega_{\mathrm{reg}}$ satisfying $c \leqslant \int \mathrm{d}\rho$ and $\iint_{|x-y| \geqslant R} \mathrm{d}\rho(x)\mathrm{d}\rho(y) \leqslant \delta$ for given $R, c, \delta > 0$. Furthermore let q be a constant satisfying $q + \frac{\alpha^{-2}}{c} \leqslant \frac{1}{2} - \frac{\delta}{c^2}$. Then we have for any $n \geqslant 1$ and function of the form $F(\rho) = f(m_q(\rho_1))$ the estimate*

$$\sup_{x \in \Omega_n} \left\| (F^{n,\bar{x}})' \right\| \leqslant \alpha^{-2} \frac{\|f'\|_\infty}{2qc} \sqrt{2R}, \tag{4.3.9}$$

where m_q is defined in Eq. (4.3.8) and Ω_n below Eq. (4.3.5).

Proof. Given $x \in \Omega_n$, let us define $\nu_t := \alpha^{-2} \left(\delta_t + \sum_{j=2}^n \delta_{x_1^j}\right)$, which allows us to rewrite $F^{n,\bar{x}}(t) = f(m_q(\nu_t))$. Let us first compute the derivative $\frac{\mathrm{d}}{\mathrm{d}t} m_q(\nu_t)$ for $t \in \mathbb{R} \backslash \{x_1^2, \ldots, x_1^n\}$. For such t, there clearly exists an $\epsilon > 0$ such that $(t - \epsilon, t + \epsilon) \subset \mathbb{R} \backslash \{x_1^2, \ldots, x_1^n\}$. It will be useful in the following that the set $Y := \{x_1^2, \ldots, x_1^n\} \cap K_q(\nu_s)$ is independent of $s \in (t - \epsilon, t + \epsilon)$, with $K_q(\nu)$ being defined below Eq. (4.3.8). Furthermore we have for $s \in (t - \epsilon, t + \epsilon)$ that $s \in K_q(s)$ if and only if $t \in K_q(t)$. Therefore $\alpha^2 \int_{K_q(v_s)} h \, \mathrm{d}\nu_s(h) = \sum_{h \in Y} h + s \mathbb{1}_{K_q(s)}(s) = \sum_{h \in Y} h + s \mathbb{1}_{K_q(t)}(t)$ and $\alpha^2 \int_{K_q(v_s)} \mathrm{d}\nu_s = |Y| + \mathbb{1}_{K_q(s)}(s) = \alpha^2 \int_{K_q(v_t)} \mathrm{d}\nu_t$ for $s \in (t - \epsilon, t + \epsilon)$, and consequently we obtain for $t \in \mathbb{R} \backslash \{x_1^2, \ldots, x_1^n\}$

$$\frac{\mathrm{d}}{\mathrm{d}t} m_q(\nu_t) = \alpha^{-2} \frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=t} \frac{\sum_{h \in Y} h + s \mathbb{1}_{K_q(t)}(t)}{\int_{K_q(v_t)} \mathrm{d}\nu_t} = \alpha^{-2} \frac{\mathbb{1}_{K_q(t)}(t)}{\int_{K_q(v_t)} \mathrm{d}\nu_t}.$$

Note that due to our assumption $\rho \in \Omega_{\mathrm{reg}}$, $m_q(\nu_t)$ can be continuously extended from $\mathbb{R} \backslash \{x_1^2, \ldots, x_1^n\}$ to all of $\mathbb{R}$, and therefore $\frac{\mathrm{d}}{\mathrm{d}t} m_q(\nu_t) = \alpha^{-2} \frac{\mathbb{1}_{K_q(t)}(t)}{\int_{K_q(v_t)} \mathrm{d}\nu_t}$ in the sense of distributions. Since $\int_{K_q(v_t)} \mathrm{d}\nu_t \geqslant 2qc$ we conclude $|(F^{n,\bar{x}})'(t)| \leqslant \alpha^{-2} \frac{\|f'\|_\infty}{2qc} \mathbb{1}_{K_q(t)}(t)$ for almost every t. In order to obtain from this the upper bound on the $L^2(\mathbb{R})$-norm in Eq. (4.3.9), we are going to verify that the support of $t \mapsto \mathbb{1}_{K_q(t)}(t)$ is contained in an interval of the form $(\xi - R, \xi + R)$ for a suitable $\xi \in \mathbb{R}$. Let us start by verifying that

$$x^\kappa(\nu_{t_1}) \geqslant x^{\kappa - \frac{\alpha^{-2}}{c}}(\nu_{t_2}) \tag{4.3.10}$$

for $0 < \kappa < 1$ and $t_1, t_2 \in \mathbb{R}$. Note that any $y \in \mathbb{R}$ satisfying the inequality $\int_{-\infty}^y \mathrm{d}\nu_{t_2} \leqslant \left(\kappa - \frac{\alpha^{-2}}{c}\right) \int \mathrm{d}\nu_{t_2}$, also satisfies

$$\int_{-\infty}^y \mathrm{d}\nu_{t_1} \leqslant \alpha^{-2} + \int_{-\infty}^y \mathrm{d}\nu_{t_2} \leqslant \alpha^{-2} + \left(\kappa - \frac{\alpha^{-2}}{c}\right) \int \mathrm{d}\nu_{t_2} \leqslant \kappa \int \mathrm{d}\nu_{t_2} = \kappa \int \mathrm{d}\nu_{t_1},$$

where we have used $\alpha^{-2} \leqslant \frac{\alpha^{-2}}{c} \int \mathrm{d}\nu_{t_2}$, and therefore $y \leqslant x^{\kappa}(\nu_{t_1})$. Using that $x^{\kappa - \frac{\alpha^{-2}}{c}}(\nu_{t_2})$ is the supremum over all such y, we conclude with the desired Eq. (4.3.10). Furthermore observe that $\nu_{t_0} = \rho_1$ with $t_0 := x_1^1$ and $\rho := \alpha^{-2} \sum_{j=1}^{n} \delta_{x^j} \in \Omega$, and therefore we know by [17, Lemma 3.9] that there exists a $\xi \in \mathbb{R}$ such that $\xi - R \leqslant x^{\frac{1}{2}-q'}(\nu_{t_0}) \leqslant x^{\frac{1}{2}+q'}(\nu_{t_0}) \leqslant \xi + R$ for $q' \leqslant \frac{1}{2} - \frac{\delta}{c^2}$. By our assumptions, $q' := q + \frac{\alpha^{-2}}{c}$ satisfies this condition, and therefore we obtain using Eq. (4.3.10) with $t_1 := t$, $t_2 := t_0$ and $\kappa := \frac{1}{2} - q$, respectively $t_1 := t_0$, $t_2 := t$ and $\kappa := \frac{1}{2} + q + \frac{\alpha^{-2}}{c}$, that

$$\xi - R \leqslant x^{\frac{1}{2}-q}(\nu_t) \leqslant x^{\frac{1}{2}+q}(\nu_t) \leqslant \xi + R$$

for all $t \in \mathbb{R}$, and consequently $\mathbb{1}_{K_q(t)}(t) = 0$ for $|t - \xi| > R$. ■

Lemma 4.3.6. *Given $0 < \sigma < \frac{1}{9}$ and $C > 0$, let $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ and $L = \alpha^{1+\sigma}$, and assume p satisfies $|p| \leqslant \frac{C}{\alpha}$ and $E_{\alpha,\Lambda}(\alpha^2 p) \leqslant E_\alpha + C|p|^2$ for a given $C > 0$. Then there exist $r', c_+ > 0$ and states Ψ'''_α with $\langle \Psi'''_\alpha | (\Upsilon_\Lambda - p)^2 | \Psi'''_\alpha \rangle \lesssim \alpha^{-(2+r')}$, $\langle \Psi'''_\alpha | \mathbb{H}_\Lambda | \Psi'''_\alpha \rangle - E_{\alpha,\Lambda}(\alpha^2 p) \lesssim \alpha^{-(2+r')}$, $\operatorname{supp}(\Psi'''_\alpha) \subseteq B_{4L}(0)$ and $\chi(\mathcal{N} \leqslant c_+)\Psi'''_\alpha = \Psi'''_\alpha$, such that*

$$\left\langle \Psi'''_\alpha \middle| W^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \middle| \Psi'''_\alpha \right\rangle \lesssim \alpha^{-r'}, \tag{4.3.11}$$

where $W_{\varphi^{\mathrm{Pek}}}$ is the Weyl operator corresponding to the Pekar minimizer φ^{Pek}, characterized by $W^{-1}_{\varphi^{\mathrm{Pek}}} a(f) W_{\varphi^{\mathrm{Pek}}} = a(f) - \langle f | \varphi^{\mathrm{Pek}} \rangle$ for all $f \in L^2(\mathbb{R}^3)$.

Proof. For $u > 0$, let us define the functions $f_\ell(y) := \chi^{\frac{1}{2}}\left(\ell - \frac{1}{2} < \alpha^u y \leqslant \ell + \frac{1}{2}\right)$ for $\ell \in \mathbb{Z}$ satisfying $|\ell| \leqslant \frac{3}{2}\alpha^u L$, as well as $f_{-\infty}(y) := \chi^{\frac{1}{2}}\left(\alpha^u y \leqslant -\lfloor \frac{3}{2}\alpha^u L \rfloor - \frac{1}{2}\right)$ and $f_\infty(\rho) := \chi^{\frac{1}{2}}\left(\lfloor \frac{3}{2}\alpha^u L \rfloor + \frac{1}{2} < \alpha^u y\right)$. With these functions at hand we define for $i \in \{1,2,3\}$ and $v > 0$ the partitions $\mathcal{P}_i := \{F_{\ell,i} : \ell \in A\}$, where $F_{\ell,i}(\rho) := f_\ell(m_{\alpha^{-v}}(\rho_i))$ and $A := \{-\infty, -\lfloor \frac{3}{2}\alpha^u L \rfloor, -\lfloor \frac{3}{2}\alpha^u L \rfloor + 1, \dots, \lfloor \frac{3}{2}\alpha^u L \rfloor, \infty\} \subseteq \mathbb{Z} \cup \{-\infty, \infty\}$, as well as $\mathcal{P} := \{F_z : z \in A^3\}$ with $F_z := F_{z_3,3} F_{z_2,2} F_{z_1,1}$. In the following let Ψ''_α be as in Lemma 4.3.4 with $\delta < \frac{c_-^2}{2}$ and let Ω_{reg} and Ω be the sets from Lemma 4.3.5 with δ and R as in Lemma 4.3.4, $q := \alpha^{-v}$ and $c := c_-$. Due to the straightforward result [17, Lemma 3.6] we have $\widehat{\mathbb{1}_{\Omega_{\mathrm{reg}}}} \Psi''_\alpha = \Psi''_\alpha$, and by the definition of Ψ''_α in Eq. (4.3.6) it is clear that we furthermore have $\widehat{\mathbb{1}_\Omega} \Psi''_\alpha = \Psi''_\alpha$. Therefore we can apply Lemma 4.3.3 together with Eq. (4.3.9) in order to obtain

$$\sum_{z_1 \in A} \left\langle \widehat{F}_{z_1,1} \Psi''_\alpha \middle| (\Upsilon_\Lambda - p)^2 \middle| \widehat{F}_{z_1,1} \Psi''_\alpha \right\rangle \leqslant \langle \Psi''_\alpha | (\Upsilon_\Lambda - p)^2 | \Psi''_\alpha \rangle + T \alpha^{\frac{4}{5}(1+\sigma)} \sum_{z_1 \in A} \alpha^{-4} \frac{\left\| f'_{z_1} \right\|_\infty^2}{2\alpha^{-2v} c_-^2} R$$
$$\lesssim \alpha^{\frac{4}{5}\sigma - \frac{16}{5}} + \alpha^{\frac{4}{5}\sigma - \frac{16}{5} + 2v} \sup_{z_1 \in A} \left\| f'_{z_1} \right\|_\infty^2 \sum_{z_1 \in A} 1 \lesssim \alpha^{\frac{9}{5}\sigma + 2v + 3u - \frac{1}{5}} \alpha^{-2}$$

for all α large enough such that $\alpha^{-v} + \frac{\alpha^{-2}}{c_-} < \frac{1}{2} - \frac{\delta}{c_-^2}$, where we have used $\sup_{z_1 \in A} \left\| f'_{z_1} \right\| \lesssim \alpha^u$, as well as $\sum_{z_1 \in A} 1 \leqslant 3(\alpha^u L + 1) \lesssim \alpha^{u+1+\sigma}$. Since the functions $F^n_{\ell,i}$ are independent of x_1^1 for $i \in \{2,3\}$, we furthermore obtain

$$\left\langle \widehat{F}_{z_1,1} \Psi''_\alpha \middle| (\Upsilon_\Lambda - p)^2 \middle| \widehat{F}_{z_1,1} \Psi''_\alpha \right\rangle = \sum_{z_2, z_3 \in A} \left\langle \widehat{F}_{z_3,3} \widehat{F}_{z_2,2} \widehat{F}_{z_1,1} \Psi''_\alpha \middle| (\Upsilon_\Lambda - p)^2 \middle| \widehat{F}_{z_3,3} \widehat{F}_{z_2,2} \widehat{F}_{z_1,1} \Psi''_\alpha \right\rangle$$

and therefore

$$\sum_{z \in A^3} Z_z^2 \langle \Psi_z | (\Upsilon_\Lambda - p)^2 | \Psi_z \rangle \lesssim \alpha^{\frac{9}{5}\sigma + 2v + 3u - \frac{1}{5}} \alpha^{-2} \tag{4.3.12}$$

with $\Psi_z := Z_z^{-1}\widehat{F}_z\Psi''_\alpha$ and $Z_z := \left\|\widehat{F}_z\Psi''_\alpha\right\|$.

Regarding the localization error of the energy, we obtain by [17, Lemma 3.3] and [17, Lemma 3.10] (see also the proof of [17, Eq. (3.22)]) that

$$\sum_{z\in A^3} Z_z^2\left\langle \Psi_z|\mathbb{H}_\Lambda|\Psi_z\right\rangle \leqslant \left\langle \Psi''_\alpha|\mathbb{H}_\Lambda|\Psi''_\alpha\right\rangle + O_{\alpha\to\infty}\left(\alpha^{-3}\right) \leqslant E_{\alpha,\Lambda}\left(\alpha^2 p\right) + C\alpha^{-2(1+\sigma)} \quad (4.3.13)$$

for a suitable constant $C > 0$, as long as $u + v \leqslant \frac{1}{2}$. In the following, let S be the set of all $z \in A^3$ such that $\langle \Psi_z|\mathbb{H}_\Lambda|\Psi_z\rangle > E_{\alpha,\Lambda}(\alpha^2 p) + \alpha^{-(2+w)}$ for a given $w > 0$, and define $M := \sum_{z\in S} Z_z^2$. By Eq. (4.3.13), we have

$$M\left(E_{\alpha,\Lambda}\left(\alpha^2 p\right) + \alpha^{-(2+w)}\right) + (1-M)E_\alpha \leqslant E_{\alpha,\Lambda}\left(\alpha^2 p\right) + C\alpha^{-2(1+\sigma)},$$

and therefore $1 - M \geqslant \frac{\alpha^{-(2+w)} - C\alpha^{-2(1+\sigma)}}{E_{\alpha,\Lambda}(\alpha^2 p) - E_\alpha + \alpha^{-(2+w)}} \geqslant C_1\alpha^{-w}$ for $w < 2\sigma$, α large enough and a suitable constant C_1, where we have used the assumption $E_{\alpha,\Lambda}(\alpha^2 p) - E_\alpha \lesssim |p|^2 \lesssim \alpha^{-2}$. Moreover, let us define S' as the set containing all $z \in A^3$, such that $\langle \Psi_z|\left(\Upsilon_\Lambda - p\right)^2|\Psi_z\rangle > \alpha^{\frac{1}{2}\left(\frac{9}{5}\sigma+2v+3u-\frac{1}{5}\right)}\alpha^{-2}$ and $M' := \sum_{z\in S'} Z_z^2$. By Eq. (4.3.12) we see that $M' \leqslant C_2\alpha^{\frac{1}{2}\left(\frac{9}{5}\sigma+2v+3u-\frac{1}{5}\right)}$ for a suitable constant C_2. Consequently

$$\sum_{z\notin S\cup S'} Z_z^2 \geqslant 1 - M - M' \geqslant C_1\alpha^{-w} - C_2\alpha^{\frac{1}{2}\left(\frac{9}{5}\sigma+2v+3u-\frac{1}{5}\right)}$$

for α large enough. Since $\sigma < \frac{1}{9}$, we can take u, v and w small enough, such that $2w + \frac{9}{5}\sigma + 2v + 3u < \frac{1}{5}$, and consequently $\sum_{z\notin S\cup S'} Z_z^2 > 0$ for α large enough, which implies the existence of a $z^* \notin S \cup S'$ with $Z_{z*} > 0$, i.e. $\langle \Psi_{z^*}|\mathbb{H}_\Lambda|\Psi_{z^*}\rangle \leqslant E_{\alpha,\Lambda}(\alpha^2 p) + \alpha^{-(2+w)}$ and $\langle \Psi_{z^*}|\left(\Upsilon_\Lambda - p\right)^2|\Psi_{z^*}\rangle \leqslant \alpha^{\frac{1}{2}\left(\frac{9}{5}\sigma+2v+3u-\frac{1}{5}\right)-2}$.

In order to rule out that one of the components z_i^* is infinite, let us verify that $\langle \Psi_z|\mathbb{H}_\Lambda|\Psi_z\rangle > E_{\alpha,\Lambda}(\alpha^2 p) + \alpha^{-(2+w)}$ for α large enough in case there exists an $i \in \{1,2,3\}$ with $z_i = \pm\infty$. Note that $\rho \in \mathrm{supp}\,(F_{-\infty,i})$ implies $m_{\alpha^{-v}}(\rho_i) < -\frac{3}{2}L$ and therefore $\int_{|x|>\frac{3}{2}L}\mathrm{d}\rho \geqslant \int_{-\infty}^{-\frac{3}{2}L}\mathrm{d}\rho_i \geqslant \int_{-\infty}^{m_{\alpha^{-v}}(\rho_i)}\mathrm{d}\rho_i \geqslant \left(\frac{1}{2} - \alpha^{-v}\right)\int \mathrm{d}\rho$. Similarly $\int_{|x|>\frac{3}{2}L}\mathrm{d}\rho \geqslant \left(\frac{1}{2} - \alpha^{-v}\right)\int\mathrm{d}\rho$ for $\rho \in \mathrm{supp}\,(F_{\infty,i})$. Consequently we have for any z with $z_i = \pm\infty$ for some $i \in \{1,2,3\}$

$$\langle \Psi_z|\mathcal{N}_{\mathbb{R}^3\setminus B_{\frac{3}{2}L}(0)}|\Psi_z\rangle \geqslant \left(\frac{1}{2} - \alpha^{-v}\right)\langle \Psi_z|\mathcal{N}|\Psi_z\rangle,$$

where $\mathcal{N}_{\mathbb{R}^3\setminus B_{\frac{3}{2}L}(0)} := \widehat{G}$ with $G(\rho) := \int_{|x|>\frac{3}{2}L}\mathrm{d}\rho$. Therefore [17, Corollary B.7] together with the fact that $\mathrm{supp}\,(\Psi_z) \subset \mathrm{supp}\,(\Psi''_\alpha) \subset B_L(0)$, yields

$$\begin{aligned}\langle \Psi_z|\mathbb{H}_\Lambda|\Psi_z\rangle &\geqslant E_\alpha + \left(\frac{1}{2} - \alpha^{-v}\right)\langle \Psi_z|\mathcal{N}|\Psi_z\rangle - \sqrt{\frac{D}{\frac{3}{2}L - L}} \geqslant E_\alpha + \left(\frac{1}{2} - \alpha^{-v}\right)c_- - \sqrt{2D\alpha^{-(1+\sigma)}}\\ &= E_{\alpha,\Lambda}\left(\alpha^2 p\right) + \frac{1}{2} + O_{\alpha\to\infty}\left(\alpha^{-v}\right) > E_{\alpha,\Lambda}\left(\alpha^2 p\right) + \alpha^{-(2+w)}\end{aligned}$$

for a suitable constant $D > 0$ and α large enough. Hence we obtain that all components z_i^* are finite, i.e. $m_{\alpha^{-v}}(\rho) \in B_{\sqrt{3}\alpha^{-u}}\left(\alpha^{-u}z^*\right) \subseteq \mathbb{R}^3$ for $\rho \in \mathrm{supp}\left(F_{z_3^*,3}F_{z_2^*,2}F_{z_1^*,1}\right)$.

Let $\Psi'''_\alpha := \mathcal{T}_{-\alpha^{-u}z^*}\Psi_{z^*}$, where $\mathcal{T}_z$ is a joint translation in the electron and phonon component, i.e. $(\mathcal{T}_z\Psi)(x) := U_z\Psi(x-z)$ with U_z being defined by $U_z^{-1}a(f)U_z = a(f_z)$ and $f_z(y) := f(y-z)$. Using the fact that $\langle \Psi_{z^*}|\mathbb{H}_\Lambda|\Psi_{z^*}\rangle \leqslant E_{\alpha,\Lambda}(\alpha^2 p) + \alpha^{-(2+w)} \lesssim E_\alpha + \alpha^{-\frac{2}{29}}$ as well as $\mathbb{1}_{\Omega^*}\Psi'''_\alpha = \Psi'''_\alpha$, where Ω^* is the set of all ρ satisfying $\int \mathrm{d}\rho \leqslant c_+$ and $m_{\alpha^{-v}}(\rho) \in B_{\sqrt{3}\alpha^{-u}}(0)$, we can apply [17, Lemma 3.11], which yields

$$\left\langle \Psi'''_\alpha \middle| W^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \middle| \Psi'''_\alpha \right\rangle \lesssim \alpha^{-\frac{2}{29}} + \alpha^{-u} + \alpha^{-v}.$$

By taking $r' > 0$ small enough such that $r' \leqslant \frac{1}{2}\left(\frac{1}{5} - \frac{9}{5}\sigma - 2v - 3u\right)$, $r' \leqslant w$ and $r' \leqslant \min\{\frac{2}{29}, u, v\}$, we conclude that $\left\langle \Psi'''_\alpha \middle| W^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \middle| \Psi'''_\alpha \right\rangle \lesssim \alpha^{-r'}$. Since $\mathrm{supp}(\Psi'''_\alpha) \subset B_L(-\alpha^{-u}z^*) \subset B_{L+\alpha^{-u}|z^*|}(0) \subset B_{4L}(0)$, this concludes the proof. ■

In the following Theorem 4.3.7, which is the main result of this section, we will lift the (weak) condensation from Eq. (4.3.11) to a strong one without introducing a large energy penalty, using an argument in [72]. We will verify that the momentum error due to the localization is negligibly small as well.

Theorem 4.3.7. *Given $0 < \sigma < \frac{1}{9}$ and $C > 0$, let $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ and $L = \alpha^{1+\sigma}$, and assume p satisfies $|p| \leqslant \frac{C}{\alpha}$ and $E_{\alpha,\Lambda}(\alpha^2 p) \leqslant E_\alpha + C|p|^2$ for a given $C > 0$. Then there exists a $r > 0$ and states Ψ_α with $\langle \Psi_\alpha | (\Upsilon_\Lambda - p)^2 |\Psi_\alpha\rangle \lesssim \alpha^{-(2+r)}$, $\langle \Psi_\alpha|\mathbb{H}_\Lambda|\Psi_\alpha\rangle - E_{\alpha,\Lambda}(\alpha^2 p) \lesssim \alpha^{-(2+r)}$ and $\mathrm{supp}(\Psi_\alpha) \subseteq B_{4L}(0)$, such that*

$$\chi\left(W^{-1}_{\varphi^{\mathrm{Pek}}-i\xi} \mathcal{N} W_{\varphi^{\mathrm{Pek}}-i\xi} \leqslant \alpha^{-r}\right)\Psi_\alpha = \Psi_\alpha, \tag{4.3.14}$$

where $\xi := \frac{p}{m}\widetilde{\nabla}_{x_1}\varphi^{\mathrm{Pek}}$ with $\widetilde{\nabla}_{x_1} := \chi^1\left(\Lambda^{-1}|\nabla_{x_1}| \leqslant 2\right)\nabla_{x_1}$.

Note that ξ is small in magnitude, $\|\xi\| \lesssim |p| \lesssim \alpha^{-1}$. The statement of Theorem 4.3.7 is also valid for $\xi = 0$, i.e., in case we conjugate by the Weyl transformation $W_{\varphi^{\mathrm{Pek}}}$ instead of $W_{\varphi^{\mathrm{Pek}}-i\xi}$. For technical reasons, it will however be useful in the proof of Theorem 4.2.1 to use $\varphi^{\mathrm{Pek}} - i\xi \approx \varphi^{\mathrm{Pek}} - i\frac{p}{m}\nabla_{x_1}\varphi^{\mathrm{Pek}}$ as a reference state, since the latter satisfies the momentum constraint $\langle \varphi^{\mathrm{Pek}} - i\frac{p}{m}\nabla_{x_1}\varphi^{\mathrm{Pek}}|\frac{1}{i}\nabla|\varphi^{\mathrm{Pek}} - i\frac{p}{m}\nabla_{x_1}\varphi^{\mathrm{Pek}}\rangle = p$.

Proof. Let Ψ'''_α be as in Lemma 4.3.6 and let us define for $0 < \epsilon < \frac{1}{2}$ and $0 < h < \min\left\{r', \frac{1}{4}\right\}$

$$\Psi_\alpha := Z_\alpha^{-1}\chi^\epsilon\left(\alpha^h W^{-1}_{\varphi^{\mathrm{Pek}}-i\xi}\mathcal{N}W_{\varphi^{\mathrm{Pek}}-i\xi} \leqslant \frac{1}{2}\right)\Psi'''_\alpha,$$

where $Z_\alpha := \|\chi^\epsilon\left(\alpha^h W^{-1}_{\varphi^{\mathrm{Pek}}-i\xi}\mathcal{N}W_{\varphi^{\mathrm{Pek}}-i\xi} \leqslant \frac{1}{2}\right)\Psi'''_\alpha\|$ is a normalization constant. Clearly the states Ψ_α satisfy Eq. (4.3.14) for $r \leqslant h$. Let us furthermore define the states $\widetilde{\Psi}_\alpha := \frac{1}{\sqrt{1-Z_\alpha^2}}\chi^\epsilon\left(\frac{1}{2} \leqslant \alpha^h W^{-1}_{\varphi^{\mathrm{Pek}}-i\xi}\mathcal{N}W_{\varphi^{\mathrm{Pek}}-i\xi}\right)\Psi'''_\alpha$. An application of [17, Lemma 3.3] yields

$$\begin{aligned} Z_\alpha^2\langle\Psi_\alpha|\mathbb{H}_\Lambda|\Psi_\alpha\rangle + (1-Z_\alpha^2)\langle\widetilde{\Psi}_\alpha|\mathbb{H}_\Lambda|\widetilde{\Psi}_\alpha\rangle &\leqslant \langle\Psi'''_\alpha|\mathbb{H}_\Lambda|\Psi'''_\alpha\rangle + C_0\alpha^{2h-\frac{7}{2}}\langle\Psi'''_\alpha|\sqrt{\mathcal{N}+1}|\Psi'''_\alpha\rangle \\ &\leqslant E_{\alpha,\Lambda}\left(\alpha^2 p\right) + C_1\alpha^{-(2+r'')} \end{aligned}$$

for suitable constants $C_0, C_1 > 0$ and $r'' := \min\{r', \frac{3}{2} - 2h\} > 0$. We have

$$\begin{aligned} 1 - Z_\alpha^2 &= \left\langle \Psi'''_\alpha \middle| \chi^\epsilon \left(\frac{1}{2} \leqslant \alpha^h W^{-1}_{\varphi^{\mathrm{Pek}} - i\xi} \mathcal{N} W_{\varphi^{\mathrm{Pek}} - i\xi} \right)^2 \middle| \Psi'''_\alpha \right\rangle \\ &\leqslant \frac{2\alpha^h}{1-2\epsilon} \left\langle \Psi'''_\alpha \middle| W^{-1}_{\varphi^{\mathrm{Pek}} - i\xi} \mathcal{N} W_{\varphi^{\mathrm{Pek}} - i\xi} \middle| \Psi'''_\alpha \right\rangle \leqslant \frac{4\alpha^h}{1-2\epsilon} \left\langle \Psi'''_\alpha \middle| W^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \middle| \Psi'''_\alpha \right\rangle + \frac{4\alpha^h \|\xi\|^2}{1-2\epsilon} \\ &\lesssim \frac{1}{1-2\epsilon} \left(\alpha^{h-r'} + \alpha^{h-2} \right) \underset{\alpha \to \infty}{\longrightarrow} 0, \end{aligned}$$

where we used the operator inequality $W^{-1}_{\varphi^{\mathrm{Pek}} - i\xi} \mathcal{N} W_{\varphi^{\mathrm{Pek}} - i\xi} \leqslant 2 \left(W^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} + \|\xi\|^2 \right)$, $\|\xi\|^2 \leqslant |p|^2 \|\nabla \varphi^{\mathrm{Pek}}\|^2 \lesssim \alpha^{-2}$ and Eq. (4.3.11). Making use of $\langle \widetilde{\Psi}_\alpha | \mathbb{H}_\Lambda | \widetilde{\Psi}_\alpha \rangle \geqslant E_\alpha$ and $E_{\alpha,\Lambda}(\alpha^2 p) - E_\alpha \lesssim |p|^2 \lesssim \alpha^{-2}$, we therefore obtain

$$\begin{aligned} \langle \Psi_\alpha | \mathbb{H}_\Lambda | \Psi_\alpha \rangle - E_{\alpha,\Lambda}(\alpha^2 p) &\leqslant Z_\alpha^{-2} \left(C_1 \alpha^{-(2+r'')} + (1 - Z_\alpha^2) \left(E_{\alpha,\Lambda}(\alpha^2 p) - E_\alpha \right) \right) \\ &\lesssim \alpha^{-(2+r'')} + \left(\alpha^{h-r'} + \alpha^{h-2} \right) \left(E_{\alpha,\Lambda}(\alpha^2 p) - E_\alpha \right) \lesssim \alpha^{-(2+r''')} \end{aligned}$$

with $r''' := \min\{r'', r' - h, 2 - h\} > 0$.

In order to estimate $\left\langle \Psi_\alpha \right| (\Upsilon_\Lambda - p)^2 \left| \Psi_\alpha \right\rangle$, let us apply the IMS identity

$$Z_\alpha^2 \left\langle \Psi_\alpha \middle| (\Upsilon_\Lambda - p)^2 \middle| \Psi_\alpha \right\rangle + (1 - Z_\alpha^2) \left\langle \widetilde{\Psi}_\alpha \middle| (\Upsilon_\Lambda - p)^2 \middle| \widetilde{\Psi}_\alpha \right\rangle = \left\langle \Psi'''_\alpha \middle| (\Upsilon_\Lambda - p)^2 \middle| \Psi'''_\alpha \right\rangle - \left\langle \Psi'''_\alpha \middle| X \middle| \Psi'''_\alpha \right\rangle, \tag{4.3.15}$$

where we define $X := \frac{1}{2} \left[\left[(\Upsilon_\Lambda - p)^2, A_1 \right], A_1 \right] + \frac{1}{2} \left[\left[(\Upsilon_\Lambda - p)^2, A_2 \right], A_2 \right]$ using the operators $A_1 := f_1 \left(W^{-1}_{\varphi^{\mathrm{Pek}} - i\xi} \mathcal{N} W_{\varphi^{\mathrm{Pek}} - i\xi} \right)$ and $A_2 := f_2 \left(W^{-1}_{\varphi^{\mathrm{Pek}} - i\xi} \mathcal{N} W_{\varphi^{\mathrm{Pek}} - i\xi} \right)$ with $f_1(x) := \chi^\epsilon\big(\alpha^h x \leqslant \frac{1}{2}\big)$ and $f_2 := \chi^\epsilon\big(\frac{1}{2} \leqslant \alpha^h x\big)$. In the following let us compute

$$\begin{aligned} \left[\left[(\Upsilon_\Lambda - p)^2, A_j \right], A_j \right] &= W^{-1}_{\varphi^{\mathrm{Pek}} - i\xi} \left[\left[\left(W_{\varphi^{\mathrm{Pek}} - i\xi} \Upsilon_\Lambda W^{-1}_{\varphi^{\mathrm{Pek}} - i\xi} - p \right)^2, f_j(\mathcal{N}) \right], f_j(\mathcal{N}) \right] W_{\varphi^{\mathrm{Pek}} - i\xi} \\ &= W^{-1}_{\varphi^{\mathrm{Pek}} - i\xi} \left[\left[\left(\Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re}\, a^\dagger(\varphi) \right)^2, f_j(\mathcal{N}) \right], f_j(\mathcal{N}) \right] W_{\varphi^{\mathrm{Pek}} - i\xi} \end{aligned}$$

where $\varphi := \frac{1}{i} \widetilde{\nabla}_{x_1} \left(\varphi^{\mathrm{Pek}} - i\xi \right)$ and $\widetilde{p} := p - \langle \varphi^{\mathrm{Pek}} - i\xi | \frac{1}{i} \widetilde{\nabla}_{x_1} | \varphi^{\mathrm{Pek}} - i\xi \rangle = p\big(1 - \frac{2}{m} \|\widetilde{\nabla}_{x_1} \varphi^{\mathrm{Pek}}\|^2\big)$. We have $|\widetilde{p}| \leqslant |p| \leqslant \frac{C}{\alpha}$ since $m = \frac{2}{3} \|\nabla \varphi^{\mathrm{Pek}}\|^2 = 2 \|\nabla_{x_1} \varphi^{\mathrm{Pek}}\|^2 \geqslant 2 \|\widetilde{\nabla}_{x_1} \varphi^{\mathrm{Pek}}\|^2$. Defining the discrete derivative $\delta f_j(x) := \alpha^2 \big(f_j(x + \alpha^{-2}) - f_j(x) \big)$, we can further write

$$\begin{aligned} \left[\left[\left(\Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re}\, a^\dagger(\varphi) \right)^2, f_j(\mathcal{N}) \right], f_j(\mathcal{N}) \right] &= 8 \left[\mathfrak{Re}\, a^\dagger(\varphi), f(\mathcal{N}) \right]^2 \\ &\quad + 2 \left\{ \Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re}\, a^\dagger(\varphi), \left[\left[\mathfrak{Re}\, a^\dagger(\varphi), f_j(\mathcal{N}) \right], f_j(\mathcal{N}) \right] \right\} \\ &= -8\alpha^{-4} \left(\mathfrak{Im} \left(a^\dagger(\varphi)\, \delta f_j(\mathcal{N}) \right) \right)^2 + 2\alpha^{-4} \left\{ \Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re}\, a^\dagger(\varphi), \mathfrak{Re} \left(a^\dagger(\varphi) (\delta f_j)^2(\mathcal{N}) \right) \right\} \end{aligned}$$

where we used $\left[\Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re}\, a^\dagger(\varphi), f_j(\mathcal{N}) \right] = 2 \left[\mathfrak{Re}\, a^\dagger(\varphi), f_j(\mathcal{N}) \right]$, $\left[\mathfrak{Re}\, a^\dagger(\varphi), f_j(\mathcal{N}) \right] = \alpha^{-2} i \mathfrak{Im} \left(a^\dagger(\varphi)\, \delta f_j(\mathcal{N}) \right)$ and $\left[\left[\mathfrak{Re}\, a^\dagger(\varphi), f_j(\mathcal{N}) \right], f_j(\mathcal{N}) \right] = \alpha^{-4} \mathfrak{Re} \left(a^\dagger(\varphi) (\delta f_j)^2(\mathcal{N}) \right)$. Hence

$$\begin{aligned} -\left[\left[\left(\Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re}\, a^\dagger(\varphi) \right)^2, f_j(\mathcal{N}) \right], f_j(\mathcal{N}) \right] &\leqslant 8\alpha^{-4} \mathfrak{Im} \left(a^\dagger(\varphi)\, \delta f_j(\mathcal{N}) \right)^2 \\ &\quad + 4\alpha^{-3}\, \mathfrak{Re} \left(a^\dagger(\varphi) (\delta f_j)^2(\mathcal{N}) \right)^2 + \alpha^{-5} \left(\Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re}\, a^\dagger(\varphi) \right)^2 \\ &\leqslant 2\|\varphi\|^2 \left(2\alpha^{-4} \|\delta f_j\|_\infty^2 + 2\alpha^{-3} \|\delta f_j\|_\infty^4 + 3\alpha^{-5} \right) \left(2\mathcal{N} + \alpha^{-2} \right) + 27\alpha^{-3} \mathcal{N}^2 + 3\alpha^{-5} |\widetilde{p}|^2 \end{aligned} \tag{4.3.16}$$

where we have applied multiple Cauchy–Schwarz estimates and used $\Upsilon_\Lambda^2 \leqslant 9\alpha^2\mathcal{N}^2$. Note that the expression in the last line of Eq. (4.3.16) is of order $\alpha^{4h-3}(\mathcal{N}+1)^2$, since $\|\delta f_j\|_\infty \lesssim \alpha^h$ and $\|\varphi\| \lesssim 1$. Using $W_{\varphi^{\mathrm{Pek}}-i\xi}^{-1}(\mathcal{N}+1)^2 W_{\varphi^{\mathrm{Pek}}-i\xi} \lesssim (\mathcal{N}+1)^2$ we therefore obtain

$$-X = -\frac{1}{2}\sum_{j=1}^{2}\left[\left[(\Upsilon_\Lambda - p)^2, A_j\right], A_j\right] \lesssim \alpha^{4h-3}(\mathcal{N}+1)^2.$$

Using this together with Eq. (4.3.15) and the observation $\langle\widetilde{\Psi}_\alpha|(\Upsilon_\Lambda - p)^2|\widetilde{\Psi}_\alpha\rangle \geqslant 0$, yields

$$\begin{aligned}\langle\Psi_\alpha|(\Upsilon_\Lambda - p)^2|\Psi_\alpha\rangle &\leqslant Z_\alpha^{-2}\left(\langle\Psi_\alpha'''|(\Upsilon_\Lambda - p)^2|\Psi_\alpha'''\rangle - \langle\Psi_\alpha'''|X|\Psi_\alpha'''\rangle\right)\\ &\lesssim \alpha^{-(2+r')} + \alpha^{4h-3}\langle\Psi_\alpha'''|(\mathcal{N}+1)^2|\Psi_\alpha'''\rangle \lesssim \alpha^{-(2+r')} + \alpha^{4h-3}.\end{aligned}$$

Since $h < \frac{1}{4}$ we have $\min\{r', 1-4h\} > 0$, and therefore we can choose $r > 0$ small enough such that $r \leqslant \min\{r', 1-4h\}$, $r \leqslant r'''$ and $r \leqslant h$, which concludes the proof. ■

4.4 Proof of Theorem 4.2.1

In this section we shall prove the main technical Theorem 4.2.1, using the results of the previous sections as well as the results in the previous part of this paper series [17]. Before we do this let us recall some definitions from [17].

Definition 4.4.1 (Finite dimensional Projection Π)**.** Given $\sigma > 0$, let $\Lambda := \alpha^{\frac{4}{5}(1+\sigma)}$ and $\ell := \alpha^{-4(1+\sigma)}$, and let us introduce the cubes $C_z := [z_1 - \ell, z_1 + \ell) \times [z_2 - \ell, z_2 + \ell) \times [z_3 - \ell, z_3 + \ell)$ for $z = (z_1, z_2, z_3) \in 2\ell\,\mathbb{Z}^3$. Then we define Π as the orthogonal projection onto the subspace spanned by the functions $x \mapsto \int_{C_z} \frac{e^{i\,k\cdot x}}{|k|}\,\mathrm{d}k$ for $z \in 2\ell\,\mathbb{Z}^3\backslash\{0\}$ satisfying $C_z \subset B_\Lambda(0)$. Furthermore, let $\varphi_1, \ldots, \varphi_N$ be a real orthonormal basis of $\Pi L^2(\mathbb{R}^3)$, such that $\varphi_n = \frac{\Pi\nabla_{x_n}\varphi^{\mathrm{Pek}}}{\|\Pi\nabla_{x_n}\varphi^{\mathrm{Pek}}\|}$ for $n \in \{1,2,3\}$.

Definition 4.4.2 (Coordinate Transformation τ)**.** Let $\varphi_x^{\mathrm{Pek}}(y) := \varphi^{\mathrm{Pek}}(y - x)$ and let $t \mapsto x_t$ be the local inverse of the function $x \mapsto (\langle\varphi_n|\varphi_x^{\mathrm{Pek}}\rangle)_{n=1}^3 \in \mathbb{R}^3$ defined for $t \in B_{\delta_*}(0)$ with a suitable $\delta_* > 0$. Note that we can take $B_{\delta_*}(0)$ as the domain of the local inverse, since $\langle\varphi_n|\varphi_0^{\mathrm{Pek}}\rangle = 0$ for all $n \in \{1,2,3\}$ due to the fact that φ^{Pek} and Π respect the reflection symmetry $y_n \mapsto -y_n$. Then we define $f : \mathbb{R}^3 \longrightarrow \Pi L^2(\mathbb{R}^3)$ as $f(t) := \chi(|t| < \delta_*)\left(\Pi\varphi_{x_t}^{\mathrm{Pek}} - \sum_{n=1}^3 t_n\varphi_n\right)$ and the transformation $\tau : \Pi L^2(\mathbb{R}^3) \longrightarrow \Pi L^2(\mathbb{R}^3)$ as

$$\tau(\varphi) := \varphi - f(t^\varphi)$$

with $t^\varphi := (\langle\varphi_1|\varphi\rangle, \langle\varphi_2|\varphi\rangle, \langle\varphi_3|\varphi\rangle) \in \mathbb{R}^3$.

Definition 4.4.3 (Quadratic Approximation $J_{t,\epsilon}$)**.** Let us first define the operators

$$K^{\mathrm{Pek}} := 1 - H^{\mathrm{Pek}} = 4(-\Delta)^{-\frac{1}{2}}\psi^{\mathrm{Pek}}\frac{1 - |\psi^{\mathrm{Pek}}\rangle\langle\psi^{\mathrm{Pek}}|}{-\Delta + V^{\mathrm{Pek}} - \mu^{\mathrm{Pek}}}\psi^{\mathrm{Pek}}(-\Delta)^{-\frac{1}{2}}, \tag{4.4.1}$$

$$L^{\mathrm{Pek}} := 4(-\Delta)^{-\frac{1}{2}}\psi^{\mathrm{Pek}}(1-\Delta)^{-1}\psi^{\mathrm{Pek}}(-\Delta)^{-\frac{1}{2}}, \tag{4.4.2}$$

where $V^{\mathrm{Pek}} := -2(-\Delta)^{-\frac{1}{2}}\varphi^{\mathrm{Pek}}$, $\mu^{\mathrm{Pek}} := e^{\mathrm{Pek}} - \|\varphi^{\mathrm{Pek}}\|^2$ and ψ^{Pek} is the, non-negative, ground state of the operator $-\Delta + V^{\mathrm{Pek}}$. Furthermore let T_x be the translation operator, i.e. $(T_x\varphi)(y) := \varphi(y-x)$, and let $K_x^{\mathrm{Pek}} := T_x K^{\mathrm{Pek}} T_{-x}$ and $L_x^{\mathrm{Pek}} := T_x L^{\mathrm{Pek}} T_{-x}$. Then we define

$$J_{t,\epsilon} := \pi\left(1-(1+\epsilon)\left(K_{x_t}^{\mathrm{Pek}}+\epsilon L_{x_t}^{\mathrm{Pek}}\right)\right)\pi$$

for $|t|<\epsilon$ and $\epsilon<\delta_*$, where δ_* and x_t are as in Definition 4.4.2 and $\pi : L^2(\mathbb{R}^3)\longrightarrow L^2(\mathbb{R}^3)$ is the orthogonal projection on the space spanned by $\{\varphi_4,\dots,\varphi_N\}$ with φ_n as in Definition 4.4.1. Furthermore we define $J_{t,\epsilon} := \pi$ for $|t|\geqslant\epsilon$ and we will use the shorthand notation $J_{t,\epsilon}[\varphi] := \langle\varphi|J_{t,\epsilon}|\varphi\rangle$.

Recall the definition of $E_{\alpha,\Lambda}$ in Theorem 4.2.1. In the following we will assume that p satisfies the assumption $E_{\alpha,\Lambda}(\alpha^2 p)\leqslant E_\alpha + C|p|^2$ of Theorem 4.3.7 with $C\geqslant\frac{1}{2m}$, which we can do w.l.o.g., since $E_{\alpha,\Lambda}(\alpha^2 p) > E_\alpha + C|p|^2$ immediately implies the statement of Theorem 4.2.1 (compare with the comment above Lemma 4.3.1). We shall also assume in the following that $|p|\leqslant\frac{C}{\alpha}$. Due to these assumptions we can apply Theorem 4.3.7, which yields the existence of a sequence Ψ_α with $\left\langle\Psi_\alpha\middle|\left(\Upsilon_\Lambda-p\right)^2\middle|\Psi_\alpha\right\rangle\lesssim\alpha^{-(2+r)}$, $\langle\Psi_\alpha|\mathbb{H}_\Lambda|\Psi_\alpha\rangle - E_{\alpha,\Lambda}(\alpha^2 p)\lesssim\alpha^{-(2+r)}$ and $\mathrm{supp}\,(\Psi_\alpha)\subseteq B_{4L}(0)$ with $L=\alpha^{1+\sigma}$, such that $\widetilde{\Psi}_\alpha := W_{-i\xi}\Psi_\alpha$ with $\xi=\frac{p}{m}\widetilde{\nabla}_{x_1}\varphi^{\mathrm{Pek}}$ satisfies condensation with respect to φ^{Pek}, i.e.

$$\chi\left(W_{\varphi^{\mathrm{Pek}}}^{-1}\mathcal{N}W_{\varphi^{\mathrm{Pek}}}\leqslant\alpha^{-r}\right)\widetilde{\Psi}_\alpha=\widetilde{\Psi}_\alpha. \tag{4.4.3}$$

Using $\frac{p}{m}\left(p-\Upsilon_\Lambda\right)\leqslant\alpha^{-\frac{r}{2}}\frac{|p|^2}{4m^2}+\alpha^{\frac{r}{2}}\left(p-\Upsilon_\Lambda\right)^2$ and $|p|\leqslant\frac{C}{\alpha}$, we therefore have

$$E_{\alpha,\Lambda}\big(\alpha^2 p\big)\geqslant\left\langle\Psi_\alpha\middle|\mathbb{H}_\Lambda+\frac{p}{m}\left(p-\Upsilon_\Lambda\right)\middle|\Psi_\alpha\right\rangle+O_{\alpha\to\infty}\left(\alpha^{-\left(2+\frac{r}{2}\right)}\right), \tag{4.4.4}$$

where $\frac{p}{m}$ formally acts as a Lagrange multiplier for the minimization of $\mathbb{H}_\Lambda$ subject to the constraint $\Upsilon_\Lambda = p$. In the rest of this Section we will verify that $\mathbb{H}_\Lambda+\frac{p}{m}\left(p-\Upsilon_\Lambda\right)$ is bounded from below by the right hand side of Eq. (4.2.3) when tested against a state Ψ satisfying $\mathrm{supp}\,(\Psi)\subseteq B_{4L}(0)$ and complete condensation with respect to $\varphi^{\mathrm{Pek}}-i\xi$ (where we find it convenient to use $\varphi^{\mathrm{Pek}}-i\xi$ instead of φ^{Pek} for technical reasons). The momentum constraint on Ψ will not be needed for this; i.e., we have transformed our original constrained minimization problem into a global one, which we handle similarly as in the previous part [17] concerning a lower bound on the global minimum $E_\alpha=\inf\sigma\left(\mathbb{H}\right)$. As already stressed in the Section 4.1, it is essential to work with the truncated Hamiltonian $\mathbb{H}_\Lambda$ and the truncated momentum Υ_Λ here, since in contrast to $\mathbb{H}_\Lambda+\frac{p}{m}\left(p-\Upsilon_\Lambda\right)$ the operator $\mathbb{H}+\frac{p}{m}\left(p-\mathbb{P}\right)$ is not bounded from below for $p\neq 0$.

Following [17], we will identify $\mathcal{F}\left(\Pi L^2(\mathbb{R}^3)\right)$ with $L^2\big(\mathbb{R}^N\big)$ using the representation of real-valued functions $\varphi=\sum_{n=1}^N\lambda_n\varphi_n$ by points $\lambda=(\lambda_1,\dots,\lambda_N)\in\mathbb{R}^N$. With this identification, we can represent the annihilation operators $a_n := a\left(\varphi_n\right)$ as $a_n=\lambda_n+\frac{1}{2\alpha^2}\partial_{\lambda_n}$, where λ_n is the multiplication operator by the function $\lambda\mapsto\lambda_n$ on $L^2\big(\mathbb{R}^N\big)$. Let us also use for functions $\varphi\mapsto g(\varphi)$ depending on elements $\varphi\in\Pi L^2(\mathbb{R}^3)$ the convenient notation $g(\lambda) := g\left(\sum_{n=1}^N\lambda_n\varphi_n\right)$, where $\lambda\in\mathbb{R}^N$.

It is essential for our proof that $\widetilde{\Psi}_\alpha$ satisfies complete condensation in φ^{Pek}, see Eq. (4.4.3), since it allows us to apply [17, Lemma 6.1] which states that in terms of the quadratic operator

$J_{t,\epsilon}$ and the transformation τ on $\Pi L^2(\mathbb{R}^3)$ in Definitions 4.4.3 and 4.4.2 we have

$$\langle\widetilde{\Psi}_\alpha|\mathbb{H}_\Lambda|\widetilde{\Psi}_\alpha\rangle \geqslant e^{\text{Pek}} + \big\langle\widetilde{\Psi}_\alpha\big| -\frac{1}{4\alpha^4}\sum_{n=1}^{N}\partial^2_{\lambda_n} + J_{t^\lambda,\alpha^{-s}}\big[\tau(\lambda)\big] + \mathcal{N}_{>N}\big|\widetilde{\Psi}_\alpha\big\rangle - \frac{N}{2\alpha^2} + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right) \tag{4.4.5}$$

for suitable $w, s_0 > 0$ and any $0 < s < s_0$, where we define $\mathcal{N}_{>N} := \mathcal{N} - \sum_{k=1}^{N} a_k^\dagger a_k$ and t^φ is defined as in Definition 4.4.2 such that $t^\lambda = (\lambda_1, \lambda_2, \lambda_3) \in \mathbb{R}^3$. Furthermore it is shown in [17, Lemma 6.1], that there exists a $\beta > 0$, such that

$$\langle\widetilde{\Psi}_\alpha|1 - \mathbb{B}|\widetilde{\Psi}_\alpha\rangle \leqslant e^{-\beta\alpha^{2-2s}} \tag{4.4.6}$$

for all $0 < s < s_0$, where $\mathbb{B}$ is the multiplication operator by the function $\lambda \mapsto \chi(|t^\lambda| < \alpha^{-s})$. In the following we will always choose $s < 1$. We will use the symbol w for a generic, positive constant, which is allowed to vary from line to line.

4.4.1 Quasi-Quadratic Lower Bound

In order to find a good lower bound on $\langle\Psi_\alpha|\mathbb{H}_\Lambda + \frac{p}{m}(p - \Upsilon_\Lambda)|\Psi_\alpha\rangle$, and therefore on $E_{\alpha,\Lambda}(\alpha^2 p)$, it is natural to conjugate $\mathbb{H}_\Lambda + \frac{p}{m}(p - \Upsilon_\Lambda)$ with the Weyl transformation $W_{\varphi^{\text{Pek}} - i\xi} = W_{\varphi^{\text{Pek}}}W_{-i\xi}$, since $\varphi^{\text{Pek}} - i\xi$ is close to the minimizer $\varphi^{\text{Pek}} - i\frac{p}{m}\nabla_{x_1}\varphi^{\text{Pek}}$ of the corresponding classical problem, see [39]. Since $i\xi$ is purely imaginary, the interaction term in $\mathbb{H}_\Lambda$ is invariant under the transformation
$W_{-i\xi}$, i.e. $W_{-i\xi}\mathfrak{Re}\left[a\left(\chi\left(|\nabla| \leqslant \Lambda\right) w_x\right)\right]W_{-i\xi}^{-1} = \mathfrak{Re}\left[a\left(\chi\left(|\nabla| \leqslant \Lambda\right) w_x\right)\right]$, and furthermore

$$W_{-i\xi}\Upsilon_\Lambda W_{-i\xi}^{-1} = \Upsilon_\Lambda - 2\mathfrak{Re}\left[a\left(\frac{1}{i}\widetilde{\nabla}_{x_1} i\xi\right)\right] + \left\langle i\xi\middle|\frac{1}{i}\widetilde{\nabla}_{x_1}\middle|i\xi\right\rangle = \Upsilon_\Lambda - 2\mathfrak{Re}\left[a\left(\widetilde{\nabla}_{x_1}\xi\right)\right], \tag{4.4.7}$$

where we have used $\left\langle i\xi\middle|\frac{1}{i}\widetilde{\nabla}_{x_1}\middle|i\xi\right\rangle = 0$ (since $\langle h|\frac{1}{i}\widetilde{\nabla}_{x_1}|h\rangle = 0$ for any real-valued or imaginary-valued function $h \in L^2(\mathbb{R}^3)$). Therefore conjugating $\mathbb{H}_\Lambda + \frac{p}{m}(p - \Upsilon_\Lambda)$ with $W_{-i\xi}$ yields

$$\begin{aligned}\left\langle\Psi_\alpha\middle|\mathbb{H}_\Lambda + \frac{p}{m}(p - \Upsilon_\Lambda)\middle|\Psi_\alpha\right\rangle &= \left\langle\widetilde{\Psi}_\alpha\middle|\mathbb{H}_\Lambda - \frac{p}{m}\Upsilon_\Lambda + 2\mathfrak{Re}\left[a\left(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi - i\xi\right)\right]\middle|\widetilde{\Psi}_\alpha\right\rangle + \frac{|p|^2}{m} + \|\xi\|^2\\ &\geqslant e^{\text{Pek}} + \big\langle\widetilde{\Psi}_\alpha\big| - \frac{1}{4\alpha^4}\sum_{n=1}^{N}\partial^2_{\lambda_n} + J_{t^\lambda,\alpha^{-s}}\big[\tau(\lambda)\big] + \mathcal{N}_{>N} - \frac{p}{m}\Upsilon_\Lambda\big|\widetilde{\Psi}_\alpha\big\rangle - \frac{N}{2\alpha^2}\\ &\quad + 2\mathfrak{Re}\left\langle\widetilde{\Psi}_\alpha\middle|a\left(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi - i\xi\right)\middle|\widetilde{\Psi}_\alpha\right\rangle + \frac{|p|^2}{m} + \|\xi\|^2 + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right),\end{aligned}$$

where we have used Eq. (4.4.5). In the next step we apply the Weyl transformation $W_{\varphi^{\text{Pek}}}$, which satisfies $W_{\varphi^{\text{Pek}}}\lambda W_{\varphi^{\text{Pek}}}^{-1} = \lambda + \lambda^{\text{Pek}}$ and hence

$$\begin{aligned} W_{\varphi^{\text{Pek}}}\frac{p}{m}\Upsilon_\Lambda W_{\varphi^{\text{Pek}}}^{-1} &= \frac{p}{m}\Upsilon_\Lambda + 2\mathfrak{Re}\left[a\left(\frac{p}{im}\widetilde{\nabla}_{x_1}\varphi^{\text{Pek}}\right)\right] = \frac{p}{m}\Upsilon_\Lambda - 2\mathfrak{Re}\left[a\left(i\xi\right)\right],\\ W_{\varphi^{\text{Pek}}}\mathfrak{Re}\left[a\left(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi - i\xi\right)\right]W_{\varphi^{\text{Pek}}}^{-1} &= \mathfrak{Re}\left[a\left(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi - i\xi\right)\right] - \|\xi\|^2,\end{aligned}$$

where we have used $\mathfrak{Re}\,\langle\varphi^{\text{Pek}}|\frac{p}{m}\widetilde{\nabla}_{x_1}\xi - i\xi\rangle = \langle\varphi^{\text{Pek}}|\frac{p}{m}\widetilde{\nabla}_{x_1}\xi\rangle = -\|\xi\|^2$. Furthermore
$W_{\varphi^{\text{Pek}}}t^\lambda W_{\varphi^{\text{Pek}}}^{-1} = (\lambda_1 + \lambda_1^{\text{Pek}}, \lambda_2 + \lambda_2^{\text{Pek}}, \lambda_3 + \lambda_3^{\text{Pek}}) = (\lambda_1, \lambda_2, \lambda_3) = t^\lambda$ with

$\lambda^{\mathrm{Pek}} := \left(\langle\varphi_n|\Pi\varphi^{\mathrm{Pek}}\rangle\right)_{n=1}^N$. Therefore defining $\Psi_\alpha^* := W_{\varphi^{\mathrm{Pek}}}\widetilde{\Psi}_\alpha = W_{\varphi^{\mathrm{Pek}}-i\xi}\Psi_\alpha$ and conjugating with $W_{\varphi^{\mathrm{Pek}}}$ yields the lower bound

$$\begin{aligned}&\langle\Psi_\alpha|\mathbb{H}_\Lambda + \frac{p}{m}\left(p-\Upsilon_\Lambda\right)|\Psi_\alpha\rangle \\ &\geqslant e^{\mathrm{Pek}} + \left\langle\Psi_\alpha^*\middle| -\frac{1}{4\alpha^4}\sum_{n=1}^N \partial_{\lambda_n}^2 + J_{t^\lambda,\alpha^{-s}}\left[\tau\left(\lambda+\lambda^{\mathrm{Pek}}\right)\right] + W_{\varphi^{\mathrm{Pek}}}\mathcal{N}_{>N}W_{\varphi^{\mathrm{Pek}}}^{-1} - \frac{p}{m}\Upsilon_\Lambda\middle|\Psi_\alpha^*\right\rangle \\ &\quad -\frac{N}{2\alpha^2} + 2\mathfrak{Re}\left\langle\Psi_\alpha^*\middle|a\left(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi\right)\middle|\Psi_\alpha^*\right\rangle + \frac{|p|^2}{m} - \|\xi\|^2 + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right).\end{aligned} \tag{4.4.8}$$

The advantage of conjugating with the Weyl transformation $W_{\varphi^{\mathrm{Pek}}-i\xi} = W_{\varphi^{\mathrm{Pek}}}W_{-i\xi}$ stems from the observation that we have an almost complete cancellation of linear terms, i.e., as we will verify below, the term linear in creation and annihilation operators $\mathfrak{Re}\left\langle\Psi_\alpha^*\middle|a\left(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi\right)\middle|\Psi_\alpha^*\right\rangle$ in Eq. (4.4.8) is of negligible order, and the function $\lambda \mapsto J_{t^\lambda,\alpha^{-s}}\left[\tau\left(\lambda+\lambda^{\mathrm{Pek}}\right)\right]$ vanishes quadratically at $\lambda = 0$. The latter follows from the fact that $\tau\left(\lambda^{\mathrm{Pek}}\right) = 0$. Utilizing the inequalities $\langle\Psi_\alpha^*|\mathcal{N}|\Psi_\alpha^*\rangle = \langle\Psi_\alpha|W_{\varphi^{\mathrm{Pek}}-i\xi}^{-1}\mathcal{N}W_{\varphi^{\mathrm{Pek}}-i\xi}|\Psi_\alpha\rangle \leqslant \alpha^{-r}$, see Eq. (4.3.14), and $\|\frac{p}{m}\widetilde{\nabla}_{x_1}\xi\| \lesssim |p|^2$, where we have used that $\varphi^{\mathrm{Pek}} \in H^2(\mathbb{R}^3)$, see [76, 95], we obtain that

$$2\mathfrak{Re}\left\langle\Psi_\alpha^*\middle|a\left(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi\right)\middle|\Psi_\alpha^*\right\rangle \lesssim \alpha^{-\frac{r}{2}}|p|^2 \lesssim \alpha^{-(2+\frac{r}{2})} \tag{4.4.9}$$

is indeed negligible small. Furthermore we can estimate, up to a term of order $\alpha^{-(2+\frac{2}{5})}$, $W_{\varphi^{\mathrm{Pek}}}\mathcal{N}_{>N}W_{\varphi^{\mathrm{Pek}}}^{-1}$ from below by a proper quadratic expression

$$\begin{aligned}W_{\varphi^{\mathrm{Pek}}}\mathcal{N}_{>N}W_{\varphi^{\mathrm{Pek}}}^{-1} &= \mathcal{N}_{>N} + a\left((1-\Pi)\varphi^{\mathrm{Pek}}\right) + a^\dagger\left((1-\Pi)\varphi^{\mathrm{Pek}}\right) + \left\|(1-\Pi)\varphi^{\mathrm{Pek}}\right\|^2 \\ &\geqslant \frac{1}{2}\mathcal{N}_{>N} - 2\left\|(1-\Pi)\varphi^{\mathrm{Pek}}\right\|^2 = \frac{1}{2}\mathcal{N}_{>N} + O_{\alpha\to\infty}\left(\alpha^{-(2+\frac{2}{5})}\right),\end{aligned} \tag{4.4.10}$$

where we have used $\|(1-\Pi)\varphi^{\mathrm{Pek}}\|^2 \lesssim \alpha^{-(2+\frac{2}{5})}$, see [17, Lemma A.1]. In the following let us use the convenient notation $e_p^{\mathrm{Pek}} := e^{\mathrm{Pek}} + \frac{|p|^2}{2m}$. Combining Eq. (4.4.8) with Eq. (4.4.9), Eq. (4.4.10) and the observation that $\frac{|p|^2}{m} - \|\xi\|^2 \geqslant \frac{|p|^2}{2m}$, and using the fact that $E_{\alpha,\Lambda}(\alpha^2 p) \geqslant \left\langle\Psi_\alpha\middle|\mathbb{H}_\Lambda + \frac{p}{m}(p-\Upsilon_\Lambda)\middle|\Psi_\alpha\right\rangle + O_{\alpha\to\infty}\left(\alpha^{-\left(2+\frac{r}{2}\right)}\right)$, see Eq. (4.4.4), we obtain

$$\begin{aligned}E_{\alpha,\Lambda}(\alpha^2 p) \geqslant\ & e_p^{\mathrm{Pek}} + \left\langle\Psi_\alpha^*\middle| -\frac{1}{4\alpha^4}\sum_{n=1}^N \partial_{\lambda_n}^2 + J_{t^\lambda,\alpha^{-s}}\left[\tau\left(\lambda+\lambda^{\mathrm{Pek}}\right)\right] + \frac{1}{2}\mathcal{N}_{>N} - \frac{p}{m}\Upsilon_\Lambda\middle|\Psi_\alpha^*\right\rangle \\ & -\frac{N}{2\alpha^2} + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right).\end{aligned} \tag{4.4.11}$$

The right hand side of Eq. (4.4.11) is up to a coordinate transformation in the argument of $J_{t^\lambda,\alpha^{-s}}$ quadratic in creation and annihilation operators. In the next subsection we will apply a unitary transformation in order to arrive at a proper quadratic expression.

4.4.2 Conjugation with the Unitary $\mathcal{U}$

In order to get rid of the coordinate transformation τ in the argument of $J_{t^\lambda,\alpha^{-s}}$, let us define the unitary operator $\mathcal{U}$ on $\mathcal{F}\left(\Pi L^2(\mathbb{R}^3)\right) \cong L^2\left(\mathbb{R}^N\right)$ as $\mathcal{U}\left(\Psi\right)(\lambda) := \Psi\left(\Xi(\lambda)\right)$, where $\Xi : \mathbb{R}^N \longrightarrow \mathbb{R}^N$ is defined as $\Xi(\lambda) := \tau\left(\lambda + \lambda^{\mathrm{Pek}}\right) \in \Pi L^2(\mathbb{R}^3) \cong \mathbb{R}^N$. Note that the inverse of τ is simply given by $\tau^{-1}(\varphi) = \varphi + f(t^\varphi)$ where $f : \mathbb{R}^3 \longrightarrow \Pi L^2(\mathbb{R}^3)$ is defined in Definition 4.4.2, which can be checked easily using the fact that $\langle \varphi_n | f(t) \rangle = 0$ for $n \in \{1,2,3\}$ and consequently $t^{\tau(\varphi)} = t^\varphi$. Hence

$$\mathcal{U}^{-1}\lambda_n \mathcal{U} = \langle \varphi_n | \tau^{-1}(\lambda)\rangle - \lambda_n^{\mathrm{Pek}} = \lambda_n + \langle \varphi_n | f(t^\lambda)\rangle - \lambda_n^{\mathrm{Pek}} \tag{4.4.12}$$

and therefore $\mathcal{U}^{-1} t^\lambda \mathcal{U} = (\langle \varphi_1 | \tau^{-1}(\lambda)\rangle - \lambda_1^{\mathrm{Pek}}, \dots, \langle \varphi_3 | \tau^{-1}(\lambda)\rangle - \lambda_3^{\mathrm{Pek}}) = (\lambda_1, \dots, \lambda_3) = t^\lambda$. Defining the matrix $(J_{t,\epsilon})_{n,m} := \langle \varphi_n | J_{t,\epsilon} | \varphi_m \rangle$ we furthermore have

$$\mathcal{U}^{-1} J_{t^\lambda,\alpha^{-s}}\big[\tau\big(\lambda + \lambda^{\mathrm{Pek}}\big)\big]\mathcal{U} = J_{t^\lambda,\alpha^{-s}}\big[\lambda\big] = \sum_{n,m=4}^{N} \big(J_{t^\lambda,\alpha^{-s}}\big)_{n,m} \lambda_n \lambda_m$$

as well as $\mathcal{U}^{-1} i\partial_{\lambda_n} \mathcal{U} = i\partial_{\lambda_n}$ for $3 < n \leqslant N$, which immediately follows from the observation that Ξ is a $t^\lambda = (\lambda_1, \lambda_2, \lambda_3)$-dependent shift. In the following let us extend $\{\varphi_1, \dots, \varphi_N\}$ to an orthonormal basis $\{\varphi_n : n \in \mathbb{N}\}$ of $L^2(\mathbb{R}^3)$ and introduce $a_n := a(\varphi_n)$ for all $n \in \mathbb{N}$, and let us extend the action of $\mathcal{U}$ to all of $\mathcal{F}(L^2(\mathbb{R}^3))$ such that $\mathcal{U}^{-1} a_n \mathcal{U} = a_n$ for $n > N$. Defining $\Psi'_\alpha := \mathcal{U}^{-1}\Psi^*_\alpha$, we obtain by Eq. (4.4.11)

$$\begin{aligned} E_{\alpha,\Lambda}(\alpha^2 p) \geqslant e_p^{\mathrm{Pek}} + \Big\langle \Psi'_\alpha \Big| &- \frac{1}{4\alpha^4}\sum_{n=1}^{3} \mathcal{U}^{-1}\partial_{\lambda_n}^2 \mathcal{U} - \frac{1}{4\alpha^4}\sum_{n=4}^{N} \partial_{\lambda_n}^2 + \sum_{n,m=4}^{N} \big(J_{t^\lambda,\alpha^{-s}}\big)_{n,m} \lambda_n \lambda_m \\ &+ \frac{1}{2}\mathcal{N}_{>N} - \mathcal{U}^{-1}\frac{p}{m}\Upsilon_\Lambda \mathcal{U}\Big|\Psi'_\alpha\Big\rangle - \frac{N}{2\alpha^2} + O_{\alpha\to\infty}\big(\alpha^{-(2+w)}\big). \end{aligned} \tag{4.4.13}$$

Using Eq. (4.4.12) and $\mathcal{U}^{-1} i\partial_{\lambda_n} \mathcal{U} = i\partial_{\lambda_n}$ for $3 < n \leqslant N$, we further obtain the transformation law $\mathcal{U}^{-1} a_n \mathcal{U} = a_n + \langle \varphi_n | f(t^\lambda) - \Pi\varphi^{\mathrm{Pek}}\rangle$ for all $n > 3$.

In order to express $\mathcal{U}^{-1}\frac{p}{m}\Upsilon_\Lambda \mathcal{U}$, let us introduce the operators c_n defined as $c_n := \frac{1}{2\alpha^2}\mathcal{U}^{-1}\partial_{\lambda_n}\mathcal{U}$ for $n \in \{1,2,3\}$ and $c_n := a_n$ for $n > 3$, as well as $g(t) := f(t) - \Pi\varphi^{\mathrm{Pek}} + \sum_{n=1}^{3} t_n \varphi_n \in \Pi L^2(\mathbb{R}^3)$ and $g_n(t) := \langle \varphi_n | g(t)\rangle$. With these definitions at hand we obtain

$$\begin{aligned} \mathcal{U}^{-1} a_n \mathcal{U} &= \mathcal{U}^{-1}\left(\frac{1}{2\alpha^2}\partial_{\lambda_n} + \lambda_n\right)\mathcal{U} = \frac{1}{2\alpha^2}\mathcal{U}^{-1}\partial_{\lambda_n}\mathcal{U} + \lambda_n = c_n + g_n\big(t^\lambda\big), \text{ for } 1 \leqslant n \leqslant 3, \\ \mathcal{U}^{-1} a_n \mathcal{U} &= a_n + \langle \varphi_n | f(t^\lambda) - \Pi\varphi^{\mathrm{Pek}}\rangle = c_n + g_n\big(t^\lambda\big), \text{ for } 4 \leqslant n \leqslant N \end{aligned}$$

and $\mathcal{U}^{-1} a_n \mathcal{U} = c_n = c_n + g_n\big(t^\lambda\big)$ for $n > N$, and therefore $\mathcal{U}^{-1} a_n \mathcal{U} = c_n + g_n\big(t^\lambda\big)$ for all $n \in \mathbb{N}$. In the following we want to think of c_n as being a variable of magnitude α^{-1} and t^λ as being of order α^{-r} for some $r > 0$, and consequently we think of $g_n\big(t^\lambda\big)$ as being of order α^{-r} as well, since $g(0) = 0$. While the former will be a consequence of the proof presented below, the control on t^λ follows from our assumption that we have condensation with respect to the state φ^{Pek}.

In the following we want to show that for suitable $w, w' > 0$, $\frac{p}{m}\Upsilon_\Lambda$ is bounded by $\epsilon\left(-\frac{1}{4\alpha^4}\sum_{n=1}^{3}\mathcal{U}^{-1}\partial_{\lambda_n}^2\mathcal{U} + \sum_{n=4}^{N} a_n^\dagger a_n + \mathcal{N}_{>N}\right)$ with $\epsilon = \alpha^{-w'}$, up to a term of negligible magnitude, see Eq. (4.4.16). Since $-\frac{1}{4\alpha^4}\sum_{n=1}^{3}\mathcal{U}^{-1}\partial_{\lambda_n}^2\mathcal{U}$ and $\mathcal{N}_{>N}$ appear in the expression on the right hand side of Eq. (4.4.13) as well, and since they are non-negative, this will leave us with the study of $-\frac{1}{4\alpha^4}\sum_{n=4}^{N}\partial_{\lambda_n}^2 + \sum_{n,m=4}^{N}\big(J_{t^\lambda,\alpha^{-s}}\big)_{n,m}\lambda_n\lambda_m - \epsilon\sum_{n=4}^{N} a_n^\dagger a_n$ for a lower bound on the expression on the right hand side of Eq. (4.4.13). Using the representation

$\frac{p}{m}\Upsilon_\Lambda = \sum_{n,m=1}^{\infty} \langle \varphi_n | \frac{p}{i\,m}\widetilde{\nabla}_{x_1}|\varphi_m\rangle\, a_n^\dagger a_m$, we obtain

$$\mathcal{U}^{-1}\frac{p}{m}\Upsilon_\Lambda\mathcal{U} = \sum_{n,m=1}^{\infty}\langle\varphi_n|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}|\varphi_m\rangle \left(c_n + g_n\big(t^\lambda\big)\right)^\dagger \left(c_m + g_m\big(t^\lambda\big)\right)$$
$$= \sum_{n,m=1}^{\infty}\langle\varphi_n|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}|\varphi_m\rangle\, c_n^\dagger c_m + \sum_{n,m=1}^{\infty}\langle\varphi_n|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}|\varphi_m\rangle \left(c_n^\dagger\, g_m\big(t^\lambda\big) + g_n\big(t^\lambda\big)\; c_m\right), \tag{4.4.14}$$

where we have used $\sum_{n,m=1}^{\infty}\langle\varphi_n|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}|\varphi_m\rangle\, g_n\big(t^\lambda\big)\, g_m\big(t^\lambda\big) = \langle g\big(t^\lambda\big)\,|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}|g\big(t^\lambda\big)\rangle = 0$, see the comment below Eq. (4.4.7). Using the bound on the operator norm $\|\frac{p}{m}\widetilde{\nabla}_{x_1}\|_{\mathrm{op}} \leqslant \frac{|p|}{m}3\Lambda = \frac{|p|}{m}3\alpha^{\frac{4}{5}(1+\sigma)} \lesssim \alpha^{\frac{4}{5}(1+\sigma)-1}$ yields

$$\pm\sum_{n,m=1}^{\infty}\langle\varphi_n|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}|\varphi_m\rangle\, c_n^\dagger c_m \lesssim \alpha^{\frac{4}{5}(1+\sigma)-1}\sum_{n=1}^{\infty} c_n^\dagger c_n. \tag{4.4.15}$$

For the bound in Eq. (4.4.15) it is essential that we are using the truncated momentum Υ_Λ defined in terms of the bounded operator $\widetilde{\nabla}_{x_1}$ instead of the unbounded operator ∇_{x_1}. Defining the coefficients $h_n(t) := \sum_{m=1}^{\infty}\langle\varphi_n|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}|\varphi_m\rangle\, g_m(t)$ and applying Cauchy–Schwarz furthermore yields for all $\epsilon > 0$

$$\pm\sum_{n,m=1}^{\infty}\langle\varphi_n|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}|\varphi_m\rangle \left(c_n^\dagger\, g_m\big(t^\lambda\big) + g_n\big(t^\lambda\big)\; c_m\right) = \sum_{n=1}^{\infty}\left(c_n^\dagger h_n\big(t^\lambda\big) + \overline{h_n(t^\lambda)}c_n\right)$$
$$\leqslant \epsilon\sum_{n=1}^{\infty} c_n^\dagger c_n + \epsilon^{-1}\sum_{n=1}^{\infty}\left|h_n\big(t^\lambda\big)\right|^2 = \epsilon\sum_{n=1}^{\infty} c_n^\dagger c_n + \epsilon^{-1}\left\|\frac{p}{m}\widetilde{\nabla}_{x_1} g\big(t^\lambda\big)\right\|^2.$$

Note that $\left\|\frac{p}{m}\widetilde{\nabla}_{x_1} g(t)\right\| \leqslant \frac{|p|}{m}\|\nabla g(t)\|$. Making use of $\nabla g(t) = \nabla\Pi\eta(t)$ with

$$\eta(t) := \chi\left(|t| < \delta_*\right)\left(\varphi_{x_t}^{\mathrm{Pek}} - \varphi^{\mathrm{Pek}}\right) + \chi\left(\delta_* \leqslant |t|\right)\left(\sum_{n=1}^{3} t_n \frac{\nabla_{x_n}\varphi^{\mathrm{Pek}}}{\|\Pi\nabla_{x_n}\varphi^{\mathrm{Pek}}\|} - \varphi^{\mathrm{Pek}}\right),$$

we obtain $\|\nabla g(t)\| \lesssim \|\nabla\eta(t)\| + \alpha^{-4(1+\sigma)}\|\eta(t)\|$ by Lemma 4.5.3. Using again $\varphi^{\mathrm{Pek}} \in H^2(\mathbb{R}^3)$, we have $\|\eta(t)\| + \|\nabla\eta(t)\| \lesssim 1 + |t|$, as well as $\|\nabla\eta(t)\| = \|\nabla\varphi_{x_t}^{\mathrm{Pek}} - \nabla\varphi^{\mathrm{Pek}}\| \leqslant |x_t|\|\Delta\varphi^{\mathrm{Pek}}\| \lesssim |t|$ for $|t| < \delta_*$. Consequently, $\left\|\frac{p}{m}\widetilde{\nabla}_{x_1} g(t)\right\| \leqslant C_0|p|\left(|t| + \alpha^{-4(1+\sigma)}(1+|t|)\right)$ for a suitable constant C_0. The choice $\epsilon := \alpha^{-\min\{\frac{r}{2},1\}}$ yields for α large enough

$$\pm\mathcal{U}^{-1}\frac{p}{m}\Upsilon_\Lambda\mathcal{U} \leqslant \alpha^{-w'}\sum_{n=1}^{\infty} c_n^\dagger c_n + C_0 C^2\left(\alpha^{-2}\alpha^{\min\{\frac{r}{2},1\}}\left|t^\lambda\right|^2 + \alpha^{-5-4\sigma}\left(1 + \left|t^\lambda\right|\right)^2\right) \tag{4.4.16}$$

with $w' < \min\{\frac{r}{2}, 1 - \frac{4}{5}(1+\sigma)\}$. In the following let α be large enough such that $\alpha^{-w'} \leqslant \frac{1}{2}$. Then we have

$$\alpha^{-w'}\sum_{n\notin\{4,\dots,N\}} c_n^\dagger c_n = \alpha^{-w'}\left(\sum_{n>N} a_n^\dagger a_n - \frac{1}{4\alpha^4}\sum_{n=1}^{3}\mathcal{U}^{-1}\partial_{\lambda_n}^2\mathcal{U}\right) \leqslant \frac{1}{2}\mathcal{N}_{>N} - \frac{1}{4\alpha^4}\sum_{n=1}^{3}\mathcal{U}^{-1}\partial_{\lambda_n}^2\mathcal{U}.$$

Using Eq. (4.4.13), Eq. (4.4.16) and $\langle \Psi'_\alpha||t^\lambda|^2|\Psi'_\alpha\rangle = \langle \widetilde{\Psi}_\alpha||t^\lambda|^2|\widetilde{\Psi}_\alpha\rangle \leqslant \langle \widetilde{\Psi}_\alpha|\mathcal{N}|\widetilde{\Psi}_\alpha\rangle + \frac{3}{2\alpha^2} \leqslant \alpha^{-r} + \frac{3}{2\alpha^2}$, see Theorem 4.3.7 for the last estimate, we obtain for a suitable $w > 0$

$$
\begin{aligned}
E_{\alpha,\Lambda}(\alpha^2 p) \geqslant e_p^{\mathrm{Pek}} + \Big\langle \Psi'_\alpha \Big| &- \frac{1}{4\alpha^4}\sum_{n=4}^{N} \partial_{\lambda_n}^2 + \sum_{n,m=4}^{N} \left(J_{t^\lambda,\alpha^{-s}}\right)_{n,m} \lambda_n \lambda_m \\
&- \alpha^{-w'} \sum_{n=4}^{N} a_n^\dagger a_n \Big| \Psi'_\alpha \Big\rangle - \frac{N}{2\alpha^2} + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right) \\
= e_p^{\mathrm{Pek}} + \left(1 - \alpha^{-w'}\right) &\Big\langle \Psi'_\alpha \Big| \mathbb{Q}_{t^\lambda,\alpha^{-s}}^{\alpha^{-w'}} - \frac{N}{2\alpha^2} \Big| \Psi'_\alpha \Big\rangle + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right)
\end{aligned}
$$

with $\mathbb{Q}_{t,\epsilon}^{\kappa} := -\frac{1}{4\alpha^4}\sum_{n=4}^{N} \partial_{\lambda_n}^2 + \frac{1}{1-\kappa}\sum_{n,m=4}^{N}\Big(\left(J_{t,\epsilon}\right)_{n,m} - \kappa\delta_{n,m}\Big)\lambda_n\lambda_m$, where we made use of the fact that $\sum_{n=4}^{N} a_n^\dagger a_n = -\frac{1}{4\alpha^4}\sum_{n=4}^{N}\partial_{\lambda_n}^2 + \sum_{n=4}^{N}\lambda_n^2 - \frac{N-3}{2\alpha^2}$.

4.4.3 Properties of the Harmonic Oscillators $\mathbb{Q}_{t,\epsilon}^{\kappa}$

Let π be the projection from Definition 4.4.3 and note that $J_{t,\epsilon} \geqslant c\,\pi$ for suitable $c > 0$, ϵ small enough and α large enough by [17, Lemma B.5]. Therefore $\mathbb{Q}_{t,\alpha^{-s}}^{\alpha^{-w'}} \geqslant 0$ for α large enough. Since $J_{t,\epsilon} \leqslant 1$, we furthermore have $(1-\kappa)\inf\sigma\left(\mathbb{Q}_{t,\epsilon}^{\kappa}\right) \leqslant \frac{N}{2\alpha^2} \lesssim \alpha^{-2}\left(\frac{\Lambda}{\ell}\right)^3 \leqslant \alpha^q$ for a suitable exponent q, see Definition 4.4.1. Combining this with the estimate $\langle \Psi'_\alpha|1-\mathbb{B}|\Psi'_\alpha\rangle = \langle \widetilde{\Psi}_\alpha|1-\mathbb{B}|\widetilde{\Psi}_\alpha\rangle \leqslant e^{-\beta\alpha^{2-2s}}$ for a suitable $\beta > 0$, where $\mathbb{B} := \chi(|t^\lambda| < \alpha^{-s})$, see Eq. (4.4.6), yields

$$
\inf_{|t|<\alpha^{-s}} \inf\sigma\left(\mathbb{Q}_{t,\alpha^{-s}}^{\alpha^{-w'}}\right)\langle \Psi_\alpha|\mathbb{B}|\Psi_\alpha\rangle \geqslant \inf_{|t|<\alpha^{-s}} \inf\sigma\left(\mathbb{Q}_{t,\alpha^{-s}}^{\alpha^{-w'}}\right) + O_{\alpha\to\infty}\left(\alpha^q e^{-\beta\alpha^{2-2s}}\right).
$$

Therefore we obtain for a suitable $w > 0$

$$
\begin{aligned}
E_{\alpha,\Lambda}(\alpha^2 p) &\geqslant e_p^{\mathrm{Pek}} + \left(1-\alpha^{-w'}\right)\Big\langle \Psi'_\alpha \Big| \mathbb{Q}_{t^\lambda,\alpha^{-s}}^{\alpha^{-w'}}\mathbb{B} - \frac{N}{2\alpha^2}\Big|\Psi'_\alpha\Big\rangle + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right) \\
&\geqslant e_p^{\mathrm{Pek}} + \left(1-\alpha^{-w'}\right)\left(\inf_{|t|<\alpha^{-s}}\inf\sigma\left(\mathbb{Q}_{t,\alpha^{-s}}^{\alpha^{-w'}}\right)\langle\Psi_\alpha|\mathbb{B}|\Psi_\alpha\rangle - \frac{N}{2\alpha^2}\right) + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right) \\
&\geqslant e_p^{\mathrm{Pek}} + \left(1-\alpha^{-w'}\right)\left(\inf_{|t|<\alpha^{-s}}\inf\sigma\left(\mathbb{Q}_{t,\alpha^{-s}}^{\alpha^{-w'}}\right) - \frac{N}{2\alpha^2}\right) + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right). \qquad (4.4.17)
\end{aligned}
$$

Since $\mathbb{Q}_{t,\epsilon}^{\kappa}$ is a harmonic oscillator, we can write its ground state energy explicitly as

$$
\begin{aligned}
\inf\sigma\left(\mathbb{Q}_{t,\epsilon}^{\kappa}\right) &= \frac{1}{2\alpha^2}\mathrm{Tr}_{\Pi L^2(\mathbb{R}^3)}\sqrt{\frac{J_{t,\epsilon}-\kappa\pi}{1-\kappa}} \\
&= \inf\sigma\left(\mathbb{Q}_{t,\epsilon}^{0}\right) + \frac{1}{2\alpha^2}\mathrm{Tr}_{\Pi L^2(\mathbb{R}^3)}\left[\sqrt{\frac{J_{t,\epsilon}-\kappa\pi}{1-\kappa}} - \sqrt{J_{t,\epsilon}}\right].
\end{aligned}
$$

Using $J_{t,\epsilon}\pi = J_{t,\epsilon}$, and therefore $[J_{t,\epsilon},\pi] = 0$, and again the fact that $J_{t,\epsilon} \geqslant c\,\pi$ for ϵ small enough and α large enough, as well as $|\sqrt{x}-\sqrt{y}| \leqslant \frac{1}{\sqrt{c}}|x-y|$ for $x \geqslant 0$ and $y \geqslant c$, we obtain for such ϵ, α, and $\kappa \leqslant c$

$$
\begin{aligned}
\pm\mathrm{Tr}_{\Pi L^2(\mathbb{R}^3)}\left[\sqrt{\frac{J_{t,\epsilon}-\kappa\pi}{1-\kappa}} - \sqrt{J_{t,\epsilon}}\right] &\leqslant \frac{1}{\sqrt{c}}\mathrm{Tr}_{\Pi L^2(\mathbb{R}^3)}\left|\frac{J_{t,\epsilon}-\kappa\pi}{1-\kappa} - J_{t,\epsilon}\right| \\
= \frac{\kappa}{\sqrt{c}(1-\kappa)}\mathrm{Tr}\left|J_{t,\epsilon}-\pi\right| &= \frac{\kappa(1+\epsilon)}{\sqrt{c}(1-\kappa)}\mathrm{Tr}\left[K^{\mathrm{Pek}} + \epsilon L^{\mathrm{Pek}}\right] \lesssim \frac{\kappa}{1-\kappa},
\end{aligned}
$$

where we have used that K^{Pek} and L^{Pek} defined in Definition 4.4.3 are trace-class. Combining what we have so far with the bound

$$\inf \sigma\left(\mathbb{Q}^0_{t,\epsilon}\right) \geqslant \frac{N}{2\alpha^2} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1-\sqrt{H^{\mathrm{Pek}}}\right] - D\left(\alpha^{-2}\epsilon + \alpha^{-\left(2+\frac{1}{5}\right)}\right)$$

for small ϵ, $|t| < \epsilon$ and large α, and a suitable $D > 0$, see [17, Lemma B.5], yields

$$\inf_{|t|<\alpha^{-s}} \inf \sigma\left(\mathbb{Q}^{\alpha^{-w'}}_{t,\alpha^{-s}}\right) - \frac{N}{2\alpha^2} + \frac{1}{2\alpha^2}\mathrm{Tr}\left[1-\sqrt{H^{\mathrm{Pek}}}\right] \gtrsim -\left(\alpha^{-(2+s)} + \alpha^{-\left(2+\frac{1}{5}\right)} + \alpha^{-(2+w')}\right).$$

In combination with Eq. (4.4.17) we therefore obtain for a suitable $w > 0$

$$E_{\alpha,\Lambda}(\alpha^2 p) \geqslant e^{\mathrm{Pek}}_p - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1-\sqrt{H^{\mathrm{Pek}}}\right] + O_{\alpha\to\infty}\left(\alpha^{-(2+w)}\right),$$

which concludes the proof of Eq. (4.2.3).

4.5 Auxiliary Results

Lemma 4.5.1. *Let $g(k) := \chi^1(K^{-1}|k| \leqslant 2)k$ for $k \in \mathbb{R}$. Then there exists a constant $C > 0$ such that for any bounded function $f : \mathbb{R} \to \mathbb{R}$ with $f' \in L^2(\mathbb{R})$ and $K > 0$, the double commutator is bounded by*

$$\left\|\left[\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), f(t)\right], f(t)\right]\right\|_{\mathrm{op}} \leqslant C\|f'\|^2,$$

where we write $f(t)$ for the multiplication operator with respect to the function $t \mapsto f(t)$. Furthermore we can choose the constant $C > 0$ such that $\left\|\left[g(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}), f(t)\right]\right\|_{\mathrm{op}} \leqslant C\sqrt{K}\|f'\|$.

Proof. Let us start by defining the sequence $f_n(t) := \chi^1\left(\frac{|t|}{n} \leqslant 2\right) f(t)$, which is compactly supported and therefore $f_n \in H^1(B_R(0))$ by our assumptions. Hence there exist smooth and compactly supported $\widetilde{f}_n$ such that $\|f_n - \widetilde{f}_n\|_\infty + \|(f_n)' - (\widetilde{f}_n)'\| \underset{n\to\infty}{\longrightarrow} 0$. Clearly the sequence $\widetilde{f}_n$ is uniformly bounded and approximates $f(t)$ in the strong operator topology, and consequently $\left[\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), \widetilde{f}_n(t)\right], \widetilde{f}_n(t)\right]$ approximates $\left[\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), f(t)\right], f(t)\right]$ in the strong operator topology as well. Hence $\left\|\left[\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), f(t)\right], f(t)\right]\right\|_{\mathrm{op}}$ is bounded from above by $\limsup_{n\to\infty}\left\|\left[\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), \widetilde{f}_n(t)\right], \widetilde{f}_n(t)\right]\right\|_{\mathrm{op}}$. Together with the observation $\|f' - (\widetilde{f}_n)'\| \underset{n\to\infty}{\longrightarrow} 0$, we can therefore assume w.l.o.g. that f is smooth and compactly supported.

Going to Fourier space and defining $M(k,k') := \sup_p \left|g(p+k+k') - g(p+k) - g(p+k') + g(p)\right|$, we can write

$$2\pi\left\|\left[\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), f(t)\right], f(t)\right]\right\|_{\mathrm{op}} = \left\|\int\int \widehat{f}(k)\widehat{f}(k')e^{it(k+k')}\left(g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t} + k + k'\right)\right.\right.$$
$$\left.\left. - g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t} + k\right) - g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t} + k'\right) + g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right)\right)\mathrm{d}k\mathrm{d}k'\right\|_{\mathrm{op}} \leqslant \iint \left|\widehat{f}(k)\widehat{f}(k')\right| M(k,k')\mathrm{d}k\mathrm{d}k'$$
$$= \int_{|k'|\leqslant K}\int_{|k|\leqslant K} \left|k\widehat{f}(k)k'\widehat{f}(k')\right| \frac{M(k,k')}{|kk'|}\mathrm{d}k\mathrm{d}k' + 2\int_{|k'|\leqslant K}\int_{|k|>K} \left|\widehat{f}(k)k'\widehat{f}(k')\right| \frac{M(k,k')}{|k'|}\mathrm{d}k\mathrm{d}k'$$
$$+ \int_{|k'|>K}\int_{|k|>K} \left|\widehat{f}(k)\widehat{f}(k')\right| M(k,k')\mathrm{d}k\mathrm{d}k'.$$

Making use of the fact that $\left|\frac{M(k,k')}{kk'}\right| \leqslant \|g''\|_\infty \lesssim \frac{1}{K}$, $\left|\frac{M(k,k')}{k'}\right| \leqslant 2\|g'\|_\infty \lesssim 1$ and $|M(k,k')| \leqslant 4\|g\|_\infty \lesssim K$, we obtain

$$\begin{aligned}
2\pi \|[[g(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}), f(t)], f(t)]\|_{\mathrm{op}} &\lesssim \frac{1}{K}\left(\int_{|k|\leqslant K} |k\widehat{f}(k)|\mathrm{d}k\right)^2 \\
&+ 2\int_{|k'|\leqslant K} |k'\widehat{f}(k')|\mathrm{d}k' \int_{|k|>K} \frac{1}{|k|}|k\widehat{f}(k)|\mathrm{d}k + K\left(\int_{|k|>K} \frac{1}{|k|}|k\widehat{f}(k)|\mathrm{d}k\right)^2 \\
&\leqslant \frac{2}{K}\left(\int_{|k|\leqslant K} |k\widehat{f}(k)|\mathrm{d}k\right)^2 + 2K\left(\int_{|k|>K} \frac{1}{|k|}|k\widehat{f}(k)|\mathrm{d}k\right)^2 \\
&\leqslant \|f'\|^2\left(\frac{2}{K}\int_{|k|\leqslant K} \mathrm{d}k + 2K\int_{|k|>K} \frac{1}{|k|^2}\mathrm{d}k\right) \leqslant 8\|f'\|^2.
\end{aligned}$$

In order to estimate the operator norm of $[g(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}), f(t)]$, we can assume as above that f is smooth and compactly supported. We compute

$$\begin{aligned}
\sqrt{2\pi}\left\|\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), f(t)\right]\right\|_{\mathrm{op}} &\leqslant \int \left|\widehat{f}(k)\right| \left\|g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t} + k\right) - g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right)\right\|_{\mathrm{op}} \mathrm{d}k \\
&\leqslant \|g'\|_\infty \int_{|k|\leqslant K} \left|k\widehat{f}(k)\right|\mathrm{d}k + 2\,\|g\|_\infty \int_{|k|>K} \frac{1}{|k|}\left|k\widehat{f}(k)\right|\mathrm{d}k \\
&\leqslant \sqrt{2K}\,\|g'\|_\infty\,\|f'\| + \sqrt{\frac{8}{K}}\,\|g\|_\infty\,\|f'\|.
\end{aligned}$$

Using $\|g'\|_\infty \lesssim 1$ and $\|g\|_\infty \lesssim K$ concludes the proof. ∎

Lemma 4.5.2. *For $K > 0$ we have the estimate $\|\chi(|\nabla| > K)\,\nabla\varphi^{\mathrm{Pek}}\| \lesssim \frac{1}{\sqrt{K}}$.*

Proof. We can write $\varphi^{\mathrm{Pek}} = 4\sqrt{\pi}\,(-\Delta)^{-\frac{1}{2}}\left|\psi^{\mathrm{Pek}}\right|^2$, where ψ^{Pek} is as in Definition 4.4.3. Hence the Fourier transform of $\nabla\varphi^{\mathrm{Pek}}$ reads $\widehat{\nabla\varphi^{\mathrm{Pek}}}(k) = \frac{ik}{|k|}\,\widehat{\left|\psi^{\mathrm{Pek}}\right|^2}(k)$, and therefore

$$\|\chi(|\nabla| > K)\,\nabla\varphi^{\mathrm{Pek}}\|^2 = \int_{|k|>K} \left|\widehat{\left|\psi^{\mathrm{Pek}}\right|^2}(k)\right|^2 \mathrm{d}k \leqslant \left\||k|^2\,\widehat{\left|\psi^{\mathrm{Pek}}\right|^2}(k)\right\|_\infty^2 \int_{|k|>K} \frac{1}{|k|^4}\mathrm{d}k \lesssim \frac{1}{K},$$

where we used $\psi^{\mathrm{Pek}} \in H^2(\mathbb{R}^3)$ and consequently $\left\||k|^2\,\widehat{\left|\psi^{\mathrm{Pek}}\right|^2}(k)\right\|_\infty < \infty$. ∎

Lemma 4.5.3. *With Π the projection defined in Definition 4.4.1, we have*

$$\|[|\nabla|, \Pi]\|_{\mathrm{op}} \lesssim \alpha^{-4(1+\sigma)}.$$

Proof. Using the Fourier transformation, we can write $\widehat{\Pi\varphi}(k) = \sum_{n=1}^N \langle f_n|\widehat{\varphi}\rangle\, f_n(k)$, with the help of non-negative functions f_n having pairwise disjoint support, which additionally satisfy $\|f_n\| = 1$ and $\mathrm{supp}\,(f_n) \subset B_{\sqrt{3}\alpha^{-4(1+\sigma)}}\left(z^n\right)$ for some $z^n \in \mathbb{R}^3$. Therefore

$$\widehat{[|\nabla|, \Pi]}\varphi(k) = \sum_{n=1}^N \left(\langle f_n|\widehat{\varphi}\rangle\,|k| - \left\langle f_n\middle|\widehat{|\nabla|\varphi}\right\rangle\right) f_n(k) = \sum_{n=1}^N \int f_n(k')\widehat{\varphi}(k')(|k| - |k'|)\,\mathrm{d}k' f_n(k).$$

Using that the functions f_n have disjoint support, as well as the fact that $||k| - |k'|| \leqslant 2\sqrt{3}\alpha^{-4(1+\sigma)}$ for $k, k' \in \operatorname{supp}(f_n)$, we obtain furthermore

$$\begin{aligned}\|[|\nabla|, \Pi]\varphi\|^2 &= \sum_{n=1}^{N} \int \left| \int f_n(k')\widehat{\varphi}(k')(|k| - |k'|)\, \mathrm{d}k' \right|^2 |f_n(k)|^2 \mathrm{d}k \\ &\leqslant 12\alpha^{-8(1+\sigma)} \sum_{n=1}^{N} \left| \int f_n(k')\, |\widehat{\varphi}(k')|\, \mathrm{d}k' \right|^2 \leqslant 12\alpha^{-8(1+\sigma)}\, \||\widehat{\varphi}|\|^2 = 12\alpha^{-8(1+\sigma)} \|\varphi\|^2,\end{aligned}$$

where we have used that f_n is an orthonormal system. ■

APPENDIX A

Molecular Impurities as a Realization of Anyons on the Two-Sphere

ABSTRACT. Studies on experimental realization of two-dimensional anyons in terms of quasiparticles have been restricted, so far, to only anyons on the plane. It is known, however, that the geometry and topology of space can have significant effects on quantum statistics for particles moving on it. Here, we have undertaken the first step towards realizing the emerging fractional statistics for particles restricted to move on the sphere, instead of on the plane. We show that such a model arises naturally in the context of quantum impurity problems. In particular, we demonstrate a setup in which the lowest-energy spectrum of two linear bosonic/fermionic molecules immersed in a quantum many-particle environment can coincide with the anyonic spectrum on the sphere. This paves the way towards experimental realization of anyons on the sphere using molecular impurities. Furthermore, since a change in the alignment of the molecules corresponds to the exchange of the particles on the sphere, such a realization reveals a novel type of exclusion principle for molecular impurities, which could also be of use as a powerful technique to measure the statistics parameter. Finally, our approach opens up a simple numerical route to investigate the spectra of many anyons on the sphere. Accordingly, we present the spectrum of two anyons on the sphere in the presence of a Dirac monopole field.

The study of quasiparticles with fractional statistics, called anyons, has been an active field of research in the past decades. This field has gained a lot of attention, due to the possible usage of these quasiparticles in quantum computation [60, 82, 42, 101]. In contrast to bosons and fermions, anyons acquire a phase $e^{i\pi\alpha}$ under the exchange of two particles, where the statistical parameter α is not necessarily an integer. The integer cases $\alpha = 0$ and $\alpha = 1$ represent bosons and fermions, respectively. For non-integer α, the transformation law $\Psi \to e^{i\pi\alpha}\Psi$ under the exchange of two particles, can only be realized by allowing the wave function Ψ to be multivalued. The idea is that the multiple values keep book of the different possible ways the particles could "braid" around each other. Due to the triviality of the braid group in $3+1$ dimensions, these particles are a purely low-dimensional phenomenon.

Although anyons are predicted to be realized in certain fractional quantum Hall systems [126, 64, 6, 121, 57, 46, 52, 83], they have not yet been unambiguously detected in experiment. Indeed there has been a recent upsurge in interest concerning the realization of anyons as emergent quasiparticles in experimentally feasible systems [25, 134, 135, 94, 127, 26]. For instance, it has been recently shown in Refs. [131, 132] how these quasiparticles emerge from impurities in standard condensed matter systems. Nevertheless, all these works focus on the particles moving on the two-dimensional plane, i.e., on $\mathbb{R}^2$. Since the theory of anyons and their statistical behavior are strongly dependent on the geometry and topology of the underlying space, investigations on curved spaces reveal novel features of quantum statistics [122, 31, 32, 109, 104, 124, 125, 111]. In particular, theoretical discussions of the fractional quantum Hall effect (FQHE) for systems having various geometry and topology have widened our understanding of the FQHE [53, 64].

In the present Letter, we explore the possibility of emerging fractional statistics for particles restricted to move on the sphere, $\mathbb{S}^2$, instead of on the plane. We show that such quasiparticles naturally arise from a system of impurities exchanging angular momentum with a many-particle bath. As a prototypical example, we consider two linear bosonic/fermionic molecules immersed in a quantum bath. In the regime of low energies, we identify the spectrum of this system with that of two anyons. This does not only allow us to realize anyons on the sphere, but also to open up various numerical approaches to investigate the spectrum of N anyons on the sphere. To illustrate this, we present the spectrum of two anyons on the sphere in the presence of a Dirac monopole field, extending the recent result of Ref. [104, 111]. Furthermore, the anyonic behavior of molecular impurities suggests that a novel type of exclusion principle holds, which concerns the alignment of the molecules, instead of the exchange of their actual position.

We start by considering a system of N free anyons on the two-sphere. The Hamiltonian is given by the sum of the Laplacian of the jth particle on the sphere: $H_0 = -\sum_{j=1}^{N} \nabla_j^2$, which acts on a multivalued wave function Ψ. By performing a singular gauge transformation, $\Psi \to e^{i\beta}\Psi$ (see Refs. [130, 96, 65, 103, 112]), one can get rid of the multivaluedness and the free anyon Hamiltonian on the sphere H_0 becomes equivalent to

$$H_{\text{anyon}} = -\sum_{j=1}^{N} \left(\nabla_j - iA_j\right)^2 \,, \tag{A.0.1}$$

which now acts on single valued bosonic/fermionic wave functions. Here anyons are depicted as bosons/fermions interacting with the magnetic gauge field A, which explains that the calculation of the anyonic spectra is very hard [84]. Note that $A = \nabla\beta$ is an almost pure gauge, up to the singularities of β, where the particles meet, and it can be found as the variational solution of the Chern-Simons (CS) Lagrangian $L_{\mathbb{S}^2} = \sum_j \left(A \cdot \dot{q}_j + A_0\right) - (4\pi\alpha)^{-1} \int_{\mathbb{S}^2} \mathrm{d}\Omega \; A \wedge \mathrm{d}A$, where q_j is the position of the nonrelativistic point particle coupled to the CS field, A_0 the time component of the gauge field, and $\wedge$ the wedge product. For anyons on the plane, one can always find a single magnetic potential A as a solution. However, due to the non trivial homology of $\mathbb{S}^2$, the CS Lagrangian on the sphere can only be solved in two different stereographic coordinate charts: north and south patches, A^N and A^S. As the fields A^N and A^S should be a single object in the overlap patch, we require them to be gauge equivalent. This equivalence is given by the Dirac quantization condition $(N-1)\alpha \in \mathbb{Z}$ [65, 103].

In what follows, in order to simplify our expressions, we represent the stereographic coordinates (x, y) as a complex number, $z = x + iy$. In these coordinates, we define the gauge transformation $F = e^{i\beta}$, with the exponent $\beta(z_1, .., z_N) = -i\alpha \sum\limits_{j<k} \log\left(\frac{z_j - z_k}{|z_j - z_k|}\right)$. The corresponding connections (gauge fields) can be written as
$A_{\bar{z}_j} = iD_{\bar{z}_j}\beta = -\frac{\alpha(1+|z_j|^2)}{2} \sum_{k\neq j} \left(\bar{z}_j - \bar{z}_k\right)^{-1}$ and $A_{z_j} = iD_{z_j}\beta = \frac{\alpha(1+|z_j|^2)}{2} \sum_{k\neq j} \left(z_j - z_k\right)^{-1}$,

where we encode the contribution from the metric on $\mathbb{S}^2$ in the following differential operators: $D_{\bar{z}_j} = (1+|z_j|^2)\partial_{\bar{z}_j}$ and $D_{z_j} = (1+|z_j|^2)\partial_{z_j}$; see Ref. [24]. In the language of connections, F represents the holonomy of A, and it is discontinuous along the lines which connect the particles with the north (south) pole, usually called the Dirac lines. Without loss of generality, we consider the north pole, which corresponds to the choice of $z_j = \cot(\theta_j/2)\exp(i\varphi_j)$, with spherical coordinates θ_j and φ_j. These lines represent the magnetic potential in the singular gauge, by assigning the particle an additional phase factor whenever it crosses them. The Dirac quantization condition makes sure that the Dirac lines are invisible, in the sense that one cannot distinguish between the theory where the lines run to the north pole and theories where they run to any other point. This means that our system is rotational invariant, up to gauge equivalences.

The anyon Hamiltonian in our complex stereographic coordinate system can be written as

$$H_{\text{anyon}} = -\sum_{j=1}^{N}\left(D_{z_j} - \bar{z}_j - A_{z_j}\right)\left(D_{\bar{z}_j} - A_{\bar{z}_j}\right) . \tag{A.0.2}$$

Direct calculations to investigate the spectra of H_{anyon} turn out to be problematic, when the spectrum is calculated from the bosonic end. This is due to the fact that the matrix elements of $A_{z_j}A_{\bar{z}_j}$ for certain bosonic states are singular, which is similar to the case of anyons on the plane [132]. To overcome this difficulty we will use a different representation of the free anyon Hamiltonian, with the help of the non-unitary singular pseudo-gauge transformation $\Psi \to e^{\alpha\sum_{j<k}\log(z_j - z_k)}\Psi$. The advantage is that one of the two magnetic potentials $A'_{\bar{z}} = \alpha D_{\bar{z}}\log(z)$ is zero, since $\log(z)$ is a holomorphic function. Therefore, the Hamiltonian simplifies to

$$H'_{\text{anyon}} = -\sum_{j=1}^{N}\left(D_{z_j} - \bar{z}_j - A'_{z_j}\right)D_{\bar{z}_j} . \tag{A.0.3}$$

The non-zero magnetic potential is given by $A'_{z_j} = 2A_{z_j}$. Note that H'_{anyon} is a similarity transformation of H_{anyon}, i.e., $H'_{\text{anyon}} = e^{\alpha\sum_{j<k}\log|z_j - z_k|}H_{\text{anyon}}e^{-\alpha\sum_{j<k}\log|z_j-z_k|}$, therefore these two operators have the same eigenvalues. The cost for the simplification is that H'_{anyon} is self-adjoint in a weighted L^2 space. As we discuss below, while the first form of the anyon Hamiltonian (A.0.2) allows us to realize anyons in natural quantum impurity setups, the Hamiltonian (A.0.3) provides powerful numerical techniques to calculate the spectra of anyons on the sphere within the simplified impurity models.

We will now consider a general impurity problem of N bosonic/fermionic impurities on $\mathbb{S}^2$ interacting with some Fock space $\mathcal{F}$. Within the Bogoliubov-Fröhlich theory [45, 13, 108], the impurity Hamiltonian is given by

$$\begin{aligned} H_{\text{imp}} = &-\sum_{j=1}^{N}\left(D_{z_j} - \bar{z}_j\right)D_{\bar{z}_j} + \sum_v \omega_v b_v^\dagger b_v \\ &+ \sum_v \lambda_v(z_1, .., z_N)\left(e^{-i\beta_v(z_1,..,z_N)}b_v^\dagger + e^{i\beta_v(z_1,..,z_N)}b_v\right) , \end{aligned} \tag{A.0.4}$$

where $b_v^\dagger, b_v$ are the bosonic creation and annihilation operators in $\mathcal{F}$, ω_v is the energy of the corresponding mode v, and the coefficients $\lambda_v(z_1, .., z_N)$ and $\beta_v(z_1, .., z_N)$ describe the interaction of the impurities with the Fock space, depending on their coordinates $z_1, .., z_N$. In the limit of $\omega_v \to \infty$ (the adiabatic limit), one can justify that the lowest spectrum of H_{imp} is described by the Born-Oppenheimer (BO) approximation; see Ref [132] for an analysis of this assumption in the planar case. The projection of the Hamiltonian to the smaller Hilbert space manifests itself as a minimal coupling of the otherwise free particles with effective magnetic potentials $A_{z_1}, .., A_{z_N}$ and a scalar potential Φ. Therefore, it is sufficient to understand how H_{imp} acts on the vacuum sector.

Accordingly, we first apply the transformation $S(z_1, .., z_N) = e^{-i\sum_v \beta_v b_v^\dagger b_v}$ to Eq. (A.0.4), and then project the transformed Hamiltonian onto the coherent state $|\varphi(z_1, .., z_N)\rangle = e^{-\frac{1}{\sqrt{2}}\sum_v \frac{\lambda_v}{\omega_v}(b_v^\dagger - b_v)}|0\rangle$. The emerging magnetic potential in complex coordinates is then given by

$$A_{z_j}^{imp} = i\sum_v \left(\frac{\lambda_v}{\omega_v}\right)^2 D_{z_j}\beta_v\,; \tag{A.0.5}$$

see Ref [132] for the details concerning the derivation of the emerging gauge field in the analogous planar case. Let us consider the specific choice $\beta_v(z_1, .., z_N) = -ip_v \sum_{j<k} \log\left(\frac{z_j - z_k}{|z_j - z_k|}\right)$, which results in $A_{z_j}^{\text{imp}} = \frac{\alpha(1+|z_j|^2)}{2}\sum_{k\neq j}(z_j - z_k)^{-1}$ with $\alpha(z_1, .., z_N) = \sum_v p_v \left(\frac{\lambda_v}{\omega_v}\right)^2$. We thus see that $A_{\bar{z}_j}^{\text{imp}}$ is the sought CS gauge field and obeys the Dirac quantization condition if $\alpha(z_1, .., z_N)$ is a constant and satisfies $(N-1)\alpha \in \mathbb{Z}$. We emphasize, however, that for the values of α which do not satisfy the Dirac quantization condition, the impurity Hamiltonian (A.0.4) is still well-defined. The only difference for these values is that the theory is no longer fully rotational invariant, but, instead, it is invariant under rotation around the z axis. In other words, the Dirac lines, which emerge together with the statistical gauge field, are not invisible [105] and they puncture the sphere. These features have drastic effects on the physical realization of anyons on the sphere in terms of quantum impurities, in comparison to emergent anyons on the plane studied in Ref. [132].

In general, the impurity Hamiltonian (A.0.4) corresponds to *interacting* anyons due the presence of the scalar potential Φ. An impurity Hamiltonian whose lowest-energy spectrum is governed by the anyon Hamiltonian in the pseudo-gauge (A.0.3), on the other hand, describes free anyons, as the scalar potential vanishes with $A_{\bar{z}} = 0$. Although such an impurity Hamiltonian is not Hermitian and may be harder to realize experimentally, considered as a toy model its non-Hermiticity is harmless for our purposes and it opens up simple numerical approaches to calculate the spectra of anyons on the sphere.

Our numerical tools work for an arbitrary number of particles. Nevertheless, we will here study only the two-anyon case, since the computational effort strongly scales with the number of particles. Furthermore, we investigate a configuration where the impurities are subjected to a Dirac monopole field B. This allows us to investigate the spectrum for all values of α, as the Dirac quantization condition in the presence of a Dirac monopole field is given by $2B - (N-1)\alpha \in \mathbb{Z}$ [104, 111]. Accordingly, we consider the following simple model

$$\begin{aligned} H'_{\text{imp}} &= H_B + \omega\left(b^\dagger b + \frac{\alpha}{p}\right) \\ &+ \sqrt{\frac{\alpha}{p}}\omega\left(e^{-p\log(z_1 - z_2)}b^\dagger + e^{p\log(z_1 - z_2)}b\right)\,, \end{aligned} \tag{A.0.6}$$

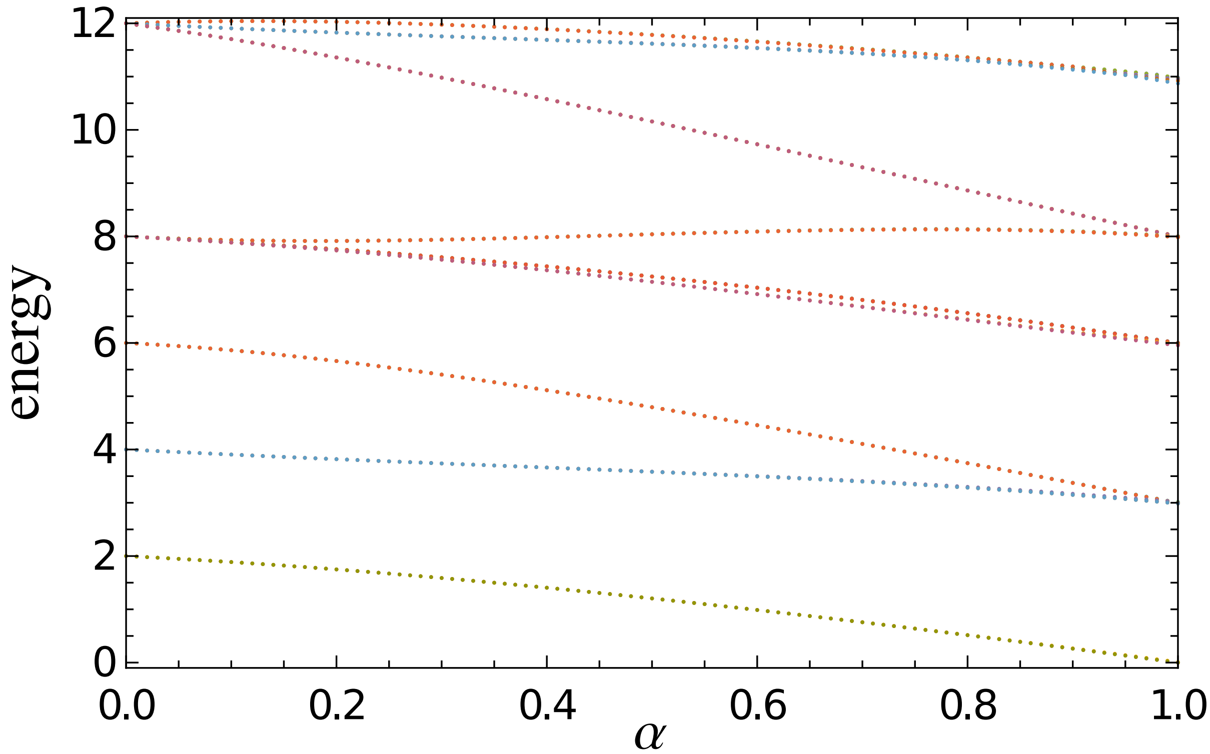

Figure A.1: Numerical computations of the energy of two anyons on the sphere in the presence of a Dirac monopole in terms of the relative statistics parameter, i.e., $\alpha = 0$ corresponds to fermions and $\alpha = 1$ to bosons. We set $2B = \alpha$ and consider spherical harmonics with the angular momentum up to $l_{\max} = 8$ for the numerics. Compare Fig. 1 in Ref. [111].

where the Hamiltonian $H_B = H_0 + \sum_{j=1}^{2} A_{z_j}^B D_{\bar{z}_j}$ governs the bosonic/fermionic particles interacting with the Dirac monopole field B generated by the gauge field $A_{z_j}^B = 2B\bar{z}_j$, p is an integer, and we subtracted the vacuum energy, $-\omega\alpha/p$, of the pure Fock space part of the Hamiltonian.

For a direct calculation, one could use, for instance, the orthonormal basis $|S(A); n\rangle$, where $|S(A)\rangle = |Y_{l_1,m_1} \otimes_{S(A)} Y_{l_2,m_2}\rangle$ are the impurity basis with $Y_{l,m}$ being the spherical harmonics, $\otimes_{S(A)}$ the (anti-)symmetric tensor product, and $|n\rangle$ the n-particle state in the Fock space. Then, one could calculate the lowest spectrum of H'_{imp} by diagonalizing the matrix $\langle S(A); n| H'_{\text{imp}} |S'(A'); n'\rangle$. Instead of this direct diagonalization technique, we first diagonalize the Fock space part of the Hamiltonian with the displacement operator. The anyon Hamiltonian (A.0.3) in the presence of a Dirac monopole field, which emerges in the limit of $\omega \to \infty$, is, then, given by

$$H'^B_{\text{anyon}} = H_B + \frac{\alpha}{p}\left(e^{p\log(z_1-z_2)} H_0 e^{-p\log(z_1-z_2)} - H_0\right) , \tag{A.0.7}$$

see Supplemental Material for the derivation. We underline that a similar form of the Hamiltonian (A.0.7) for anyons on the plane has been previously introduced in Ref. [132], where the second term of the right hand side was written in terms of composite bosons/fermions for an even integer p. Extending this approach we use here Bose-Fermi mixtures which enable us to set $p = 1$. Within such a simple choice Eq. (A.0.7) can be written as the following matrix equation

$$E^B_{\text{anyon}} = E_{\text{bos}} + 2B\, W_S + \alpha\left(Z^{-1} E_{\text{fer}} Z - E_{\text{bos}}\right) , \tag{A.0.8}$$

where the elements of the matrices are given by $E_{\text{bos}} = \langle S| H_0 |S'\rangle$, $E_{\text{fer}} = \langle A| H_0 |A'\rangle$, $W_S = \langle S| \sum_{j=1}^{2} \bar{z}_j D_{\bar{z}_j} |S'\rangle$, and $Z^{-1} = \langle S| z_1 - z_2 |A\rangle$. As the latter two terms are straightforward to calculate numerically, and the matrix Z can be obtained by taking the (pseudo)inverse of Z^{-1}, Eq. (A.0.8) opens up a powerful route to calculate the anyonic spectrum. The spectrum from the fermionic end in terms of the relative statistics parameter can be calculated simply with the replacement of the basis $|S(A)\rangle \rightarrow |A(S)\rangle$ in Eq. (A.0.8).

As an example, we compute the eigenvalues for α ranging from 0 to 1. For an easier comparison with the result existing in Ref. [111], we calculate the spectrum from the fermionic end. The result presented in Fig. A.1 is consistent with the one shown in Ref. [111], where the spectrum was calculated only for the subset of energy levels with unit total angular momentum.

The general form of the impurity Hamiltonian (A.0.4) allow us also to physically realize anyons on the sphere in terms of quantum impurities. First of all, the kinetic energy of the particles on the sphere, which is given by the Laplacian $-\left(D_{z_j} - \bar{z}_j\right) D_{\bar{z}_j}$, can be realized as the angular momentum operator $\boldsymbol{L}_j^2$. The latter can be considered as the Hamiltonian of linear molecules, which enables us to map rotation of molecules to motion of point particles on the sphere. Consequently, instead of point-like impurities, which have been considered for the planar case in Ref. [132], we consider here linear molecules and explore the angular momentum exchange with the bath. Such a realization exposes a novel correlation between molecular impurities. Specifically, the exchange of the particles on the sphere corresponds to a change in the alignment of the molecules, but not the exchange of the molecules themselves, see Fig. A.2 (Top). Therefore, the emerging statistical interaction manifests itself in the alignment of molecules.

To illustrate this in a transparent way, we consider the simple impurity Hamiltonian (A.0.6) in the absence of the Dirac monopole. We investigate the alignment $\langle (\cos\theta_1 - \cos\theta_2)^2 \rangle$ as a function of the statistics parameter for two molecules. In Fig. A.2 (Bottom) we present the alignment for the ground state, which is obtained from Eq. (A.0.8) for the case of $B = 0$. We note that the Hamiltonian is still well-defined for the values of α which do not satisfy the Dirac quantization condition as we discussed before. Thus, the alignment of the molecules could be used as an experimental measure of the statistics parameter. Such a measurement can be performed, for instance, within the technique of laser-induced molecular alignment [43, 66]. Further discussion of the alignment of molecules as a consequence of the statistical interaction will be the subject of future work.

A physical realization of the interaction between the molecules and a bath is also natural in the context of quantum impurity problems. Indeed, it was shown that the molecular impurities rotating in superfluid helium can be described within an impurity problem [113, 114, 67]. The resulting quasiparticle, which is called the angulon, represents a quantum impurity exchanging orbital angular momentum with a bath of quantum oscillators, and serves as a reliable model for the rotation of molecules in superfluids [68]. Therefore, we consider the following angulon Hamiltonian [133, 75]

$$\begin{aligned} H_{\text{angulon}} = &\sum_{j=1}^{2} \boldsymbol{L}_j^2 + V(q_1, q_2) + \sum_{k,l,m} \omega_{k,l,m} b_{k,l,m}^{\dagger} b_{k,l,m} \\ &+ \sum_{k,l,m} \lambda_{k,l,m}(q_1, q_2) \left(e^{-i\beta_{k,l,m}(q_1,q_2)} b_{k,l,m}^{\dagger} + \text{H.c.} \right) , \end{aligned} \tag{A.0.9}$$

where $\hat{b}_{k,l,m}^{\dagger}$ and $\hat{b}_{k,l,m}$ are the bosonic creation and annihilation operators written in the

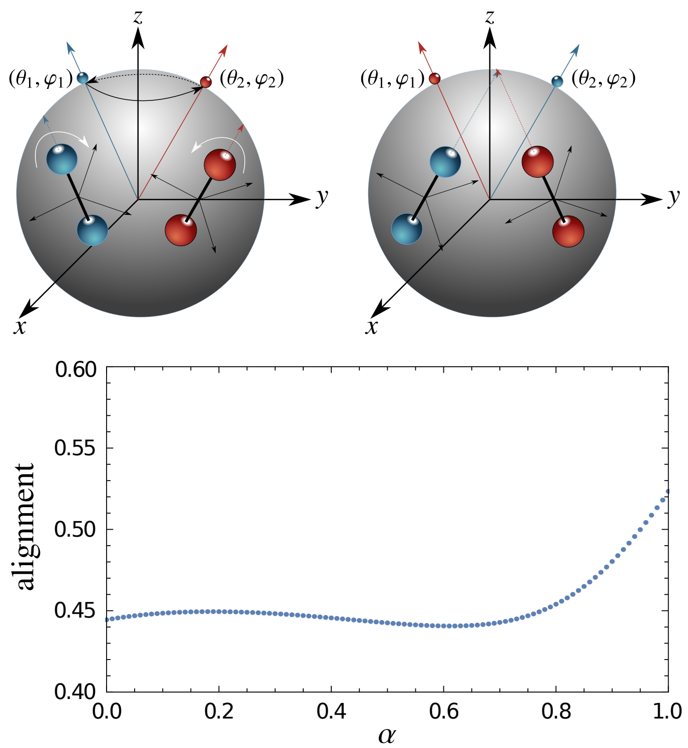

Figure A.2: (Top) Realization of anyons on the sphere in terms of linear molecules immersed in a quantum many-particle environment. A change in the alignment of the molecules (dumbbells), which is depicted by the white arrows, corresponds to the exchange of the particles on the sphere (dots), shown by the curvy black arrows. (Bottom) The alignment $\langle(\cos\theta_1 - \cos\theta_2)^2\rangle$ as a function of the absolute statistics parameter for the ground state. The curve follows the bosonic state $|Y_{0,0} \otimes_S Y_{0,0}\rangle$ at $\alpha = 0$ to the fermionic state $|Y_{1,0} \otimes_A Y_{0,0}\rangle$ at $\alpha = 1$. We consider spherical harmonics with the angular momentum up to $l_{\max} = 8$ for the numerics.

spherical basis [113], $q_i = (\theta_i, \varphi_i)$ are the angular coordinates representing the molecular rotation of the i-th molecule, V is a confining potential, and H.c. stands for Hermitian conjugate. Note that the coupling terms might depend on the intermolecular distance, as well. For heavy molecules the BO approximation can be justified with a gapped dispersion $\omega_{k,l,m}$. Furthermore, following our previous reasoning and Eq. (A.0.5), if the impurity-bath coupling satisfies the relation $i\sum_{k,l,m}\left(\frac{\lambda_{k,l,m}}{\omega_{k,l,m}}\right)^2 D_{z_j}\beta_{k,l,m} = A_{z_j}$, the lowest-energy spectrum of the two linear molecules immersed in the bath coincide with the spectrum of two anyons on the sphere. In principle, such an interaction is feasible with the state-of-art techniques in the physics of superfluid helium as well as ultracold molecules.

In order to present a simple and intuitive realization, we first neglect the intermolecular distance. This enables us to define the interaction term simply as $\lambda_{k,l,m}(q_1,q_2)e^{-i\beta_{k,l,m}(q_1,q_2)} = u_{k,l}\sum_{j=1}^{2} Y_{l,m}(q_j)$ with the impurity-bath coupling $u_{k,l}$. For a physical configuration, we consider molecular impurities in superfluid helium nanodroplets. The corresponding coupling captures the details of the molecule-helium interaction. For the form of the coupling and the relevant parameters we refer the reader to Supplemental Material and Ref. [22, 23], where the model has been used in order to describe angulon instabilities and oscillations observed in the experiment. Furthermore, the dispersion relation of superfluid helium allows us to achieve a gapped dispersion at the roton minimum ω_r [67]. Following the experimental realization

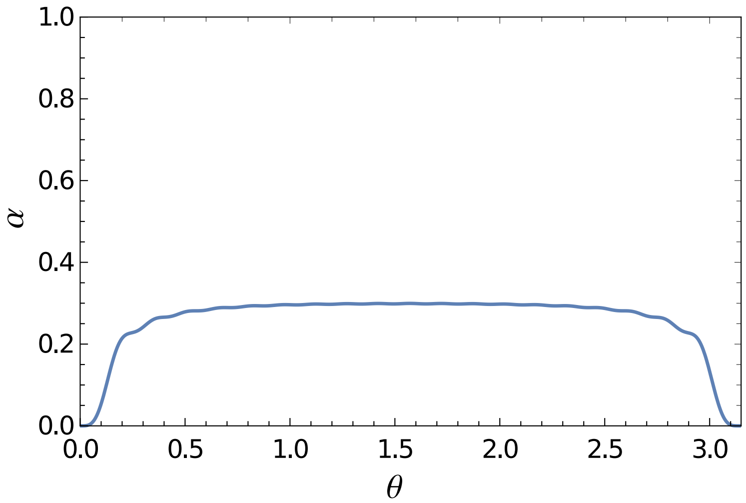

Figure A.3: The dependence of the statistical parameter α on the relative angle θ. The computation is performed for the parameters modeling the molecule-helium interaction, given in Supplemental Material. The other parameters are $\omega_r = 1$, $\Omega = 1.1$, and $l_{\text{max}} = 20$.

proposed in Ref. [132] for anyons on the plane, we also couple the impurities to an additional constant magnetic field and rotate the whole system at the cyclotron frequency Ω, which breaks time reversal symmetry so that anyons can emerge on the lowest-energy spectrum.

A priori, the emerging statistics parameter $\alpha = \alpha(\theta)$ depends on the relative angle θ between the points q_1 and q_2. However, with a careful choice of the model parameters, α becomes approximately constant with the condition $\Omega\, l_{\text{max}}/\omega_r \gg 1$, see Supplemental Material. The condition imposes that the cyclotron frequency should be at the order of the roton minimum. This implies that molecular impurities should be subjected to a strong magnetic field at the order of $M\omega_r$ with M being the mass of the molecules. The θ dependence of α is demonstrated in Fig. A.3. In general, the statistics parameter does not satisfy the Dirac quantization condition. Therefore, the molecular impurities correspond to anyons interacting with the magnetic potential depicted by the Dirac lines, with broken rotational symmetry. We also note that with the additional confining potential, V, the particles are confined to one of the half spheres so that the statistics parameter becomes accessible to the experiment.

Thus, we see that a system of two linear molecules exchanging angular momentum with a many-particle bath can give rise to a system of quasiparticles with anyonic statistics, and can be realized by considering molecular impurities in superfluid helium droplets. It would be interesting to continue this approach and investigate, whether one can generalize the results above e.g. to non-Abelian Chern-Simons particles with the help of a higher order Born-Oppenheimer approximation.

APPENDIX B

Characterisation of Gradient Flows for a given Functional

ABSTRACT. Let X be a vector field and Y be a co-vector field on a smooth manifold M. Does there exist a smooth Riemannian metric $g_{\alpha\beta}$ on M such that $Y_\beta = g_{\alpha\beta}X^\alpha$? The main result of this note gives necessary and sufficient conditions for this to be true. As an application of this result we show that a finite-dimensional ergodic Lindblad equation admits a gradient flow structure for the von Neumann relative entropy if and only if the condition of BKM-detailed balance holds.

B.1 Introduction

This paper deals with the following general question:

> *Let $X^\alpha \in \Gamma(TM)$ be a vector field and $Y_\beta \in \Gamma(T^*M)$ be a co-vector field on a smooth manifold M. Does there exist a smooth Riemannian metric $g_{\alpha\beta}$ on M such that $Y_\beta = g_{\alpha\beta}X^\alpha$?* [1]

Clearly, this is not always true: X^α and Y_β will have to satisfy some compatibility conditions. Firstly, X^α and Y_β need to have the same set of zeroes (critical points). Secondly, at all other points $m \in M$, they need to satisfy $X^\alpha Y_\alpha|_m > 0$. A third (and slightly less obvious) compatibility condition is obtained by differentiating the equation $Y_\beta = g_{\alpha\beta}X^\alpha$: at each critical point $m \in M$ there should exist a scalar product $\bar{g}_{\alpha\beta} \in T^*_m M \otimes_S T^*_m M$ such that $\nabla_\alpha Y_\gamma|_m = \bar{g}_{\beta\gamma}\nabla_\alpha X^\beta|_m$ for some (equivalently, any) connection ∇_α. This condition does not hold automatically: it represents a compatibility constraint on X^α and Y_β with a natural interpretation in some examples below.

While these three conditions are clearly necessary, it is not obvious that they are also sufficient. The main result of this paper shows that this is indeed the case, under mild smoothness and non-degeneracy assumptions; namely, at all critical points, we require non-degeneracy of the derivative of Y_β and we assume that X^α and Y_β are real analytic in suitable local coordinates; cf. Section B.2 for the details.

[1] Throughout the paper we use index notation and Einstein's summation convention. Greek letters denote abstract indices, Roman letters denotes concrete indices.

Theorem B.1.1 (Main result). *Let $X^\alpha \in \Gamma(TM)$ and $Y_\beta \in \Gamma(T^*M)$ satisfy Assumption B.2.1 below. Then there exists a metric $g_{\alpha\beta} \in \Gamma(T^*M \otimes T^*M)$ satisfying $Y_\beta = g_{\alpha\beta}X^\alpha$ if and only if the following conditions hold:*

(i) *For all $m \in M$ with $Y_\beta|_m \neq 0$ we have $X^\alpha Y_\alpha|_m > 0$;*

(ii) *For all $m \in M$ with $Y_\beta|_m = 0$ we have $X^\alpha|_m = 0$;*

(iii) *For all $m \in M$ with $Y_\beta|_m = 0$ there exists a scalar product $\bar{g}_{\alpha\beta} \in T^*_m M \otimes_S T^*_m M$ such that*

$$\nabla_\alpha Y_\gamma|_m = \bar{g}_{\beta\gamma}\nabla_\alpha X^\beta|_m.$$

The choice of the connection ∇ in *(iii)* is arbitrary.

We shall also prove a variant of this result where X^α and Y_β are of class C^{k+1} for some $k \in \mathbb{N}$. In this case, the metric $g_{\alpha\beta}$ is of class C^k; see Theorem B.2.6 below.

While Theorem B.1.1 is of independent interest, our motivation comes from an open question on gradient flow structures for dissipative quantum systems, that will be discussed below.

Let us first briefly sketch the structure of the proof. To prove the sufficiency of conditions *(i)–(iii)*, it suffices to construct a *local* metric around every point of M. The global metric can then be constructed using a partition of unity. Around non-critical points the construction is straightforward: in local coordinates, it corresponds to constructing a positive definite matrix that maps one given vector to another one. However, it is *not* trivial to construct a smooth metric satisfying $Y_\beta = g_{\alpha\beta}X^\alpha$ in a neighbourhood of a critical point.

To solve this problem, we assume that the sought metric has a power series expansion in a suitable chart around the critical point. We then derive an infinite hierarchy of tensor equations, which express power series coefficients of degree N in terms of coefficients of degree at most $N-1$ for $N \geqslant 1$. Solvability of the lowest order equation is guaranteed by compatibility condition *(iii)*. We then prove that higher order equations can be solved iteratively. Moreover, the norms of the solutions are exponentially bounded in the degree, which allows us to construct a convergent power series that satisfies the desired equation in a neighbourhood of the critical point.

Application to gradient structures

Consider now the special case where $Y \in \Gamma(T^*M)$ is the derivative of a smooth function $f \in C^\infty$, i.e, $Y_\beta = \nabla_\beta f$. Then our question becomes: *Does there exist a smooth Riemannian metric $g_{\alpha\beta}$ such that X is the gradient of f with respect to the metric g, i.e., $X^\alpha = g^{\alpha\beta}\nabla_\beta f$?* In other words, the question is whether the ODE $\dot{u} = -X(u)$ on M can be formulated as a gradient flow equation $\dot{u}(t) = -\nabla f\big(u(t)\big)$ for a suitable Riemannian metric. Our main result yields necessary and suffcient conditions.

Gradient flows describe motion in the direction of steepest descent of the function f in the geometry defined by the metric g. The identification of an ODE as a gradient flow equation is often fruitful, as there are powerful techniques available for the analysis of gradient flows [4].

As an application of our main result, we address an open question on the gradient flow structure of finite-dimensional dissipative quantum systems. To put this result into context, let us first discuss the corresponding classical setting.

Classical Markov semigroups

Consider an irreducible continuous-time Markov chain on a finite set $\mathcal{X}$ with transition rates $q_{xy} \geqslant 0$ for $x, y \in \mathcal{X}$ with $x \neq y$. The associated Markov semigroup $(P_t)_{t\geqslant 0}$ is a C_0-semigroup of positive operators on $\mathbb{R}^{\mathcal{X}}$ that preserves the constant functions. Its infinitesimal generator $L : \mathbb{R}^{\mathcal{X}} \to \mathbb{R}^{\mathcal{X}}$ is given by

$$\big(L\psi\big)(x) := \sum_{y\in\mathcal{X}} q_{xy}\big(\psi(y) - \psi(x)\big).$$

As time evolves, the marginal law of the Markov chain describes a curve $(\mu_t)_{t>0}$ in $\mathscr{P}_*(\mathcal{X})$, the simplex of probability densities with positive density. It evolves according to the Kolmogorov forward equation (KFE)

$$\partial_t \mu_t = L^* \mu_t, \qquad \text{where } \big(L^*\mu\big)(x) = \sum_{y\neq x} \mu(y) q_{yx} - \mu(x) q_{xy}$$

for $\mu \in \mathscr{P}(\mathcal{X})$. Let $\pi \in \mathscr{P}_*(\mathcal{X})$ be the unique stationary distribution. It is well known and easy to verify that the relative entropy

$$\mathrm{Ent}_\pi(\mu) := \sum_{x\in\mathcal{X}} \mu(x) \log\Big(\frac{\mu(x)}{\pi(x)}\Big)$$

decreases along trajectories of the KFE.

Much more is true if the Markov chain is *reversible*, i.e., the *detailed balance* condition $\pi_x q_{xy} = \pi_y q_{yx}$ holds for all $x \neq y$. Equivalently, this means that the generator L is selfadjoint in the Hilbert space $L^2(\mathcal{X}, \pi)$. In this case, it was shown in [85, 88] that the KFE can be written as the gradient flow equation of Ent_π with respect to a Riemannian metric on $\mathscr{P}_*(\mathcal{X})$. The associated Riemannian distance is given by a discrete dynamical optimal transport problem, in the spirit of the Benamou–Brenier formulation for the Wasserstein distance [8]. This gradient flow structure is a discrete version of the Wasserstein gradient flow structure for the Fokker–Planck equation discovered by Jordan, Kinderlehrer, and Otto [56]. This construction has been the starting point for the development of discrete Ricci curvature based on geodesic convexity with applications to functional inequalities [34, 90, 35, 36, 33]

It was shown by Dietert [28] that the reversibility assumption is also necessary: if the KFE can be written as gradient flow equation for Ent_π with respect to *some* Riemannian metric on $\mathscr{P}_*(\mathcal{X})$, then the underlying Markov chain is necessarily reversible. Combined with the results from [85, 88], this result characterises reversible Markov chains as exactly those that admit a gradient flow structure for the relative entropy Ent_π.

In this paper we provide a noncommutative analogue of this result.

Quantum Markov semigroups

Let $(\mathscr{P}_t)_{t\geqslant 0}$ be a quantum Markov semigroup on a finite-dimensional C^*-algebra $\mathcal{A}$, i.e., $(\mathscr{P}_t)_{t\geqslant 0}$ is a C_0-semigroup of linear operators on $\mathcal{A}$ such that $\mathscr{P}_t \mathbb{1} = \mathbb{1}$ and the operators $\mathscr{P}_t$ are completely positive, i.e., $\mathscr{P}_t \otimes I_n$ is a positive operator on $\mathcal{A} \otimes \mathbb{M}_n(\mathbb{C})$ for all $n \geqslant 1$. (Here, $\mathbb{1} \in \mathcal{A}$ denotes the unit element, and I_n denotes the identity operator on the algebra of $n \times n$-matrices $\mathbb{M}_n(\mathbb{C})$.) The infinitesimal generator of $(\mathscr{P}_t)_{t\geqslant 0}$ will be denoted by $\mathscr{L}$.

Let $(\mathscr{P}_t^\dagger)_{t\geqslant 0}$ be the adjoint semigroup with respect to the duality pairing $\langle A, B\rangle = \mathrm{Tr}[A^*B]$. This is a C_0-semigroup of completely positive and trace-preserving linear operators with generator $\mathscr{L}^\dagger$. In particular, the operators $\mathscr{P}_t^\dagger$ map the set of density matrices $\mathfrak{P} := \{\rho \in \mathcal{A} \ : \ \rho \geqslant 0$ and $\mathrm{Tr}[\rho] = 1\}$ into itself. Here we restrict our attention to the *ergodic* setting: we assume that there exists a unique stationary state, i.e., a unique density matrix $\sigma \in \mathfrak{P}$ satisfying $\mathscr{L}^\dagger\sigma = 0$. We shall assume that σ is invertible.

The non-commutative analogue of the KFE is the *Lindblad equation* $\partial_t\rho_t = \mathscr{L}^\dagger\rho_t$. It is well known [117, 118] that the *von Neumann relative entropy*

$$H_\sigma(\rho) := \mathrm{Tr}[\rho(\log\rho - \log\sigma)]$$

decreases along solutions to this equation. Moreover, following the earlier works [19, 89], it was shown in [20, 92] that the Lindblad equation $\partial_t\rho = \mathscr{L}^\dagger\rho$ can be written as gradient flow equation for H_σ under the condition of GNS-*detailed balance*. This condition means that the generator $\mathscr{L}$ is selfadjoint with respect to the weighted L^2-type scalar product

$$\langle A, B\rangle_\sigma^{\mathrm{GNS}} := \mathrm{Tr}[\sigma A^* B]$$

named after Gelfand, Naimark, and Segal. As in the discrete setting above, the associated Riemannian metric is related to a dynamical optimal transport problem.

It is now natural to ask whether the condition of GNS-detailed balance is also necessary for the existence of a gradient flow structure for the von Neumann relative entropy. However, it was shown in [21] that a different symmetry condition is necessary, namely the condition of BKM-*detailed balance*. This condition corresponds to the selfadjointness of $\mathscr{L}$ with respect to another weighted L^2-type scalar product

$$\langle A, B\rangle_\sigma^{\mathrm{BKM}} := \int_0^1 \mathrm{Tr}[\sigma^{1-s}A^*\sigma^s B]\,\mathrm{d}s,$$

named after Bogoliubov, Kubo, and Mori. As the condition of BKM-detailed balance is strictly weaker than GNS-detailed balance [21], there was a gap between the known necessary and sufficient conditions. As an application of Theorem B.1.1 we prove the following result, which closes this gap.

Theorem B.1.2. *Let $\mathscr{L}$ be the generator of an ergodic quantum Markov semigroup on a finite dimensional C^*-algebra $\mathcal{A}$, and let $\sigma \in \mathfrak{P}_+$ be its stationary state. The following statements are equivalent:*

(1) The operator $\mathscr{L}$ is selfadjoint with respect to the BKM *scalar product $\langle\cdot,\cdot\rangle_\sigma^{\mathrm{BKM}}$.*

(2) There exists a Riemannian metric on the interior of $\mathfrak{P}$ for which the Lindblad equation $\dot\rho_t = \mathscr{L}^\dagger\rho_t$ is the gradient flow equation of the von Neumann relative entropy H_σ.

The implication *(2) $\Rightarrow$ (1)* was proved in [21, Theorem 2.9]. The converse implication is new.

Structure of the paper

Section B.2 contains the main result and a reformulation of the result in the gradient case. The proof of the main result is contained in Section B.3, except for the construction of the local metric, which is presented in Section B.4. Section B.5 deals with the construction of a metric of class C^k under the assumption that the fields X^α and Y_β are of class C^{k+1}. The application to quantum Markov semigroups is contained in Section B.6.

B.2 Main results

Let $X^\alpha \in \Gamma(TM)$ be a vector field and $Y_\beta \in \Gamma(T^*M)$ be a co-vector field on a smooth manifold M. Let $\mathsf{N}_Y := \{m \in M \ : \ Y|_m = 0\}$ be the set of critical points of Y.

In the sequel we impose the following mild assumptions on the fields X^α and Y_β.

Assumption B.2.1. (i) *(Non-degeneracy) The bilinear form $\nabla_\alpha Y_\beta|_m$ is non-degenerate for all $m \in \mathsf{N}_Y$ for some (equivalently, any) connection ∇.*

(ii) *(Real analyticity) For all $m \in \mathsf{N}_Y$ there exists a neighbourhood $U_m \ni m$, an open set $\Omega \subset \mathbb{R}^n$, and a coordinate chart $\varphi_m : U_m \to \Omega$, such that the fields $\widetilde{X}^a := X^a \circ \varphi_m^{-1} : \Omega \to \mathbb{R}$ and $\widetilde{Y}_a := Y_a \circ \varphi_m^{-1} : \Omega \to \mathbb{R}$ have a converging power series expansion around $\varphi_m(m)$ for all $a \in \{1, \ldots, n\}$.*

Remark B.2.2. The choice of the connection in *(i)* above is irrelevant, since the difference of two connections ∇ and $\tilde{\nabla}$ satisfies $\tilde{\nabla}_\alpha Y_\beta - \nabla_\alpha Y_\beta = \Gamma^\gamma_{\alpha\beta} Y_\gamma$, where $\Gamma^\gamma_{\alpha\beta}$ is a $(1,2)$ tensor. In particular, $\tilde{\nabla}_\alpha Y_\beta = \nabla_\alpha Y_\beta$ for $m \in \mathsf{N}_Y$. For the same reason, the choice of the connection is irrelevant in *(iii)* in the following result.

Using the notation introduced above, we restate our main result (Theorem B.1.1) for the convenience of the reader.

Theorem B.2.3 (Main result)**.** *Let $X^\alpha \in \Gamma(TM)$ and $Y_\beta \in \Gamma(T^*M)$ satisfy Assumption B.2.1. Then there exists a smooth metric $g_{\alpha\beta} \in \Gamma(T^*M \otimes T^*M)$ satisfying $Y_\beta = g_{\alpha\beta} X^\alpha$, if and only if the following conditions hold:*

(i) *$X^\alpha Y_\alpha|_m > 0$ for all $m \in M \backslash \mathsf{N}_Y$;*

(ii) *$X^\alpha|_m = 0$ for all $m \in \mathsf{N}_Y$;*

(iii) *For all $m \in \mathsf{N}_Y$ there exists a scalar product $\bar{g}_{\alpha\beta} \in T^*_m M \otimes_S T^*_m M$, such that*

$$\nabla_\alpha Y_\gamma|_m = \bar{g}_{\beta\gamma} \nabla_\alpha X^\beta|_m,$$

where ∇_α is an arbitrary connection.

Remark B.2.4. As the necessity of the three conditions has been discussed above, it remains to prove their sufficiency. This will be done in Section B.3 below.

In the special case where the co-vector field $Y_\alpha := \nabla_\alpha F \in \Gamma(T^*M)$ is the derivative of a scalar function $f : M \to \mathbb{R}$, the above result admits a convenient reformulation. Assuming that f attains its minimum at a unique critical point $\bar{m} \in M$, the next results shows that property *(iii)* above is equivalent to the symmetry and positivity of the linearised map $\Lambda : T_{\bar{m}}M \to T_{\bar{m}}M$, $Z \mapsto \nabla_Z X$, at the critical point $\bar{m}$. The relevant scalar product is given by the Hessian of f.

Corollary B.2.5 (Gradient case)**.** *Let $f \in C^\infty(M)$ be a function and $X^\alpha \in \Gamma(TM)$ be a vector field, such that X^α and $Y_\alpha := \nabla_\alpha f$ satisfy Assumption B.2.1. Suppose that Y has a unique zero, $\bar{m} \in M$, at which f attains its minimum. Then there exists a Riemannian metric $g_{\alpha\beta} \in \Gamma(T^*M \otimes T^*M)$ satisfying*

$$\nabla_\beta f = g_{\alpha\beta} X^\alpha,$$

if and only if the following conditions hold:

(i) $\nabla_{X^\alpha} f|_m < 0$ *for all* $m \in M$ *with* $m \neq \bar{m}$*;*

(ii) $X^\alpha|_{\bar{m}} = 0$*;*

(iii) The linear map $\Lambda := \nabla_\alpha X^\beta|_{\bar{m}} : T_{\bar{m}}M \to T_{\bar{m}}M$ *is positive and symmetric with respect to the Hessian scalar product* $h_{\alpha\beta} := \nabla_\alpha \nabla_\beta f|_{\bar{m}}$ *on* $T_{\bar{m}}M$*.*

Proof. It is clear that the conditions *(i)* and *(ii)* match the corresponding conditions in Theorem B.2.3.

Suppose now that condition *(iii)* from Theorem B.2.3 holds, for some scalar product $\bar{g}^{\alpha\beta} \in T_{\bar{m}}M \otimes_S T_{\bar{m}}M$. We have to show that

$$h_{\alpha\beta}(\Lambda Z)^\alpha W^\beta = h_{\alpha\beta} Z^\alpha (\Lambda W)^\beta \qquad \text{for all } Z^\alpha, W^\alpha \in T_{\bar{m}}M, \text{ and}$$
$$h_{\alpha\beta}(\Lambda Z)^\alpha Z^\beta > 0 \qquad \text{for all } Z^\alpha \in T_{\bar{m}}M,\ Z^\alpha \neq 0.$$

To show this, note that $(\Lambda Z)^\alpha = Z^\gamma \nabla_\gamma X^\alpha = Z^\gamma \bar{g}^{\alpha\delta} h_{\delta\gamma}$ for $Z^\alpha \in T_{\bar{m}}M$. Hence, for $W^\alpha \in T_{\bar{m}}M$, we see that the expression

$$h_{\alpha\beta}(\Lambda Z)^\alpha W^\beta = h_{\alpha\beta} \bar{g}^{\alpha\delta} h_{\delta\gamma} Z^\gamma W^\beta$$

is invariant under interchanging Z and W, which proves the desired symmetry. Moreover, this expression implies that $h_{\alpha\beta}(\Lambda Z)^\alpha Z^\beta = \bar{g}^{\alpha\beta} \widetilde{Z}_\alpha \widetilde{Z}_\beta$ where $\widetilde{Z}_\alpha = h_{\alpha\beta} Z^\beta$. Since $h_{\alpha\beta}$ is invertible by Assumption B.2.1 and $\bar{g}^{\alpha\beta}$ is positive definite, it follows that $h_{\alpha\beta}(\Lambda Z)^\alpha Z^\beta > 0$ whenever $Z^\alpha \neq 0$.

Conversely, suppose that condition *(iii)* of the corollary holds. For all $Z^\alpha, W^\alpha \in T_{\bar{m}}M$ it follows that $h_{\alpha\beta}(\Lambda Z)^\alpha W^\beta = \widetilde{g}_{\alpha\beta} Z^\alpha W^\beta$ for a positive and symmetric tensor $\widetilde{g}_{\alpha\beta} \in T^*_{\bar{m}}M \otimes_S T^*_{\bar{m}}M$. Since $h_{\alpha\beta}(\Lambda Z)^\alpha W^\beta = h_{\alpha\beta} Z^\gamma \nabla_\gamma X^\alpha W^\beta$ we infer that $\widetilde{g}_{\alpha\beta} = h_{\gamma\beta} \nabla_\alpha X^\gamma$. Now define

$$\bar{g}^{\alpha\beta} := h^{\alpha\delta} \widetilde{g}_{\delta\gamma} h^{\gamma\beta} \in T_{\bar{m}}M \otimes T_{\bar{m}}M.$$

Since $\widetilde{g}_{\alpha\beta}$ is positive and symmetric and $h^{\alpha\delta}$ is invertible, $\bar{g}^{\alpha\beta}$ defines a scalar product. Moreover, we have the desired identity $\nabla_\alpha X^\beta|_{\bar{m}} = \bar{g}^{\beta\gamma} h_{\alpha\gamma}$, which completes the proof. ∎

In the special case were Y_β is the derivative of a scalar function f, the existence of a metric satisfying $\nabla_\beta f = g_{\alpha\beta} X^\alpha$ was proved in [7] on the complement of the set of critical points. The existence of a metric with the desired property on the whole manifold was stated as an open question [7, Question 1]. Subsequently, under an additional assumption, which corresponds to (iii) in Theorem B.2.3, the existence of a *continuous* extension of $g_{\alpha\beta}$ to all of M was obtained in [10]; cf. Section B.5 below for more details. However, the metric constructed [10] is in general *not* differentiable, even if the fields X^α and Y_β are smooth; see Example B.5.2 below.

Here we show that C^k-regularity of the metric can be obtained if the fields X^α and Y_β are assumed to be of class C^{k+1}.

Theorem B.2.6 (Existence of a metric of class C^k)**.** *Let* X^α *and* Y_β *be of class* C^{k+1} *on* M *for some* $k \in \mathbb{N}$ *and assume that* $\nabla_\alpha Y_\beta|_m$ *is non-degenerate for all* $m \in \mathsf{N}_Y$ *for some (equivalently, any) connection* ∇*. Then there exists a metric* $g_{\alpha\beta}$ *of class* C^k *on* M *satisfying* $Y_\beta = g_{\alpha\beta} X^\alpha$ *if and only if conditions* (i)*,* (ii)*, and* (iii) *of Theorem B.2.3 hold.*

The proof of this result will be given in Section B.5 below. It relies on the construction based on tensor equations that we develop in the proof of Theorem B.2.3.

B.3 Proof of the main result

Our main result (Theorem B.2.3) relies on two local versions of this result. First we construct a local solution around any non-critical point $m \in M \backslash \mathsf{N}_Y$. In the special case were Y_β is the derivative of a scalar function, a different construction of a metric away from critical points was carried out in [7]; see Section B.5 below.

Theorem B.3.1 (Local solutions around non-critical points)**.** *Suppose that $X^\alpha \in \Gamma(TM)$ and $Y_\beta \in \Gamma(T^*M)$ satisfy $X^\alpha Y_\alpha|_{\bar{m}} > 0$ for some $\bar{m} \in M$. Then there exists a neighbourhood U of $\bar{m}$ and a smooth local metric $g_{\alpha\beta} : U \to T^*M \otimes T^*M$ such that*

$$X^\alpha|_m = g^{\alpha\beta} Y_\beta|_m \tag{B.3.1}$$

for all $m \in U$.

Proof. Since $X^\alpha Y_\alpha|_m > 0$, we have $Y_\alpha|_m \neq 0$. Therefore, we can complete the co-vector field $e^1_\alpha := Y_\alpha \in T^*M$ to a dual frame $E := (e^1_\alpha, \dots, e^n_\alpha)$ in a neighbourhood V of m, i.e., $(e^1_\alpha|_m, \dots, e^n_\alpha|_m)$ is a basis of $T^*_m M$ for all $m \in V$. The coordinates of X^α with respect to this frame are given by $X^j := X^\alpha e^j_\alpha : V \to \mathbb{R}$ for $j = 1, \dots, n$. Since $X^1|_{\bar{m}} > 0$, the set $U := V \cap \{X^1 > 0\}$ is still a neighbourhood of $\bar{m}$. Let us define $\bar{X} : U \to \mathbb{R}^{n-1}$ and $f : U \to \mathbb{R}$ by

$$\bar{X} := (X^2, \dots, X^n), \qquad f := \frac{X^1}{2} + \frac{2}{X^1}|\bar{X}|^2.$$

We then define the bilinear form $g^{\alpha\beta}$ in coordinates $G = (g^{ij})^n_{i,j=1}$ as

$$G := \begin{bmatrix} X^1 & \bar{X}^\intercal \\ \bar{X} & f I_{n-1} \end{bmatrix},$$

where I_n is the identity matrix. Since the matrix G is symmetric, the bilinear form g is symmetric as well. To verify that $G > 0$, we write

$$\begin{aligned} G &= \begin{bmatrix} \sqrt{\frac{X^1}{2}} \\ \sqrt{\frac{2}{X^1}}\bar{X} \end{bmatrix} \begin{bmatrix} \sqrt{\frac{X^1}{2}} & \sqrt{\frac{2}{X^1}}\bar{X}^\intercal \end{bmatrix} + \begin{bmatrix} \frac{X^1}{2} & 0 \\ 0 & f I_{n-1} - \frac{2}{X^1}\bar{X}\bar{X}^\intercal \end{bmatrix} \\ &\geqslant \begin{bmatrix} \frac{X^1}{2} & 0 \\ 0 & \left(f - \frac{2}{X^1}|\bar{X}|^2\right) I_{n-1} \end{bmatrix} = \frac{X^1}{2} I_n > 0, \end{aligned}$$

as desired. To complete the proof, note that the coordinates of Y_α are given by $Y_1 = 1$ and $Y_j = 0$ for $j \neq 1$. Consequently,

$$(g^{\alpha\beta} Y_\beta)^i = \sum_j g^{ij} Y_j = g^{i1} = X^i,$$

which shows (B.3.1). ∎

The second local version of Theorem B.2.3 concerns the construction of a smooth local metric in a neighbourhood of a critical point.

Theorem B.3.2 (Local solutions around critical points). *Let $X^\alpha \in \Gamma(TM)$ and $Y_\beta \in \Gamma(T^*M)$ satisfy Assumption B.2.1. Suppose that $X^\alpha|_{\bar{m}} = Y_\alpha|_{\bar{m}} = 0$ for some $\bar{m} \in M$, and suppose that there exists a scalar product $\bar{g} \in T_{\bar{m}}M \otimes_S T_{\bar{m}}M$, such that*

$$\nabla_\alpha X^\beta|_{\bar{m}} = \bar{g}^{\beta\gamma}\nabla_\alpha Y_\gamma|_{\bar{m}}.$$

Then there exists a neighbourhood U of m and a smooth local metric $g_{\alpha\beta} : U \to T^*M \otimes T^*M$ such that

$$X^\alpha|_m = g^{\alpha\beta}Y_\beta|_m$$

for all $m \in U$.

The proof of Theorem B.3.2 is the main challenge of this paper and will be carried out in section B.4.

We now show that the main result (Theorem B.2.3) follows readily from the local Theorems B.3.1 and B.3.2 using a partition of unity argument; see, e.g., [47, Theorem 1.131] for the existence of a partition of unity.

Proof of Theorem B.2.3. The local results Theorems B.3.1 and B.3.2 guarantee that for any $m \in M$ there exists a neighbourhood U_m and a local metric $g_{\alpha\beta}$ defined on U_m, such that the desired identity

$$X^\alpha = g^{\alpha\beta}Y_\beta,$$

holds on U_m.

Let $\{f_k\}_{k\in\mathbb{N}}$ be a partition of unity subordinated to the cover $\{U_m : m \in M\}$ of the manifold M, i.e., there exists a locally finite open covering $\{V_k\}_{k\in\mathbb{N}}$ of M, such that each V_k is contained in U_{m_k} for some $m_k \in M$, each function $f_k : M \to \mathbb{R}$ is nonnegative and smooth and its support is contained in V_k, and we have $\sum_{k\in\mathbb{N}} f_k(m) = 1$ for all $m \in M$ (where the sum is finite for each m). We then define

$$g^{\alpha\beta} := \sum_{k\in\mathbb{N}} f_k g^{\alpha\beta}_{m_k}.$$

As $g^{\alpha\beta}$ is a finite convex combination of the scalar products $g^{\alpha\beta}_{m_k}$, it is a scalar product. By linearity, $g^{\alpha\beta}$ satisfies the desired equation $X^\alpha = g^{\alpha\beta}Y_\beta$. ■

B.4 Local solutions around critical points

In this section we give the proof of Theorem B.3.2, which deals with the construction of the metric around critical points.

Fix $\bar{m} \in M$ and let $\varphi : U \to \Omega$ be a coordinate chart which maps a neighbourhood U of $\bar{m}$ onto an open set $\Omega \subseteq \mathbb{R}^n$. Using this chart we can identify the vector field $X^\alpha \in \Gamma(TM)$ defined on $U \subseteq M$ with the function $\widetilde{X}^\alpha : \Omega \to V := \mathbb{R}^n$, where $\widetilde{X}^\alpha := X^\alpha \circ \varphi^{-1}$. Similarly, the co-vector field $Y_\beta \in \Gamma(T^*M)$ defined on $U \subseteq M$ can be identified with a function $\widetilde{Y}_\beta : \Omega \to V^*$, and the metric $g_{\alpha\beta} \in \Gamma(T^*M \otimes_S T^*M)$ can be identified with a function $\widetilde{g}_{\alpha\beta} : \Omega \to V^* \otimes_S V^*$. In the remainder of this section, we will work on a fixed chart and remove the tildes to lighten notation.

B.4.1 Motivation of the tensor equations

Let $\bar{x} \in \Omega$ be such that $Y_\beta|_{\bar{x}} = 0$, and suppose that the identity $X^\alpha = g^{\alpha\beta} Y_\beta$ holds in a neighbourhood of $\bar{x}$. For $N \in \mathbb{N}$ and all indices $c_1, \ldots, c_N \in \{1, \ldots, n\}$ we will derive a system of equations that the partial derivatives $T^{ab}_{c_1 \cdots c_N} := \partial_{c_1} \cdots \partial_{c_N} g^{ab}$ satisfy at $x = \bar{x}$.

Taking partial differentives ∂_c for $c \in \{1, \ldots, n\}$ yields

$$\partial_c X^a = \partial_c g^{ab} Y_b + g^{ab} \partial_c Y_b.$$

Since $Y_b|_{\bar{x}} = 0$, we find that

$$\partial_c X^a = g^{ab} \partial_c Y_b$$

at $x = \bar{x}$. Taking second order derivatives, we find, for $c_1, c_2 \in \{1, \ldots, n\}$,

$$\partial_{c_1} \partial_{c_2} X^a = \partial_{c_1} \partial_{c_2} g^{ab} Y_b + \partial_{c_1} g^{ab} \partial_{c_2} Y_b + \partial_{c_2} g^{ab} \partial_{c_1} Y_b + g^{ab} \partial_{c_1} \partial_{c_2} Y_b.$$

As $Y_b|_{\bar{x}} = 0$, the first term on the right-hand side vanishes, and we infer that the tensor of first-order derivatives $T^{ab}_c := \partial_c g^{ab}$ is a solution to the system

$$U_{c_2 b} T^{ab}_{c_1} + U_{c_1 b} T^{ab}_{c_2} = R^a_{c_1 c_2},$$

where $U_{ab} := \partial_a Y_b$ and $R^a_{c_1 c_2} := \partial_{c_1} \partial_{c_2} X^a - g^{ab} \partial_{c_1} \partial_{c_2} Y_b$.

More generally, for $N = 1, 2, \ldots$, we find

$$\partial_{c_1} \cdots \partial_{c_N} X^a = \sum_{S \subseteq [N]} \partial_{c_S} g^{ab} \partial_{c_{[N] \setminus S}} Y_b,$$

where we use the shorthand notation $\partial_{c_S} = \partial_{c_{i_1}} \cdots \partial_{c_{i_k}}$ for $S = \{i_1, \ldots, i_k\} \subseteq \{1, \ldots, N\}$ with $i_\mu \neq i_\nu$ for $\mu \neq \nu$. Since $Y_b = 0$, the term with $|S| = N$ vanishes. Thus, the derivatives of order $(N-1)$, given by $T^{ab}_{c_1 \cdots c_{N-1}} := \partial_{c_1} \cdots \partial_{c_{N-1}} g^{ab}$ solve the system

$$\sum_{i=1}^{N} U_{c_i b} T^{ab}_{c_1 \cdots \check{c}_i \cdots c_N} = R^a_{c_1 \cdots c_N}, \tag{B.4.1}$$

where $U_{cb} := \partial_c Y_b$, and

$$R^a_{c_1 \cdots c_N} := \partial_{c_1} \cdots \partial_{c_N} X^a - \sum_{\substack{S \subseteq [N] \\ |S| < N-1}} \partial_{c_S} g^{ab} \partial_{c_{[N] \setminus S}} Y_b$$

depends on (derivatives of) X and Y, and on derivatives of g of order at most $N-2$. The notation $T^{ab}_{c_1 \cdots \check{c}_i \cdots c_N}$ means that the index c_i is removed.

The identity (B.4.1) suggests an iterative scheme to construct a local solution $g^{\alpha\beta}$ to the equation $X^\alpha = g^{\alpha\beta} Y_\beta$ around a critical point $\bar{x} \in U$ as a power series

$$g^{ab}|_{\bar{x}} := \sum_{N=0}^{\infty} \frac{1}{N!} T^{ab}_{c_1 \cdots c_N} (x - \bar{x})^{c_1} \cdots (x - \bar{x})^{c_N}$$

with coefficients $T^{\alpha\beta}_{\gamma_1 \cdots \gamma_N} \in V^{\otimes_S 2} \otimes (V^*)^{\otimes_S N}$ The idea is to define, for $N = 0$, $T^{ab} := \bar{g}^{ab}$, where $\bar{g} \in T^*_{\bar{x}} M \otimes_S T^*_{\bar{x}} M$ is the scalar product satisfying

$$\partial_c X^a|_{\bar{x}} = \bar{g}^{ab} \, \partial_c Y_b|_{\bar{x}},$$

which exists by assumption. Higher order Taylor coefficients $T^{ab}_{c_1 \ldots c_N}$ are then constructed by iteratively solving a system of tensor equations of the form (B.4.1).

Section B.4.2 deals with the existence of a solution to these equations. The construction and the convergence of the iterative scheme is contained in Section B.4.3.

B.4.2 Solving the tensor equations

We start by formulating an explicit solution to the tensor equation (B.4.1) of order $N = 2$.

Lemma B.4.1. *Let V be a finite-dimensional vector space, and let $R^{\alpha}_{\gamma\delta} \in V \otimes (V^* \otimes_S V^*)$ and $U_{\alpha\beta} \in V^* \otimes V^*$ be given. We assume that $U_{a\beta}$ is invertible with inverse $U^{\alpha\beta} \in V \otimes V$. Then the tensor $T^{\alpha\beta}_{\gamma} \in (V \otimes V) \otimes V^*$ defined by*

$$T^{\alpha\beta}_{\gamma} := \frac{1}{2}\Big(U^{\beta\delta} R^{\alpha}_{\gamma\delta} + U^{\alpha\delta} R^{\beta}_{\gamma\delta} - U_{\gamma\gamma'} U^{\alpha\alpha'} U^{\beta\beta'} R^{\gamma'}_{\alpha'\beta'}\Big)$$

satisfies the equations $T^{\alpha\beta}_{\gamma} = T^{\beta\alpha}_{\gamma}$ and

$$U_{\delta\beta} T^{\alpha\beta}_{\gamma} + U_{\gamma\beta} T^{\alpha\beta}_{\delta} = R^{\alpha}_{\gamma\delta}. \tag{B.4.2}$$

Proof. The fact that $T^{\alpha\beta}_{\gamma} = T^{\beta\alpha}_{\gamma}$ follows readily from the definition. To show that (B.4.2) holds, note that by definition of T,

$$2U_{\delta\beta} T^{\alpha\beta}_{\gamma} = R^{\alpha}_{\gamma\delta} + U_{\delta\beta} U^{\alpha\epsilon} R^{\beta}_{\gamma\epsilon} - U_{\gamma\gamma'} U^{\alpha\alpha'} R^{\gamma'}_{\alpha'\delta}, \tag{B.4.3}$$

$$2U_{\gamma\beta} T^{\alpha\beta}_{d} = R^{\alpha}_{\delta\gamma} + U_{\gamma\beta} U^{\alpha\epsilon} R^{\beta}_{\delta\epsilon} - U_{\delta\delta'} U^{\alpha\alpha'} R^{\delta'}_{\alpha'\gamma}. \tag{B.4.4}$$

Relabeling indices on the right-hand side and using the symmetry of R, we observe that the second term in (B.4.3) equals the third term in (B.4.4), and the second term in (B.4.4) equals the third term in (B.4.3). Summing these identities, we thus obtain (B.4.2). ∎

We also need the following multilinear generalisation.

Lemma B.4.2. *Fix $N \geqslant 2$. Let V be a finite-dimensional vector space, and let $R^{\alpha}_{\gamma_1\cdots\gamma_N} \in V \otimes (V^*)^{\otimes_s N}$ and $U_{\alpha\beta} \in V^* \otimes V^*$ be given. We assume that $U_{\alpha\beta}$ is invertible with inverse $U^{\alpha\beta} \in V \otimes V$. Then the tensor $T^{\alpha\beta}_{\gamma_1\cdots\gamma_{N-1}} \in V^{\otimes_s 2} \otimes (V^*)^{\otimes_s (N-1)}$ defined by*

$$T^{\alpha\beta}_{\gamma_1\cdots\gamma_{N-1}} := \frac{1}{N}\left(U^{\beta\delta} R^{\alpha}_{\delta\gamma_1\cdots\gamma_{N-1}} + U^{\alpha\delta} R^{\beta}_{\delta\gamma_1\cdots\gamma_{N-1}} - \frac{1}{N-1}\sum_{i=1}^{N-1} U_{\gamma_i\gamma_i'} U^{\alpha\alpha'} U^{\beta\beta'} R^{\gamma_i'}_{\alpha'\beta'\gamma_1\cdots\check{\gamma}_i\cdots\gamma_{N-1}}\right) \tag{B.4.5}$$

satisfies

$$\sum_{i=1}^{N} U_{\gamma_i\beta} T^{\alpha\beta}_{\gamma_1\cdots\check{\gamma}_i\cdots\gamma_N} = R^{\alpha}_{\gamma_1\cdots\gamma_N}. \tag{B.4.6}$$

Proof. The fact that T belongs to $V^{\otimes_s 2} \otimes (V^*)^{\otimes_s (N-1)}$ follows readily from the definition. To show that (B.4.6) holds, note that

$$\begin{aligned}\sum_{i=1}^{N} U_{\gamma_i\beta} T^{\alpha\beta}_{\gamma_1\cdots\check{\gamma}_i\cdots\gamma_N} &= \frac{1}{N}\sum_{i=1}^{N}\Big\{U_{\gamma_i\beta} U^{\beta\delta} R^{\alpha}_{\delta\gamma_1\cdots\check{\gamma}_i\cdots\gamma_N} + U_{\gamma_i\beta} U^{\alpha\delta} R^{\beta}_{\delta\gamma_1\cdots\check{\gamma}_i\cdots\gamma_N} \\ &\qquad - \frac{1}{N-1}\sum_{j:j\neq i} U_{\gamma_i\beta} U^{\beta\beta'} U_{\gamma_j\gamma_j'} U^{\alpha\alpha'} R^{\gamma_j'}_{\alpha'\beta'\gamma_1\cdots\check{\gamma}_i\cdots\check{\gamma}_j\cdots\gamma_N}\Big\} \\ &= \frac{1}{N}\sum_{i=1}^{N}\Big\{R^{\alpha}_{\gamma_1\cdots\gamma_N} + U_{\gamma_i\beta} U^{\alpha\delta} R^{\beta}_{\delta\gamma_1\cdots\check{\gamma}_i\cdots\gamma_N} - \frac{1}{N-1}\sum_{j:j\neq i} U_{\gamma_j\gamma_j'} U^{\alpha\alpha'} R^{\gamma_j'}_{\alpha'\gamma_1\cdots\check{\gamma}_j\cdots\gamma_N}\Big\}.\end{aligned}$$

This yields the result, as the first term has the desired form, and the second term cancels against the third term, as can be seen by renaming indices (α', γ_j') into (δ, β). ∎

B.4.3 Iterative construction of the power series & Proof of Theorem B.3.2

We now place ourselves in the setting of Theorem B.3.2. Thus, let $X^\alpha \in \Gamma(TM)$ and $Y_\beta \in \Gamma(T^*M)$ satisfy Assumption B.2.1, and suppose that $X^\alpha|_{\bar{m}} = Y_\alpha|_{\bar{m}} = 0$ for some fixed $\bar{m} \in M$. We assume that there exists a scalar product $\bar{g} \in T_{\bar{m}}M \otimes_S T_{\bar{m}}M$ satisfying

$$\nabla_\alpha X^\beta|_{\bar{m}} = \bar{g}^{\beta\gamma}\nabla_\alpha Y_\gamma|_{\bar{m}}.$$

Our goal is to construct the local metric $g^{\alpha\beta}$ around $\bar{m}$ as a convergent power series centered at $\bar{x} = \varphi(\bar{m})$. We now present the definition of its coeffients $T^{ab}_{c_1\cdots c_N}$, which is motivated by the equations (B.4.1). Our computations will be performed in a fixed chart $\varphi : U \to \Omega$ around $\bar{m}$ which satisfies Assumption B.2.1.

Definition B.4.3 (The power series coeffients $T^{ab}_{c_1\cdots c_N}$)**.** *Write $U_{\alpha\beta} := \nabla_\alpha Y_\beta|_{\bar{m}}$ for brevity.*

- Initialisation: *We define the initial tensor $T^{\alpha\beta} \in V \otimes_S V$ of our iteration as*

$$T^{ab} := \bar{g}^{ab}.$$

- Iterative step (special case $N = 2$): *We first define $R^\alpha_{\gamma\delta} \in V \otimes (V^* \otimes_S V^*)$ by*

$$R^a_{cd} := \partial_c\partial_d X^a - T^{ab}\partial_c\partial_d Y_b$$

  and then define $T^{\alpha\beta}_\gamma \in (V \otimes_S V) \otimes V^*$ as the solution to the system

$$U_{db}T^{ab}_c + U_{cb}T^{ab}_d = R^a_{cd}$$

  constructed in Lemma B.4.1.

- Iterative step ($N = 2, 3, \ldots$): *We first define $R^\alpha_{\gamma_1\cdots\gamma_N} \in V \otimes (V^*)^{\otimes_S N}$ in terms of the lower order tensors $T^{\alpha\beta}, T^{\alpha\beta}_{\gamma_1}, \ldots, T^{\alpha\beta}_{\gamma_1\cdots\gamma_{N-2}}$ by*

$$R^a_{c_1\cdots c_N} := \partial_{c_1}\cdots\partial_{c_N}X^a - \sum_{\substack{S\subseteq[N]\\ |S|<N-1}} T^{ab}_{c_S}\,\partial_{c_{[N]\setminus S}}Y_b. \tag{B.4.7}$$

  Here we use the shorthand notation $T_{c_S} := T_{c_{i_1}\cdots c_{i_k}}$ for $S := \{i_1, \ldots, i_k\}$ with $i_\mu \neq i_\nu$ for $\mu \neq \nu$. Then we define the tensor $T^{\alpha\beta}_{\gamma_1\cdots\gamma_{N-1}} \in V^{\otimes_S(N-1)} \otimes (V^*)^{\otimes_S 2}$ as the solution to the system

$$\sum_{i=1}^N U_{c_ib}T^{ab}_{c_1\cdots\check{c}_i\cdots c_N} = R^a_{c_1\cdots c_N},$$

  constructed in Lemma B.4.2.

Remark B.4.4. The nondegeneracy assumption on the derivative $\nabla_\alpha Y_\beta|_{\bar{m}}$ is crucially used in this construction, as the application of Lemmas B.4.1 and B.4.2 requires the invertibility of $U_{\alpha\beta}$.

Our next aim is to show that the power series

$$g^{ab}|_x := \sum_{N=0}^{\infty} \frac{1}{N!} T^{ab}_{c_1\cdots c_N} (x-\bar{x})^{c_1} \cdots (x-\bar{x})^{c_N}.$$

converges and defines a Riemannian metric in a neigbourhood of $\bar{x}$. For this purpose we equip the spaces $V^{\otimes k} \otimes (V^*)^{\otimes \ell}$ with the norm

$$\left\| W^{\beta_1\ldots\beta_\ell}_{\alpha_1\cdots\alpha_k} \right\|_\infty := \max_{a_1,\ldots,a_k,b_1,\ldots,b_\ell} \left| W^{b_1\cdots b_\ell}_{a_1\cdots a_k} \right|,$$

where $W^{b_1\cdots b_\ell}_{a_1\cdots a_k}$ are the coordinates of $W^{\beta_1\ldots\beta_\ell}_{\alpha_1\cdots\alpha_k}$ in the standard basis of $\mathbb{R}^n$. For brevity, let us write

$$r_N := \| R^{\alpha}_{\gamma_1\cdots\gamma_N} \|_\infty \quad \textit{and} \quad t_N := \| T^{\alpha\beta}_{\gamma_1\cdots\gamma_N} \|_\infty.$$

We then obtain the following crucial growth bound on the power series coefficients.

Lemma B.4.5. *There exist constants $C, p < \infty$ such that $t_N \leqslant C N! p^N$ for all $N \geqslant 1$.*

Proof. Recall that we work in a chart for which Assumption B.2.1 holds. Therefore, the real analyticity assumption implies that there exist constants $C', q < \infty$ such that

$$\left| \partial_{c_1} \cdots \partial_{c_M} \widetilde{X}^a |_{\bar{x}} \right| \leqslant C' M! q^M \quad \textit{and} \quad \left| \partial_{c_1} \cdots \partial_{c_M} \widetilde{Y}_a |_{\bar{x}} \right| \leqslant C' M! q^M \tag{B.4.8}$$

for all $m \in \mathbb{N}$ and all $c_1, \ldots, c_M \in \{1, \ldots, n\}$; see, e.g., [61, Proposition 2.2.10].

Since $U_{\alpha\beta}$ is non-degenerate by Assumption B.2.1, we have

$$K := \max\left\{ \|U_{\alpha\beta}\|_\infty, \|U^{\alpha\beta}\|_\infty \right\} < \infty.$$

Using the bounds on the power series coefficients from (B.4.8) and the definitions of T and R from (B.4.5) and (B.4.7), we obtain the following relations between the norms r_k and t_k:

$$\begin{aligned} \frac{r_N}{N!} &\leqslant C' q^N + \frac{C'n}{N!} \sum_{\substack{S \subseteq [N] \\ |S| < N-1}} t_{|S|} q^{N-|S|} \big(N - |S|\big)! \\ &= C' q^N + \frac{C'n}{N!} \sum_{k=0}^{N-2} \binom{N}{k} t_k q^{N-k} (N-k)! = C' q^N \left(1 + n \sum_{k=0}^{N-2} \frac{t_k}{k! q^k} \right) \end{aligned}$$

and

$$t_{N-1} \leqslant \frac{1}{N} \Big(2nK r_N + K^3 n^3 r_N \Big) =: \frac{\widetilde{K}}{N} r_N,$$

where $\widetilde{K} < \infty$ depends on K and n. Using these estimates we shall now prove the desired result by induction.

We thus assume, for some $N \geqslant 0$, that the desired inequality $t_k / k! \leqslant C p^k$ holds for all $k \leqslant N$, with suitable constants $C, p < \infty$. We will now show that $t_{N+1}/(N+1)! \leqslant C p^{N+1}$. Indeed, using the inequalities above and the induction assumption, we obtain

$$\frac{t_{N+1}}{(N+1)!} \leqslant \frac{\widetilde{K}}{(N+2)!} r_{N+2} \leqslant C' \widetilde{K} q^{N+2} \left(1 + n \sum_{k=0}^{N} \frac{t_k}{k! q^k} \right) \leqslant C' \widetilde{K} q^{N+2} \left(1 + Cn \sum_{k=0}^{N} \left(\frac{p}{q} \right)^k \right).$$

Assuming, without loss of generality, that $C \geqslant 1$ and $p > q$, this yields

$$\frac{t_{N+1}}{(N+1)!} \leqslant Cp^{N+1}C'\widetilde{K}q\left(\left(\frac{q}{p}\right)^{N+1} + n\sum_{k=0}^{N}\left(\frac{q}{p}\right)^{N-k+1}\right) \leqslant Cp^{N+1}C'\widetilde{K}q\left(\frac{q}{p} + \frac{nq}{p-q}\right).$$

By choosing p sufficiently large, the last term in brackets can be made smaller than $(C'\widetilde{K}q)^{-1}$. This yields the result. ■

Corollary B.4.6. *There exists a neigbourhood $U \ni \bar{x}$, such that the power series*

$$g^{ab}|_x := \sum_{N=0}^{\infty} \frac{1}{N!} T^{ab}_{c_1\cdots c_N}(x-\bar{x})^{c_1}\cdots(x-\bar{x})^{c_N} \tag{B.4.9}$$

converges for all $x \in U$, its inverse defines a Riemannian metric, and the equality $X^\alpha|_x = g^{\alpha\beta}Y_\beta|_x$ holds for all $x \in U$.

Proof. The definitions yield

$$\left|T^{ab}_{c_1\cdots c_N}(x-\bar{x})^{c_1}\cdots(x-\bar{x})^{c_N}\right| \leqslant n^N \|T^{\alpha\beta}_{\gamma_1\cdots\gamma_N}\|_\infty \|x-\bar{x}\|_1^N,$$

where $\|y\|_1 := \sum_a |y^a|$ for $y \in V^*$. Since $\|T^{\alpha\beta}_{\gamma_1\cdots\gamma_N}\|_\infty \leqslant CN!p^N$ by Lemma B.4.5, we infer that the power series (B.4.9) converges for $\|x-\bar{x}\|_1 < 1/(pn)$.

To verify that $g^{\alpha\beta}$ defines a metric, note first that $g^{ab} = g^{ba}$ by construction. To show that $g^{\alpha\beta}$ is positive definite when x is close enough to $\bar{x}$, it suffices to note that $g^{\alpha\beta}|_{\bar{x}} = \bar{g}^{\alpha\beta}$ is positive definite and the map $x \mapsto g^{\alpha\beta}|_x$ is continuous.

Since the tensor fields X^α, Y_β, and $g^{\alpha\beta}$ are given by convergent power series, and since $X^\alpha|_{\bar{x}} = g^{\alpha\beta}Y_\beta|_{\bar{x}}$ by assumption, it is enough to verify that all derivatives at $\bar{x}$ coincide, i.e.,

$$\partial_{c_1}\cdots\partial_{c_N}X^a = \partial_{c_1}\cdots\partial_{c_N}(g^{ab}Y_b)$$

for all $N \in \mathbb{N}$ and all $c_1,\ldots,c_N \in \{1,\ldots,n\}$. To prove this identity, we use the notation from Definition B.4.3, to obtain at $x = \bar{x}$,

$$\begin{aligned}
\partial_{c_1}\cdots\partial_{c_N}(g^{ab}Y_b) &= \sum_{S\subseteq[N]} \partial_{c_S}g^{ab}\partial_{c_{[N]\setminus S}}Y_b \\
&= \Big(\partial_{c_1}\cdots\partial_{c_N}g^{ab}\Big)Y_b + \sum_{i=1}^{N}\Big(\partial_{c_1}\cdots\partial_{c_{i-1}}\partial_{c_{i+1}}\cdots\partial_{c_N}g^{ab}\Big)\partial_{c_i}Y_b \\
&\qquad + \sum_{\substack{S\subseteq[N]\\|S|<N-1}} \partial_{c_S}g^{ab}\partial_{c_{[N]\setminus S}}Y_b \qquad\qquad (B.4.10)\\
&= 0 + \sum_{i=1}^{N} U_{c_ib}T^{ab}_{c_1\cdots\check{c}_i\cdots c_N} + \Big(\partial_{c_1}\cdots\partial_{c_N}X^a - R^a_{c_1\cdots c_N}\Big) \\
&= \partial_{c_1}\cdots\partial_{c_N}X^a.
\end{aligned}$$

To obtain the third equality, we use that $\bar{x}$ is a critical point, together with the definitions of R, T, and U in Definition B.4.3. In the final step we use the tensor equation (B.4.6). ■

The proof of Theorem B.3.2 is now complete, as the metric $g^{\alpha\beta}$ constructed above can be pushed back to M using the chart φ.

B.5 Construction of a metric of class C^k

Let X^α be a vector field and Y_β be a co-vector field on a smooth manifold M. As before, let $\mathsf{N}_Y := \{m \in M \ : \ Y|_m = 0\}$ be the set of critical points of Y. In this section we weaken the regularity assumptions on X and Y. In Proposition B.5.1 these fields are assumed to be merely differentiable. Subsequently we provide the proof of Theorem B.2.6, which deals with fields of class C^{k+1} for $k \in \mathbb{N}$.

The following result, which does not require an iterative scheme, is known in the special case where Y_β is the derivative of a scalar function [7, 10]. In this setting, the existence of a metric with the desired property away from critical points is proved in [7]. The construction of the metric below is taken from there. It relies on the unique decomposition of vector fields into a component parallel to X and a component annihilating Y, which only works away from critical points. The proof of the existence of a continuous extension to all of M is adapted from [10].

Proposition B.5.1 (Existence of a continuous metric)**.** *Let X^α and Y_β be differentiable fields on M and suppose that the bilinear form $\nabla_\alpha Y_\beta|_m$ is non-degenerate for all $m \in \mathsf{N}_Y$ for some (equivalently, any) connection ∇. Suppose that the following conditions hold:*

(i) $X^\alpha Y_\alpha|_m > 0$ *for all* $m \in M\backslash\mathsf{N}_Y$*;*

(ii) $X^\alpha|_m = 0$ *for all* $m \in \mathsf{N}_Y$*;*

(iii) *For all $m \in \mathsf{N}_Y$ there exists a scalar product $\bar{g}_m \in T_mM \otimes_S T_mM$, such that*

$$\nabla_\alpha Y_\gamma|_m = \bar{g}_{\beta\gamma}\nabla_\alpha X^\beta|_m,$$

where ∇_α is an arbitrary connection.

Then there exists a continuous metric $g_{\alpha\beta}$ on M satisfying $Y_\beta = g_{\alpha\beta}X^\alpha$.

Proof. Let $m \in M\backslash\mathsf{N}_Y$ be a non-critical point, hence $X|_m \neq 0$ and $Y|_m \neq 0$ by (ii). The assumption (i) implies that we have the direct sum decomposition $T_mM = Y_m^\perp \oplus \operatorname{span}\{X_m\}$, hence every vector $Z \in T_mM$ can be uniquely decomposed as

$$Z = Z^{(0)} + Z^{(1)}, \quad \text{with} \quad Z^{(0)} \in Y_m^\perp \quad and \quad Z^{(1)} := \frac{\langle Z, Y_m\rangle}{\langle X_m, Y_m\rangle}X_m \in \operatorname{span}\{X_m\}.$$

Let $g = g_{\alpha\beta}$ be an arbitrary continuous metric on M satisfying $g|_m = \bar{g}_m$ at all critical points $m \in \mathsf{N}_Y$. Following [7], we construct a perturbation of $\widetilde{g}$ as follows:

$$\widetilde{g}(Z, W) := g(Z^{(0)}, W^{(0)}) + \frac{\langle Z^{(1)}, Y\rangle\,\langle W^{(1)}, Y\rangle}{\langle X, Y\rangle}, \tag{B.5.1}$$

for $Z, W \in \Gamma(TM)$. In view of (i), it readily follows that g defines a continuous metric on $M\backslash\mathsf{N}_Y$. It remains to show that $\widetilde{g}$ can be continuously extended to all of M.

It will be convenient to use abstract index notation. Taking into account that $\langle Z^{(1)}, Y\rangle = \langle Z, Y\rangle$ and $\langle W^{(1)}, Y\rangle = \langle W, Y\rangle$, it follows from the definition that

$$\widetilde{g}_{\alpha\beta} = g_{\alpha\beta} + \frac{Y_\alpha Y_\beta - g_{\alpha\gamma}X^\gamma Y_\beta - g_{\gamma\beta}X^\gamma Y_\alpha}{X^\delta Y_\delta} + \frac{g_{\gamma\delta}X^\gamma X^\delta Y_\alpha Y_\beta}{(X^\delta Y_\delta)^2}.$$

Introducing the deficit $R_\beta := Y_\beta - g_{\alpha\beta}X^\alpha$, we can write

$$\widetilde{g}_{\alpha\beta} = g_{\alpha\beta} + \frac{R_\alpha Y_\beta + R_\beta Y_\alpha}{X^\delta Y_\delta} - \frac{R_\gamma X^\gamma Y_\alpha Y_\beta}{(X^\delta Y_\delta)^2}. \tag{B.5.2}$$

Fix a critical point $\bar{m} \in \mathsf{N}_Y$. Using assumptions (ii) and (iii) we shall show that $\widetilde{g}|_m \to g|_{\bar{m}}$ as $m \to \bar{m}$, following the arguments in [10]. Using the notation from Section B.4, we shall perform a Taylor expansion of the terms in (B.5.2) in a fixed chart, where $\bar{m} \in M$ corresponds to $\bar{x} \in \mathbb{R}^n$. As X and Y are differentiable, and $\bar{x}$ is a critical point, it follows from (ii) that

$$X^a(x) = \nabla_c X^a(\bar{x})(x-\bar{x})^c + o\big(|x-\bar{x}|\big) \quad \textit{and} \quad Y_b(x) = \nabla_c Y_b(\bar{x})(x-\bar{x})^c + o\big(|x-\bar{x}|\big). \tag{B.5.3}$$

Since $\bar{g}_{ab}(\bar{x})$ is a scalar product, there exists $\kappa > 0$ such that $\bar{g}_{ab}(\bar{x})v^a v^b \geqslant \kappa|v|^2$ for all $v \in \mathbb{R}^n$. Furthermore, $\nabla_b X^a$ is non-degenerate by assumption (iii) and the non-degeneracy assumption on $\nabla_b Y^a$. Therefore, $|\nabla_b X^a v|^2 \geqslant \widetilde{\kappa}|v|^2$ for some constant $\widetilde{\kappa} > 0$. Using these inequalities, together with (iii), yields

$$\begin{aligned} X^a Y_a(x) &= \nabla_b X^a(\bar{x})\nabla_c Y_a(\bar{x})(x-\bar{x})^b(x-\bar{x})^c + o\big(|x-\bar{x}|^2\big) \\ &= \bar{g}_{ad}(\bar{x})\nabla_b X^a(\bar{x})\nabla_c X^d(\bar{x})(x-\bar{x})^b(x-\bar{x})^c + o\big(|x-\bar{x}|^2\big) \\ &\geqslant \kappa\big|\nabla_b X^a(\bar{x})(x-\bar{x})^b\big|^2 + o\big(|x-\bar{x}|^2\big) \\ &\geqslant \kappa\widetilde{\kappa}|x-\bar{x}|^2 + o\big(|x-\bar{x}|^2\big), \end{aligned} \tag{B.5.4}$$

which bounds the denominator in (B.5.2) from below. As for the terms in the numerator, we first note that $X^a(x) = O\big(|x-\bar{x}|\big)$ and $Y_b(x) = O\big(|x-\bar{x}|\big)$. These bounds trivially imply that $R_b(x) = O\big(|x-\bar{x}|\big)$ as well, but this is not sufficient. The key point of the proof is that this bound can be improved. Indeed, using (iii) and the continuity of g at $\bar{x}$, we obtain

$$\begin{aligned} R_b(x) &= \big(Y_b - g_{ab}X^a\big)(x) \\ &= \nabla_c Y_b(\bar{x})(x-\bar{x})^c - g_{ab}(x)\nabla_c X^a(\bar{x})(x-\bar{x})^c + o(|x-\bar{x}|) \\ &= \big(\bar{g}_{ab}(x) - g_{ab}(x)\big)\nabla_c X^a(\bar{x})(x-\bar{x})^c + o(|x-\bar{x}|) \\ &= o\big(|x-\bar{x}|\big). \end{aligned} \tag{B.5.5}$$

It now follows from (B.5.4) and (B.5.5) together with the bounds on X and Y, that the fractions in (B.5.2) vanish as $x \to \bar{x}$. This shows that $\widetilde{g}$ can be continuously extended to M by setting $\widetilde{g}_{ab}(\bar{x}) := \bar{g}_{ab}(\bar{x})$. ∎

While the metric $\widetilde{g}$ constructed in the proof of Proposition B.5.1 is continuous, it is *not* in general differentiable, even if the background metric $g_{\alpha\beta}$ and the vector fields X^α and Y_β are smooth. Here is an explicit counterexample.

Example B.5.2. Let M be the open unit ball in $\mathbb{R}^2$. We work in cartesian coordinates. Set $X(x) = Y(x) = x$ for $x \in M$, and consider the background metric $g_{\alpha\beta}$ defined by

$$g_{ab}(x) := \begin{bmatrix} 1+x_2 & 0 \\ 0 & 1 \end{bmatrix}$$

for $x = (x_1, x_2) \in M$. Since g is smooth and $g|_0 = I$, it is a valid background metric. An explicit computation yields

$$\widetilde{g}_{11}(x) = 1 + \frac{x_2^5}{(x_1^2+x_2^2)^2} \quad \textit{and} \quad \nabla_1\widetilde{g}_{11}(x) = -4\frac{x_1 x_2^5}{(x_1^2+x_2^2)^3}.$$

The latter is a non-constant homogeneous function and as such discontinuous at $x = 0$, thus $\widetilde{g}_{\alpha\beta}$ does not belong to C^1.

Theorem B.2.6 shows that better regularity properties can be obtained by a careful choice of the background metric $g_{\alpha\beta}$. In the following proof we define $g_{\alpha\beta}$ by making use of the construction in Section B.4, which yields improved bounds on the deficit $R_\beta := Y_\beta - g_{\alpha\beta}X^\alpha$ around critical points. This allows us to construct a metric $\widetilde{g}_{\alpha\beta}$ of class C^k whenever X^α and Y_β are of class C^{k+1}.

Proof of Theorem B.2.6. First we note that the necessity of conditions (i) and (ii) was already observed in the introduction. The necessity of (iii) follows, even when g is assumed to be merely continuous, from the expansions for X and Y in (B.5.3) and the expansion $g(x) = g(\bar{x}) + o\big(|x - \bar{x}|\big)$ in local coordinates around a critical point $\bar{x}$. Therefore it remains to show that these three conditions are also sufficient.

As in Proposition B.5.1, we construct a metric of the form (B.5.2) on the non-critical set $M \backslash \mathsf{N}_Y$:

$$\widetilde{g}_{\alpha\beta} = g_{\alpha\beta} + \frac{R_\alpha Y_\beta + R_\beta Y_\alpha}{X^\delta Y_\delta} - \frac{R_\gamma X^\gamma Y_\alpha Y_\beta}{(X^\delta Y_\delta)^2}, \tag{B.5.6}$$

where $R_\beta := Y_\beta - g_{\alpha\beta}X^\alpha$ denotes the deficit, and $g_{\alpha\beta}$ is a background metric on M that will be carefully chosen below. As noted before, it is immediate to verify that the desired identity $Y_\beta = \widetilde{g}_{\alpha\beta}X^\alpha$ holds on $M \backslash \mathsf{N}_Y$.

Construction of the background metric. Fix $\bar{m} \in \mathsf{N}_Y$. As in Section B.4 we work in a fixed coordinate chart where $\bar{m}$ corresponds to $\bar{x} \in \mathbb{R}^n$. In these local coordinates we then define the background metric by

$$g_{\bar{m}}^{ab}(x) := \sum_{N=0}^{k} \frac{1}{N!} T^{ab}_{c_1 \cdots c_N} (x - \bar{x})^{c_1} \cdots (x - \bar{x})^{c_N}$$

for x in a small neigbourhood around $\bar{x}$. It is crucial that we use the tensors $T^{\alpha\beta}_{\gamma_1 \cdots \gamma_N}$ that were constructed in Definition B.4.3. Note that $T^{\alpha\beta}_{\gamma_1 \cdots \gamma_N}$ is indeed well defined for $N \leqslant k$ due to our assumption that X^α and Y_β are $k + 1$ times continuously differentiable. As $T^{\alpha\beta}$ is positive definite, it follows that $(g_{\bar{m}})_{\alpha\beta}$ defines a metric in a neighbourhood of $\bar{x}$.

For each cricitical point $\bar{m}$, this construction yields a Riemannian metric in an open neighbourhood $\mathcal{V}_{\bar{m}}$ of $\bar{m}$. By the non-degeneracy assumption, we may assume that the sets $\{\mathcal{V}_{\bar{m}}\}_{\bar{m} \in \mathsf{N}_Y}$ are pairwise disjoint. Let $\mathcal{U}_{\bar{m}}$ be an open neighbourhood of $\bar{m}$ satisfying $\overline{\mathcal{U}_{\bar{m}}} \subseteq \mathcal{V}_{\bar{m}}$ and let $f_{\bar{m}} : M \to [0,1]$ be a smooth function on M satisfying $f_{\bar{m}}|_{\mathcal{U}_{\bar{m}}} = 1$ and $f_{\bar{m}}|_{M \backslash \mathcal{V}_{\bar{m}}} = 0$. Using an arbitrary metric $(g_*)_{\alpha\beta}$ on M and the function $\widetilde{f} := 1 - \sum_{\bar{m} \in \mathsf{N}_Y} f_{\bar{m}}$, we define

$$g_{\alpha\beta} := \sum_{\bar{m} \in \mathsf{N}_Y} f_{\bar{m}} (g_{\bar{m}})_{\alpha\beta} + \widetilde{f}\widetilde{g}_{\alpha\beta}, \tag{B.5.7}$$

which yields a C^k metric $g_{\alpha\beta}$ on M satisfying $g_{\alpha\beta}|_m = (g_{\bar{m}})_{\alpha\beta}|_m$ for all $\bar{m} \in \mathsf{N}_Y$ and $m \in \mathcal{U}_{\bar{m}}$.

The crucial property of this background metric g, which will be used below, is that the deficit $R_\beta := Y_\beta - g_{\alpha\beta}X^\alpha$ satisfies

$$\partial_{c_1} \cdots \partial_{c_p} R_\beta|_{\bar{m}} = 0 \tag{B.5.8}$$

for all $\bar{m} \in \mathsf{N}_Y$ and $p \leqslant k+1$. This follows from the definition of the tensors $T^{ab}_{c_1 \cdots c_N}$ using the computation (B.4.10).

Differentiability of the metric. To verify that $\tilde{g}_{\alpha\beta}$ is k times continuously differentiable, we will show that the partial derivatives

$$U_{\alpha\beta\, c_1 \dots c_p} := \partial_{c_1} \cdots \partial_{c_p} \frac{R_\alpha Y_\beta}{X^\delta Y_\delta} \quad \textit{and} \quad V_{\alpha\beta\, c_1 \dots c_p} := \partial_{c_1} \cdots \partial_{c_p} \frac{R_\gamma X^\gamma Y_\alpha Y_\beta}{(X^\delta Y_\delta)^2}$$

can be continuously extended from $M \backslash \mathsf{N}_Y$ to all of M for $p \leqslant k$. In view of (B.5.6) this yields the desired result.

We use the notation from Definition B.4.3, thus $\partial_{c_S} = \partial_{c_{i_1}} \cdots \partial_{c_{i_q}}$ for $S = \{i_1, \dots, i_q\} \subseteq \{1, \dots, p\}$ with $i_\mu \neq i_\nu$ for $\mu \neq \nu$. With this notation we have

$$U_{\alpha\beta\, c_1 \dots c_p} = \sum_{\ell=0}^{p} \sum_{\{S_1, \dots, S_\ell, A, B\} \in \mathcal{X}_p} \frac{(-1)^\ell \ell!}{\left(X^\delta Y_\delta\right)^{\ell+1}} \partial_{c_{S_1}}\!\left(X^\delta Y_\delta\right) \cdots \partial_{c_{S_\ell}}\!\left(X^\delta Y_\delta\right) \partial_{c_A} R_\alpha \, \partial_{c_B} Y_\beta,$$

$$V_{\alpha\beta\, c_1 \dots c_p} = \sum_{\ell=0}^{p} \sum_{\{S_1, \dots, S_\ell, A, B\} \in \mathcal{X}_p} \frac{(-1)^\ell \ell!}{\left(X^\delta Y_\delta\right)^{2(\ell+1)}} \partial_{c_{S_1}}\!\left(X^\delta Y_\delta\right)^2 \cdots \partial_{c_{S_\ell}}\!\left(X^\delta Y_\delta\right)^2 \partial_{c_A} R_\gamma \, \partial_{c_B}\!\left(X^\gamma Y_\alpha Y_\beta\right),$$

where $\mathcal{X}_p$ is the collection of all possible partitions of $\{1, \dots, p\}$.

Let us fix a critical point $\bar{m} \in \mathsf{N}_Y$ and let $\bar{x}$ be the corresponding point in $\mathbb{R}^n$. Recall from (B.5.4) that

$$\left(X^\delta Y_\delta\right)^{-1}(x) = O\big(|x - \bar{x}|^{-2}\big).$$

Furthermore, since $X^\alpha|_{\bar{x}} = 0$ and $Y_\alpha|_{\bar{x}} = 0$, Taylor's formula yields, for any $S \subseteq \{1, \dots, p\}$,

$$\partial_{c_S}\!\left(X^\delta Y_\delta\right)(x) = O\big(|x - \bar{x}|^{(2-|S|)_+}\big), \qquad \partial_{c_S} Y_\beta(x) = O\big(|x - \bar{x}|^{(1-|S|)_+}\big),$$
$$\partial_{c_S}\!\left(X^\delta Y_\delta\right)^2(x) = O\big(|x - \bar{x}|^{(4-|S|)_+}\big), \qquad \partial_{c_S}\!\left(X^\gamma Y_\alpha Y_\beta\right)(x) = O\big(|x - \bar{x}|^{(3-|S|)_+}\big).$$

To estimate $\partial_{c_S} R_\alpha(x)$ we use the crucial point, observed in (B.5.8), that our background metric is constructed so that $\partial_{c_S} R_\beta(\bar{x}) = 0$ when $|S| \leqslant k+1$. This ensures that

$$\partial_{c_S} R_\alpha(x) = O\big(|x - \bar{x}|^{k+2-|S|}\big).$$

Combining these bounds, we estimate the right-hand sides of $U_{\alpha\beta\, c_1 \dots c_p}$ and $V_{\alpha\beta\, c_1 \dots c_p}$ as follows:

$$\frac{1}{\left(X^\delta Y_\delta\right)^{\ell+1}} \partial_{c_{S_1}}\!\left(X^\delta Y_\delta\right) \cdots \partial_{c_{S_\ell}}\!\left(X^\delta Y_\delta\right) \partial_{c_A} R_\alpha \, \partial_{c_B} Y_\beta = O\big(|x - \bar{x}|^u\big),$$
$$\frac{1}{\left(X^\delta Y_\delta\right)^{2(\ell+1)}} \partial_{c_{S_1}}\!\left(X^\delta Y_\delta\right)^2 \cdots \partial_{c_{S_\ell}}\!\left(X^\delta Y_\delta\right)^2 \partial_{c_A} R_\gamma \, \partial_{c_B}\!\left(X^\gamma Y_\alpha Y_\beta\right) = O\big(|x - \bar{x}|^v\big),$$

where the exponents u and v satisfy

$$u = -2(\ell+1) + \big(2 - |S_1|\big)_+ + \ldots + \big(2 - |S_\ell|\big)_+ + \big(k + 2 - |S_A|\big) + \big(1 - |S_B|\big)_+ \,,$$
$$v = -4(\ell+1) + \big(4 - |S_1|\big)_+ + \ldots + \big(4 - |S_\ell|\big)_+ + \big(k + 2 - |S_A|\big) + \big(3 - |S|\big)_+ \,.$$

Since $|S_1| + \cdots + |S_\ell| + |A| + |B| = p$ for $\{S_1, \dots, S_\ell, A, B\} \in \mathcal{X}_p$, we obtain $u \geqslant k - p + 1 \geqslant 1$ and $v \geqslant k - p + 1 \geqslant 1$, which shows that

$$U_{\alpha\beta\, c_1 \dots c_p} = O\big(|x - \bar{x}|\big) \quad \textit{and} \quad V_{\alpha\beta\, c_1 \dots c_p} = O\big(|x - \bar{x}|\big).$$

Therefore $U_{\alpha\beta\, c_1 \dots c_p}$ and $V_{\alpha\beta\, c_1 \dots c_p}$ can be extended continuously to all of M by assigning the value zero for $\bar{m} \in \mathsf{N}_Y$. ■

B.6 Application to Quantum Markov Semigroups (QMS)

In this section prove Theorem B.1.2 by an application of Corollary B.2.5. As in Section B.1, let $\mathscr{L}$ be the generator of an ergodic quantum Markov semigroup $(\mathscr{P}_t)_{t\geqslant 0}$ on a finite dimensional C^*-algebra $\mathcal{A}$ with stationary state $\sigma \in \mathfrak{P}_+$. The manifold under consideration is the set of strictly positive density matrices

$$\mathfrak{P}_+ = \{\rho \in \mathfrak{P} \;:\; \rho > 0\}.$$

Note that $\mathfrak{P}_+$ is a relatively open subset of the affine space $\sigma + T \subseteq \mathcal{A}$, where

$$T := \{A \in \mathcal{A} \;:\; A = A^*,\; \mathrm{Tr}[A] = 0\}.$$

Therefore, the tangent space of $\mathfrak{P}_+$ can be naturally identified with T. We will apply Corollary B.2.5 to the triple (M, f, X) where $M := \mathfrak{P}_+$ and

$$\begin{aligned} f &: \mathfrak{P}_+ \to \mathbb{R}, & f(\sigma) &:= H_\sigma(\rho) = \mathrm{Tr}[\rho(\log\rho - \log\sigma)],\\ X &: \mathfrak{P}_+ \to T, & X(\rho) &:= \mathscr{L}^\dagger \rho. \end{aligned}$$

The functional H_σ is everywhere strictly positive, except at its global minimum σ. Moreover, a standard computation shows that, for $\rho \in \mathfrak{P}_+$ and $A \in T$,

$$\partial_\varepsilon\big|_{\varepsilon=0} H_\sigma(\rho + \varepsilon A) = \mathrm{Tr}[(\log\rho - \log\sigma)A], \tag{B.6.1}$$

Therefore, the differential of H_σ is everywhere non-zero except at σ, so that we are in a position to apply Corollary B.2.5.

Recall that we are interested in the BKM-scalar product on $\mathcal{A}$ given by

$$\langle A, B\rangle_\sigma^{\mathrm{BKM}} := \mathrm{Tr}[A^* \mathscr{M}_\sigma(B)], \quad \text{where } \mathscr{M}_\sigma(B) := \int_0^1 \sigma^{1-s} B \sigma^s \,\mathrm{d}s,$$

for $A, B \in \mathcal{A}$. We refer to [5] for a recent study of this scalar product. It is natural to also consider the inner product on $\mathcal{A}$ defined in terms of the inverse operator $\mathscr{M}_\sigma^{-1} : \mathcal{A} \to \mathcal{A}$ given by

$$\langle A, B\rangle_\sigma^{\widetilde{\mathrm{BKM}}} := \mathrm{Tr}[A^* \mathscr{M}_\sigma^{-1}(B)], \quad \text{where } \mathscr{M}_\sigma^{-1}(B) := \int_0^\infty (t+\sigma)^{-1} B (t+\sigma)^{-1} \,\mathrm{d}t.$$

We will use the following simple result.

Lemma B.6.1. *For a linear operator $\mathscr{K} : \mathcal{A} \to \mathcal{A}$ the following assertions are equivalent:*

1. *$\mathscr{K}$ is selfadjoint with respect to the inner product $\langle \cdot, \cdot\rangle_\sigma^{\mathrm{BKM}}$.*
2. *$\mathscr{K}^\dagger$ is selfadjoint with respect to the inner product $\langle \cdot, \cdot\rangle_\sigma^{\widetilde{\mathrm{BKM}}}$.*

Proof. It is readily seen that both assertions are equivalent to $\mathscr{M}_\sigma \mathscr{K} = \mathscr{K}^\dagger \mathscr{M}_\sigma$. ∎

The *entropy production functional* $I_\sigma : \mathfrak{P}_+ \to \mathbb{R}$ is defined by

$$I_\sigma(\rho) = -\operatorname{Tr}[(\log\rho - \log\sigma)\mathscr{L}^\dagger\rho]$$

for $\rho \in \mathfrak{P}_+$. Note that indeed $\frac{\mathrm{d}}{\mathrm{d}t}H_\sigma(\mathscr{P}_t^\dagger\rho) = -I_\sigma(\mathscr{P}_t^\dagger\rho)$. The functional I_σ is nonnegative and convex [117, 118]. The following result shows the *strict* positivity of the entropy production (except at stationarity) under the assumption of BKM-detailed balance.

Proposition B.6.2. *Let $\mathscr{L}$ be the generator of an ergodic quantum Markov semigroup on a finite dimensional C^*-algebra $\mathcal{A}$, with invariant state $\sigma \in \mathfrak{P}_+$. If* BKM*-detailed balance holds, then $I_\sigma(\rho) > 0$ for all $\rho \in \mathfrak{P}_+$ with $\rho \neq \sigma$.*

Proof. As remarked above, I_σ is nonnegative and convex. Therefore, it suffices to show that I_σ is strictly convex at its minimum σ. Take $A \in T$ with $A \neq 0$.

For $\rho \in \mathfrak{P}_+$ we set $\rho_\varepsilon := \rho + \varepsilon A$ for $|\varepsilon|$ sufficiently small to ensure that $\rho_\varepsilon \in \mathfrak{P}_+$. Using the standard identities

$$\partial_\varepsilon\big|_{\varepsilon=0}\log\rho_\varepsilon = \int_0^\infty (t+\rho)^{-1}A(t+\rho)^{-1}\,\mathrm{d}t \quad \textit{and} \quad \partial_\varepsilon\big|_{\varepsilon=0}(s+\rho_\varepsilon)^{-1} = -(s+\rho)^{-1}A(s+\rho)^{-1}$$

for $s > 0$, we obtain

$$\partial_\varepsilon\big|_{\varepsilon=0}I_\sigma(\rho_\varepsilon) = \operatorname{Tr}[(\log\rho - \log\sigma)\mathscr{L}^\dagger A] + \operatorname{Tr}\left[\int_0^\infty (t+\rho)^{-1}A(t+\rho)^{-1}\mathscr{L}^\dagger\rho\,\mathrm{d}t\right],$$

and

$$\begin{aligned}\partial_\varepsilon^2\big|_{\varepsilon=0}I_\sigma(\rho_\varepsilon) &= 2\operatorname{Tr}\left[\int_0^\infty (t+\rho)^{-1}A(t+\rho)^{-1}\mathscr{L}^\dagger A\,\mathrm{d}t\right] \\ &\quad - 2\operatorname{Tr}\left[\int_0^\infty (t+\rho)^{-1}A(t+\rho)^{-1}A(t+\rho)^{-1}\mathscr{L}^\dagger\rho\,\mathrm{d}t\right].\end{aligned}$$

In particular, for $\sigma_\varepsilon := \sigma + \varepsilon A$, we obtain

$$\partial_\varepsilon^2\big|_{\varepsilon=0}I_\sigma(\sigma_\varepsilon) = 2\operatorname{Tr}\left[\int_0^\infty (t+\sigma)^{-1}A(t+\sigma)^{-1}\mathscr{L}^\dagger A\,\mathrm{d}t\right] = 2\langle A, \mathscr{L}^\dagger A\rangle_\sigma^{\widetilde{\mathrm{BKM}}}.$$

Since I_σ is convex, this identity implies that $\langle A, \mathscr{L}^\dagger A\rangle_\sigma^{\widetilde{\mathrm{BKM}}} \geqslant 0$.

On the other hand, $\mathscr{L}^\dagger$ is selfadjoint with respect to $\langle\cdot,\cdot\rangle_\sigma^{\widetilde{\mathrm{BKM}}}$ by Lemma B.6.1 and the assumption of BKM-detailed balance. Moreover, the restriction of $\mathscr{L}^\dagger$ to T is invertible by the ergodicity assumption. Therefore, $\langle A, \mathscr{L}^\dagger A\rangle_\sigma^{\widetilde{\mathrm{BKM}}} \neq 0$.

We thus conclude that $\langle A, \mathscr{L}^\dagger A\rangle_\sigma^{\widetilde{\mathrm{BKM}}} > 0$, which yields the result. ■

Proof of Theorem B.1.2. First we will translate condition (iii) of Corollary B.2.5, namely the selfadjointness of the linearised operator Λ with respect to the Hessian scalar product h. We claim that this is exactly the assumption of BKM-detailed balance in our setting.

Indeed, since $\mathscr{L}^\dagger$ is a linear operator, its linearisation $\Lambda : T \to T$ appearing in condition (iii) is simply given by $\Lambda := \mathscr{L}^\dagger$. Moreover, the Hessian of $\rho \mapsto H_\sigma(\rho)$ at $\rho = \sigma$ is given by

$$h(A,B) := \partial_\varepsilon\big|_{\varepsilon=0}\partial_\eta\big|_{\eta=0}H_\sigma\big(\sigma + \varepsilon A + \eta B\big) = \int_0^\infty \operatorname{Tr}\left[\frac{1}{s+\sigma}A\frac{1}{s+\sigma}B\right]\mathrm{d}s = \langle A, B\rangle_\sigma^{\widetilde{\mathrm{BKM}}}$$

for $A, B \in T$. Hence the Hessian scalar product in condition (iii) is the $\widetilde{\mathrm{BKM}}$-scalar product. Thus, condition (iii) is the $\widetilde{\mathrm{BKM}}$-selfadjointness of $\mathscr{L}^\dagger$. By Lemma B.6.1 this corresponds to the BKM-selfadjointness of $\mathscr{L}$, which is the assumption of BKM-detailed balance.

This argument shows that the necessity of BKM-detailed balance for the gradient flow structure follows from Corollary B.2.5. To show that BKM-detailed balance is also sufficient, we note first that condition (ii) of Corollary B.2.5 is simply the stationarity condition $\mathscr{L}^\dagger\sigma = 0$, which holds by assumption. Thus, it remains to show that condition (i) of Corollary B.2.5 is implied by the assumption of BKM-detailed balance. Then the existence of the gradient flow structure follows by applying Corollary B.2.5 in the opposite direction.

For this purpose, recall that $f = H_\sigma$ and $X = \mathscr{L}^\dagger$, so that

$$\nabla_X f = \mathrm{Tr}[(\log\rho - \log\sigma)\mathscr{L}^\dagger\rho] = -I_\sigma.$$

Hence, condition (i) is the strict positivity of the entropy production $I_\sigma(\rho)$ or $\rho \neq \sigma$, which follows from the assumption of BKM-detailed balance by Proposition B.6.2. ■

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