The Polaron at Strong Coupling

Classical and Quantum Behavior

by

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Abstract

This thesis is the result of the research carried out by the author during his PhD at IST Austria between 2017 and 2021. It mainly focuses on the Fröhlich polaron model, specifically to its regime of strong coupling. This model, which is rigorously introduced and discussed in the introduction, has been of great interest in condensed matter physics and field theory for more than eighty years. It is used to describe an electron interacting with the atoms of a solid material (the strength of this interaction is modeled by the presence of a coupling constant α in the Hamiltonian of the system). The particular regime examined here, which is mathematically described by considering the limit $\alpha \to \infty$, displays many interesting features related to the emergence of classical behavior, which allows for a simplified effective description of the system under analysis. The properties, the range of validity and a quantitative analysis of the precision of such classical approximations are the main object of the present work. We specify our investigation to the study of the ground state energy of the system, its dynamics and its effective mass. For each of these problems, we provide in the introduction an overview of the previously known results and a detailed account of the original contributions by the author ([32, 33, 35, 36], the content of Chapters 2, 3, 4 and 5, respectively). Here a short overview.

- **Ground State Energy**: we are particularly interested in the second order expansion in α, as $\alpha \to \infty$, of the ground state energy of the system. In order to understand it, one needs to go beyond the first order classical approximation of the system and factor in the full quantum nature of the problem. The first work successfully dealing with this question is [41], which works in the case of a polaron confined to a bounded domain. In collaboration with the PhD supervisor, the author of this thesis proves in [32] the validity of some assumptions made in [41]. Moreover, [33] represents the first investigation of the problem carried out in a translational invariant setting, namely a three dimensional torus.
- **Dynamics**: in the limit $\alpha \to \infty$, the dynamics of the polaron is approximated by simpler evolution equations, called Landau–Pekar (LP) equations. In [35], a set of initial states is identified, such that the validity (in time) of such approximation is extended in comparison to previously known results ([73, 74]).
- **Effective Mass**: [36] represents a recent attempt of investigating the effective mass of the system looking at its effective evolution equations, i.e. the LP equations.

Finally, the appendix is dedicated to [34], a project carried out by the author in the very different field of optimal tranport. It accounts for a successful attempt of extending techniques from commutative optimal transport to the quantum (and non-commutative) framework. In this sense, the appendix can be seen as yet another instance of interplay between the classical and the quantum world.

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About the Author

Dario Feliciangeli completed a BSc and a MSc in Mathematics at Sapienza University in Rome, before joining IST Austria in September 2017 and the group of Professor Robert Seiringer in 2018. His main research interests include quantum many-body problems and optimal transport.

List of Collaborators and Publications

This thesis contains the two following published papers

- Dario Feliciangeli and Robert Seiringer. Uniqueness and nondegeneracy of minimizers of the Pekar functional on a ball. *SIAM Journal on Mathematical Analysis*, 52(1):605–622, 2020,
- Dario Feliciangeli, Simone Rademacher, and Robert Seiringer. Persistence of the spectral gap for the Landau–Pekar equations. *Letters in Mathematical Physics*, 111(1):1–19, 2021.

It also contains the submitted papers

- Dario Feliciangeli and Robert Seiringer. The strongly coupled polaron on the torus: quantum corrections to the Pekar asymptotics. *arXiv preprint arXiv:2101.12566*, 2021,
- Dario Feliciangeli, Simone Rademacher, and Robert Seiringer. Effective mass of the polaron via Landau-Pekar equations. *arXiv preprint arXiv:2107.03720*, 2021.

Finally, the appendix contains the submitted paper

- Dario Feliciangeli, Augusto Gerolin, and Lorenzo Portinale. A non-commutative entropic optimal transport approach to quantum composite systems at positive temperature. *arXiv preprint arXiv:2106.11217*, 2021.

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CHAPTER 1

Introduction

Ubiquitously in mathematics and physics, one encounters situations in which the problem under consideration, in some specific regime of its parameters, displays particular or simplified behavior. A particular instance of such phenomena, arguably among the most fascinating and somewhat magical in our disciplines, is the one of a very complicated system effectively described by some simpler equation or law, again in some specific range of parameters. This case is very common in physics, where several models do simplify drastically in particular limiting regime (e.g., small or large temperature or density). Furthermore, in quantum many-body systems, where a precise study of the full system is often too complicated to be carried out, this kind of analysis is sometimes the only one possible, at the same time still being extremely interesting: it sheds light on the emergence of particular behavior and on the range of validity and the precision of approximate descriptions, like classical approximations of quantum systems. This leads, with both aesthetical and scientific motivations, to the model considered in this work, which is a prime example of these latter situations: the polaron model, particularly its strong coupling regime.

1.1 The Polaron Model

Consider a negatively charged particle, an electron, embedded in a sea of neutral particles arranged in lattice configuration, a crystal. Through its electrical field, the electron polarizes the neutral particles, which naturally arrange themselves as dipoles pointing towards the electron and generate a dipole potential on it, affecting its state. Through this interaction, the electron is coupled to the neutral particles and the resulting system is very complicated to describe in quantum-mechanical terms. In the following, we shall refer to the neutral particles and to the dipoles associated to them as *phonons* and to the whole system as the *polaron*.

We specialize to the case of a large polaron, namely one where the lattice is so fine that its spacing is much smaller than the De Broglie wavelength of the electron and therefore can be approximated by a continuous medium. In this case the relevant Hamiltonian for the system is the Fröhlich Hamiltonian, introduced in [47] and defined below in (1.1.13). A first rigorous attempt of studying this model was carried out by Landau in [67]. Later, H. Fröhlich and S. Pekar (see [48] and [95]) and Landau again (see [66]) were the main early contributors to lay the foundations of the polaron theory. It was Pekar who also coined the name polaron to describe this newly introduced quasi-particle.

The model, which we shall always consider in three dimensions but in a few different settings, has one dimensionless coupling constant α, which models the strength of the interaction between the electron and the neutral particles. This constant heavily influences the analysis of the system, there being a big difference between the two regimes of weak and strong coupling, respectively corresponding to small and large α. At weak coupling, the system is well described by perturbation theory and its behavior was rigorously understood quite early on (see [37], [60], [69], [68], [83]). At strong coupling, the polaron model displays instead the kind of classical simplifications we mentioned above and, even if some heuristic guesses (which turned out to be correct) were already made in the 50s (see [95] and [66]), it was not before the 80s that the first rigorous results were proven in this regime (see [30]). We shall thoroughly explain this after having rigorously introduced the model.

1.1.1 State Spaces

We first introduce the state spaces of the electron and of the phonons in the case of an unconfined polaron on $\mathbb{R}^3$. For the electron the situation is simple enough and the state space is given by $L^2(\mathbb{R}^3)$. On the other hand, the state space of the phonons is a bosonic Fock space over $L^2(\mathbb{R}^3)$, denoted by $\mathcal{F}(L^2(\mathbb{R}^3))$ and defined by

$$\mathcal{F}(L^2(\mathbb{R}^3)) := \bigoplus_{n=0}^{\infty} \mathfrak{h}_n, \tag{1.1.1}$$

where $\mathfrak{h}_n = \otimes^n_{\mathsf{sym.}} L^2(\mathbb{R}^3)$ denotes the permutation symmetric functions in $\otimes^n L^2(\mathbb{R}^3)$. A first motivation to use this space is given by the fact that the phonons have to be treated as a quantum field of excitations (the collective displacements of the neutral charges which arrange themselves as dipoles) but we shall below further justify this choice. Before, we recall some general facts about the bosonic Fock space. We call *vacuum* the only normalized element of $\otimes^0 L^2(\mathbb{R}^3) = \mathbb{C}$, this is customarily denoted by the symbol Ω. Furthermore, we define the number operator $\mathbb{N}$ as the operator on $\mathcal{F}(L^2(\mathbb{R}^3))$ acting on each $\mathfrak{h}_n$ as $n\mathbb{1}$. Given any $f \in L^2(\mathbb{R}^3)$, the corresponding bosonic annihilation operator is defined by

$$\begin{aligned} a(f) : \mathfrak{h}_n &\to \mathfrak{h}_{n-1} \\ \Psi_n &\mapsto \sqrt{n} \int_{\mathbb{R}^3} \overline{f(x_n)} \Psi_n(x_1, \dots, x_n) dx_n, \end{aligned} \tag{1.1.2}$$

and its adjoint, the corresponding bosonic creation operator, is defined by

$$\begin{aligned} a^\dagger(f_j) : \mathfrak{h}_{n-1} &\to \mathfrak{h}_n \\ \Psi_{n-1} &\mapsto \frac{1}{\sqrt{n}} (f \otimes_{\mathsf{sym.}} \Psi_{n-1}) := \frac{1}{\sqrt{n}} \sum_{k=1}^{n} f(x_k) \Psi_{n-1}(x_1, \dots, \not{x}_k, \dots, x_n). \end{aligned} \tag{1.1.3}$$

These operators satisfy the Canonical Commutation Relations (CCR)

$$[a(f), a^\dagger(g)] = \langle f | g \rangle_{L^2(\mathbb{R}^3)}, \quad [a(f), a(g)] = 0. \tag{1.1.4}$$

Note that one often formally writes

$$a^\dagger(f) = \int_{\mathbb{R}^3} dx\, f(x) a^\dagger_x = \int_{\mathbb{R}^3} dk\, \hat{f}(k) a^\dagger_k, \tag{1.1.5}$$

where $\hat{f}$ is the Fourier transform of f, $a^\dagger_x$ are operator valued distributions satisfying

$$[a_x, a^\dagger_{x'}] = \delta(x - x'), \quad [a_x, a_{x'}] = 0, \tag{1.1.6}$$

and $a_k^\dagger$ denotes, in a somewhat sloppy but quite useful notation, the Fourier transform of $a_x^\dagger$. Either using this formalism or defining $a_j^\dagger := a^\dagger(f_j)$ and $a_j := a(f_j)$ for a given orthonormal basis $\{f_j\}_{j\in\mathbb{N}} \subset L^2(\mathbb{R}^3)$, the number operator $\mathbb{N}$ introduced above can equivalently be written as

$$\mathbb{N} = \sum_j a_j^\dagger a_j = \int_{\mathbb{R}^3} dk\, a_k^\dagger a_k. \tag{1.1.7}$$

Observe that, given an orthonormal basis $\{f_j\}_{j\in\mathbb{N}} \subset L^2(\mathbb{R}^3)$, $\mathfrak{h}_n \subset \mathcal{F}(L^2(\mathbb{R}^3))$ is generated by all the words of length n in the symbols $\{a_j^\dagger\}_{j\in\mathbb{N}}$, modulo the permutation group $\mathcal{S}_n$, applied to the vacuum Ω.

To further justify the choice of $\mathcal{F}(L^2(\mathbb{R}^3))$ as a state space for the phonons, we first need to realize that a classical state of the phonon field is nothing else than a function which at any point in $y \in \mathbb{R}^3$ (recall that in a large polaron the lattice can be approximated by a continuous medium) gives the intensity, positive or negative, of the dipole moment centered at y (recall as well that the dipole is assumed to automatically align with the direction of the electron charge and therefore only the absolute value and the sign of its moment are relevant). As a second step, we need to introduce the Q-space representation of the bosonic Fock space (we shall here use a quite formal approach, we refer to [100] for a rigorous discussion). The key idea behind this construction is already contained in the case of a simple harmonic oscillator on $\mathbb{R}$. Given the Hamiltonian

$$H_{\mathsf{h.o.}} = -\frac{\partial_x^2}{2} + \frac{x^2}{2} \quad \text{on} \quad L^2(\mathbb{R}), \tag{1.1.8}$$

it is well known that there exists a basis $\{\varphi_j\}_{j=0}^\infty$ of eigenfunctions of $H_{\mathsf{h.o.}}$ of respective eigenvalue $1/2 + j$ and that there exist two operators $a^\dagger$ and a such that $a^\dagger\varphi_j = \sqrt{j+1}\varphi_{j+1}$ and $a\varphi_j = \sqrt{j}\varphi_{j-1}$. Therefore,

$$L^2(\mathbb{R}) = \operatorname{span}\{\varphi_j\}_{j=0}^\infty \simeq \mathcal{F}(\mathbb{C}), \tag{1.1.9}$$

with the isomorphism explicitly given by $\varphi_j = (j!)^{-1/2}(a^\dagger)^j\varphi_0 = (j!)^{-1/2}(a^\dagger)^j\Omega$, and the number operator which in this representation reads $\mathbb{N} = H_{\mathsf{h.o.}} - 1/2$. Similarly, one can see that

$$L^2(\mathbb{R}^N) = \otimes^N L^2(\mathbb{R}) \simeq \otimes^N \mathcal{F}(\mathbb{C}) = \mathcal{F}(\mathbb{C}^N), \tag{1.1.10}$$

with the difference that here there are N creation operators $a_1^\dagger, \dots, a_N^\dagger$ to apply to the vacuum to build $\mathcal{F}(\mathbb{C}^N)$, each one corresponding to one of the variables in $L^2(\mathbb{R}^N)$. The number operator on $\mathcal{F}(\mathbb{C}^N)$ can be written in this representation as $\mathbb{N} = \sum_{k=1}^N a_k^\dagger a_k = \sum_{k=1}^N [(H_{\mathsf{h.o.}})_{x_k} - 1/2] = -\Delta_{\mathbb{R}^N}/2 + \|x\|^2/2 - N/2$. This construction, which is rigorous as long as one deals with a finite number of factors, can be extended to the infinite dimensional case with some modifications and some extra effort (see [100]). Therefore, fixing an orthonormal basis $\{f_j\}_{j=1}^\infty \subset L^2(\mathbb{R}^3)$ and considering the associated $a_j^\dagger$ and a_j, allows, at least formally, to define an isomorphism between $\mathcal{F}(L^2(\mathbb{R}^3)) = \mathcal{F}(\mathbb{C}^\infty)$ and $L^2(\mathbb{R}^\infty)$. In light of this discussion, an element of $\mathcal{F}(L^2(\mathbb{R}^3))$ can be considered as a function of infinitely many variables y_j (we shall use the variable x for the spacial coordinate of the electron and prefer, to avoid confusion, to use the variables y for the position coordinates of the phonons), each one associated to the creation operator $a_j^\dagger$ corresponding to f_j. This finally allows to close the circle and justify the use of $\mathcal{F}$ as a quantum state space for the phonon field. Indeed, from this point of view, the modulus squared of any $\Psi \in \mathcal{F}(L^2(\mathbb{R}^3))$ can be thought of as a probability distribution over functions in $L^2(\mathbb{R}^3)$, i.e. classical states of the phonon field, where the expectation w.r.t. to y_k expresses the expected k-th coefficient in the fixed basis $\{f_j\}_{j=1}^{\infty}$. Note that this is in complete analogy with the case of the electron, whose classical states are positions $x \in \mathbb{R}^3$ and quantum states are functions in $L^2(\mathbb{R}^3)$ (i.e. functions whose modulus squared represent a probability distribution over classical states of the electron). Finally observe that the number operator can be written in this representation as

$$\mathbb{N} = \sum_{j=1}^{\infty}(-\partial_{y_j}^2/2 + y_j^2/2 - 1/2). \tag{1.1.11}$$

Note that this expression has to be handed carefully, since the summands are not summable individually.

1.1.2 Fröhlich Hamiltonian

Once we have introduced and discussed the state space of the electron and of the phonons, the state space of the full composite system is naturally given by the tensor product

$$\mathcal{S}_{\mathbb{R}^3} = L^2(\mathbb{R}^3) \otimes \mathcal{F}(L^2(\mathbb{R}^3)). \tag{1.1.12}$$

We are now ready to introduce the Fröhlich Hamiltonian [47] on $\mathcal{S}_{\mathbb{R}^3}$, it reads

$$H_\alpha = -\Delta \otimes \mathbb{1} + \mathbb{1} \otimes \left(\int_{\mathbb{R}^3} a_k^\dagger a_k dk\right) - \sqrt{\frac{\alpha}{2\pi^2}} \int_{\mathbb{R}^3} \frac{dk}{|k|} \left(a_k e^{ik\cdot x} + a_k^\dagger e^{-ik\cdot x}\right). \tag{1.1.13}$$

The first term accounts for the kinetic energy of the electron and the second, in which the number operator appears, for the field energy of the phonon field. The third term is an operator on $\mathcal{F}(L^2(\mathbb{R}^3))$ indexed by x, the position variable of the electron, and has to be understood as a multiplication operator on $L^2(\mathbb{R}^3)$. It explicitly depends on the coupling constant α and couples the electron with the phonons, accounting for the energy of their interaction.

For fixed $x \in \mathbb{R}^3$, the interaction term can be written as

$$-a(\sqrt{\alpha} v_x) - a^\dagger(\sqrt{\alpha} v_x) \tag{1.1.14}$$

with $\hat{v}_x(k) = (2\pi^2)^{-1/2}|k|^{-1}e^{-ik\cdot x}$, or equivalently

$$v_x(y) = (\pi^3)^{-1/2}|x-y|^{-2} = 2\pi^{1/2}(-\Delta)^{-1/2}(x,y). \tag{1.1.15}$$

Note that $v_x(y)$ coincides, up to constants, with the dipole potential exerted in the point x by a dipole pointing to x and center of mass in y. Recalling the physical picture that the polaron model describes, this makes perfect sense. Formally, we can write H_α using the Q-space representation introduced above for $\mathcal{F}(L^2(\mathbb{R}^3))$ and this justifies further its explicit expression. Fix an orthonormal basis $\{f_j\}_{j=1}^{\infty} \subset L^2(\mathbb{R}^3)$ and think of any element in $\mathcal{S}_{\mathbb{R}^3}$ as a function $\Psi(x, y_1, \dots, y_n, \dots)$ of infinitely many variables, where x is the variable corresponding to the electron and the y_j-s are the infinitely many variables corresponding to the phonons. Using that in Q-space one has $\frac{1}{\sqrt{2}}(a^\dagger(f_j) + a(f_j)) = y_j$ (see [100]), we can then write H_α as

$$\begin{aligned} H_\alpha &= -\Delta_x + \sum_{k=1}^{\infty}\left(-\frac{\Delta_{y_k}}{2} + \frac{|y_k|^2}{2} - \sqrt{2}\left\langle \sqrt{\alpha} v_x \middle| f_k\right\rangle_{L^2(\mathbb{R}^3)} y_k - 1/2\right) \\ &= -\Delta_x + \mathbb{N} + V(x, y_1, \dots, y_n, \dots), \end{aligned} \tag{1.1.16}$$

where $V(x, y_1, \dots)$ is understood as a multiplication operator which at any point $(x, y_1, \dots)$ represents, up to an α-dependent constant, the dipole potential generated at x by the classical dipole field $\sum_{j=1}^{\infty} y_j f_j$. Looking at the first expression in (1.1.16), we see that the model morally corresponds to a system of infinitely many harmonic oscillators, each interacting with the charge distribution of the electron via a dipole potential.

Going back to a more rigorous discussion of H_α, we now consider its well-posedness and domain. Since $v_x \notin L^2(\mathbb{R}^3)$, the definition of H_α is a priori ill-posed. Nevertheless, the presence of the Laplacian allows to make sense of H_α via its quadratic form, which can be shown to be closed and bounded from below. One way to show this is to use a technique which goes back to [83], known as Lieb-Yamazaki bound. The key idea is to exploit the following commutator identity

$$\frac{a_k}{|k|} e^{ik\cdot x} = \sum_{j=1}^{3} \left[p_j, \frac{k_j}{|k|^3} a_k e^{ik\cdot x} \right], \tag{1.1.17}$$

where $p = -i\nabla$. With some effort (we refer to [83, 82, 109] for details) this allows to apply an ultraviolet cutoff to the interaction term (i.e. restricting the integration only to $|k| \leq \Lambda$, for some finite Λ), at the price of a small kinetic energy contribution, which can be easily reabsorbed in H_α. Finally, this allows to show that

$$H_\alpha \geq -C\alpha^2 - 3/2. \tag{1.1.18}$$

Note that we always use the letter C to denote a generic positive constant independent of the other parameters of the problem, whereas we use the notation C_p to emphasize the dependence on a parameter p. This bound, as we shall see in Section 1.2.2, is not optimal (even if of the right order in α) but it is sufficient to show the stability of H_α and imply its well-posedness. We emphasize the importance of the Lieb-Yamazaki bound, which is used again in Section 1.2.3 in a more sophisticated manner (an idea introduced in [41] which basically consists in applying the Lieb-Yamazaki bound three times instead of just once). Another way of showing the well-posedness of the Fröhlich Hamiltonian, which also gives information about its explicit domain, utilizes a Gross transformation [58, 94], a unitary transformation on $\mathcal{S}_{\mathbb{R}^3}$ of the form

$$U = e^{a(f_x) - a^\dagger(f_x)}, \tag{1.1.19}$$

for an appropriate family of functions $f_x \subset L^2(\mathbb{R}^3)$ indexed by $x \in \mathbb{R}^3$. This approach (we refer to [57] for the details) allows to conclude

$$(1+\varepsilon)\|H_0\Psi\| + C_\varepsilon\|\Psi\| \leq \|UH_\alpha U^\dagger\Psi\| \leq (1-\varepsilon)\|H_0\Psi\| - C_\varepsilon\|\Psi\|, \tag{1.1.20}$$

where $H_0 = -\Delta + \mathbb{N}$, $0 < \varepsilon$ is arbitrary small and C_ε is a suitable α-dependent constant. In particular, this bound shows, when $\varepsilon < 1$, that the domain of $UH_\alpha U^\dagger$ coincides with the one of H_0.

Once we have discussed the well-posedness of H_α, we can define its ground state energy

$$e_\alpha := \inf \operatorname{spec} H_\alpha, \tag{1.1.21}$$

and the associated Schrödinger equation [47], which drives the dynamics of a large polaron and reads

$$i\frac{d}{dt}\Psi_t = H_\alpha \Psi_t. \tag{1.1.22}$$

We shall see, in Sections 1.2.2 and 1.3 respectively, that both e_α and equation (1.1.22) display classical behavior in the strong coupling regime.

The previous definitions and discussions apply also to the case of a confined polaron, with a few modifications which we discuss here. In particular, we are interested in the cases of a polaron confined to a bounded domain $\Omega \in \mathbb{R}^3$ with Dirichlet boundary conditions or to a three dimensional torus $\mathbb{T}^3_L$ of linear size L. The state spaces to consider are respectively

$$\mathcal{S}_\Omega := L^2(\Omega) \otimes \mathcal{F}(L^2(\Omega)), \quad \mathcal{S}_{\mathbb{T}^3_L} := L^2(\mathbb{T}^3_L) \otimes \mathcal{F}(L^2(\mathbb{T}^3_L)), \tag{1.1.23}$$

and the Fröhlich Hamiltonian reads

$$\begin{aligned} H_{\alpha,\Omega} &= -\Delta_\Omega \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{N}_\Omega - a(\sqrt{\alpha} v_x^\Omega) - a^\dagger(\sqrt{\alpha} v_x^\Omega) \\ H_{\alpha,\mathbb{T}^3_L} &= -\Delta_L \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{N}_{\mathbb{T}^3_L} - a(\sqrt{\alpha} v_x^L) - a^\dagger(\sqrt{\alpha} v_x^L). \end{aligned} \tag{1.1.24}$$

Here $-\Delta_\Omega$ and Δ_L denote respectively the Dirichlet Laplacian on Ω and the periodic Laplacian on $\mathbb{T}^3_L$, $\mathbb{N}_\Omega$ and $\mathbb{N}_{\mathbb{T}^3_L}$ are the number operators on $\mathcal{F}(L^2(\Omega))$ and $\mathcal{F}(L^2(\mathbb{T}^3_L))$, $v_x^\Omega = C(-\Delta_\Omega)^{-1/2}$ and $v_x^L = C(-\Delta_L)^{-1/2}$. Note that $(-\Delta_L)^{-1/2}$ is understood to be 0 on the kernel of $-\Delta_L$.

Before moving on to discuss the strong coupling regime of the polaron, we want to emphasize that the Fröhlich Hamiltonian for the polaron is part of a quite large family of similar Hamiltonians appearing often in physics and used as toy models for quantum field theory. These Hamiltonians are of the form

$$H = -\Delta - \int_{\mathbb{R}^3} dk\, v(k) \left(a_k e^{ik\cdot x} + a_k^\dagger e^{-ik\cdot x} \right) + \int_{\mathbb{R}^3} \omega(k) a_k^\dagger a_k, \tag{1.1.25}$$

and depend on the choice of v and ω. Examples are given by the Nelson model for quantum electrodynamics (where $v(k) \propto |k|^{-1/2}$ and $\omega(k) \propto |k|$ or more generally $\omega(k) \propto \sqrt{|k|^2 + m^2}$ for $m \geq 0$ [94]), and the spin bosons model [61] and the angulon model [107], in which the modifications are more substantial and involve also the state spaces and the couplings $e^{ik\cdot x}$.

1.1.3 The Strongly Coupled Polaron

As mentioned above, the system displays different behavior at weak and strong coupling. From now on, we specify to the regime of strong coupling, at which a very interesting classical simplification occurs. To be more precise, it is the quantum phonon field that in this regime can be treated classically, while the electron is still quantum.

We begin this discussion by giving an alternative form of H_α, retrieved by a simple change of variables. These new *strong coupling units* are the best suited to treat the strong coupling regime and immediately identify the right scalings as $\alpha \to \infty$, as we see below. We apply the following transformation

$$x \mapsto \alpha^{-1} x, \quad a_k \mapsto \alpha^{-1/2} a_{\alpha^{-1}k}. \tag{1.1.26}$$

A simple computation shows that in these units $H_\alpha = \alpha^2 \mathfrak{H}_\alpha$, where

$$\mathfrak{H}_\alpha = -\Delta \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{N} - a(v_x) - a^\dagger(v_x). \tag{1.1.27}$$

We see immediately that, in strong coupling units, all the terms of the Hamiltonian explicitly scale the same in α, namely as α^2, the prefactor relating H_α and $\mathfrak{H}_\alpha$. Nevertheless, the α

dependence is also present implicitly in the commutation relations of the rescaled creation and annihilation operators, which now satisfy

$$[a(f), a^\dagger(g)] = \frac{1}{\alpha^2} \langle f|g\rangle \,, \quad [a(f), a(g)] = 0. \tag{1.1.28}$$

Consequently, the spectrum of the number operator appearing in $\mathfrak{H}_\alpha$ is also rescaled and coincides with $\alpha^{-2}\{0, 1, 2, \dots\}$. Note that, in (1.1.28), the factor α^{-2} plays the role of an effective Planck constant, hinting to the classical behavior of the phonon field in the limit $\alpha \to \infty$, manifested by almost commuting field operators.

A multitude of questions naturally arise at this point: how can we exploit the rescaled commutation relations (1.1.28)? Is it possible to make rigorous the intuition, so far only heuristically justified, that classical behavior should arise in the limit $\alpha \to \infty$? Which properties of the system are we interested in investigating and which ones do we expect to be affected by a classical simplification in this regime? We shall carry out this discussion in three different parts, related to the three main properties of the system we are interested in:

- the first part concerns the ground state energy of the system, as defined in (1.1.21), and is the content of Section 1.2,
- the second part concerns the dynamics of a polaron, driven by equation (1.1.22), and is the content of Section 1.3
- the third part is related to the problem of defining and computing an effective mass of the polaron which, a priori, is not explicitly present in the model. This is the content of Section 1.4

1.2 The Polaron Ground State Energy at Strong Coupling

We begin with some heuristic computations, which serve as a bridge to then explain the main known results related to the computation of e_α in the strong coupling regime.

We emphasize that, instead of computing e_α, we prefer to work with

$$E_\alpha := \inf \operatorname{spec} \mathfrak{H}_\alpha = \alpha^{-2} e_\alpha, \tag{1.2.1}$$

since this quantity is order 1 to leading order in α, as we shall see. Note that the bound (1.1.18) already shows $E_\alpha \geq -C$, i.e. that E_α is at most order 1 in α as $\alpha \to \infty$.

1.2.1 $\mathbb{C}$-numbers Substitution and Classical Pekar Functionals

The rescaled commutation relations (1.1.28) suggest a classical approximation for the phonon field and this amounts to substituting the annihilation and creation operators $a_k^\dagger$ and a_k with complex valued functions $z(k)$ and $z^*(k)$ respectively. This approach, often called $\mathbb{C}$-numbers substitution in physics, was firstly adopted by Pekar in our context [95] and leads to the definition of the classical functional corresponding to $\mathfrak{H}_\alpha$, for this reason customarily called Pekar functional. For φ a complex valued functions, we write z as the Fourier transform of φ, i.e.

$$z(k) = (2\pi)^{-2/3} \int_{\mathbb{R}^3} dx (\operatorname{Re} \varphi(x) + i \operatorname{Im} \varphi(x)) e^{-ik\cdot x}, \tag{1.2.2}$$

and use this ansatz for the computation of the energy. This way, we arrive to the Pekar functional, which reads

$$\mathcal{G}(\psi,\varphi) := \int_{\mathbb{R}^3} |\nabla\psi(x)|^2 dx - 2\int\int_{\mathbb{R}^6} \frac{|\psi(x)|^2 \operatorname{Re}\varphi(y)}{\pi^{3/2}|x-y|^2} dxdy + \int_{\mathbb{R}^3} |\varphi(y)|^2 dy. \tag{1.2.3}$$

Note that $\mathcal{G}$ is minimized for real valued φ. Moreover, since $(-\Delta)^{-1/2}(x,y) = (2\pi^2)^{-1}|x-y|^{-2}$, we can equivalently write

$$\mathcal{G}(\psi,\varphi) = \|\varphi\|_2^2 + \langle\psi|h_\varphi|\psi\rangle\,, \tag{1.2.4}$$

where

$$h_\varphi := -\Delta + V_{\operatorname{Re}\varphi}, \quad V_{\operatorname{Re}\varphi} := -4\pi^{1/2}(-\Delta)^{1/2}\operatorname{Re}\varphi. \tag{1.2.5}$$

By a simple completion of the square, for fixed ψ the optimal φ is given by

$$\sigma_\psi := 2(\pi)^{1/2}(-\Delta)^{-1/2}|\psi|^2, \tag{1.2.6}$$

and we arrive at

$$\mathcal{E}(\psi) := \inf_\varphi \mathcal{G}(\psi,\varphi) = \int_{\mathbb{R}^3} |\nabla\psi(x)|^2 dx - \int\int_{\mathbb{R}^6} \frac{|\psi(x)|^2|\psi(y)|^2}{|x-y|} dxdy. \tag{1.2.7}$$

Similarly, for fixed φ the optimal ψ is given by the ground state of h_φ, if it exists, and we arrive at

$$\mathcal{F}(\varphi) := \inf_\psi \mathcal{G}(\psi,\varphi) = \|\varphi\|_2^2 + \inf\operatorname{spec} h_\varphi. \tag{1.2.8}$$

We shall refer to $\mathcal{G}$, $\mathcal{E}$ and $\mathcal{F}$ as Pekar functionals, even if strictly speaking the classical functional corresponding to the Hamiltonian $\mathfrak{H}_\alpha$ is only $\mathcal{G}$. We can here also define the Pekar energy as

$$E_P := \inf_{\psi,\varphi} \mathcal{G}(\psi,\varphi) = \inf_\psi \mathcal{E}(\psi) = \inf_\varphi \mathcal{F}(\varphi). \tag{1.2.9}$$

The same discussion can be carried out in the case of a polaron confined to a bounded domain Ω or to a torus $\mathbb{T}_L^3$, arriving to the corresponding functionals (which clearly feature $-\Delta_\Omega$ and $-\Delta_L$ in place of of $-\Delta$) and Pekar energies. We shall distinguish these from the full-space counterparts with a subscript Ω or $\mathbb{T}_L^3$, respectively. The Pekar functionals and their properties are extremely important to understand the behavior of the polaron in the strong coupling regime, as we shall see. A study of the functional $\mathcal{E}$ was carried out in [76], obtaining the following result.

Theorem 1.2.1 (Lieb 1977, [76])**.** *There exists a positive and radial minimizer ψ_P of $\mathcal{E}$ under the constraint $\|\psi\|_2 = 1$, which is unique up to translations and changes of phase.*

If we denote the sets of minimizers of $\mathcal{E}$ and $\mathcal{F}$ respectively as $\mathcal{M}^{\mathcal{E}}$ and $\mathcal{M}^{\mathcal{F}}$, Theorem 1.2.1 implies that

$$\begin{aligned} \mathcal{M}^{\mathcal{E}} &= \left\{ e^{i\theta}\psi_P^y \mid \theta\in[0,2\pi),\ y\in\mathbb{R}^3 \right\}, \\ \mathcal{M}^{\mathcal{F}} &= \left\{ \varphi_P^y \mid y\in\mathbb{R}^3 \right\}, \end{aligned} \tag{1.2.10}$$

where $\varphi_P := \sigma_{\psi_P}$ and $f^y(x) := f(x-y)$. In particular, the classical approximation leads to a self-trapping of the electron (manifested in the existence of a minimizer despite the translation invariance of the problem) which is not expected to occur in the full quantum problem [52, 31]. Note that the uniqueness part of Theorem 1.2.1 is far from trivial, as the functional is not convex. Its proof (see also [115, 84]) relies heavily on radial symmetry and is very specific to the case of the Coulomb potential, the only generalizations known involving small perturbations of either the non-linearity [122] or of the potential [103]. We shall discuss in Section 1.2.4 the modifications of Theorem 1.2.1 in the case of a bounded domain Ω or a torus $\mathbb{T}^3_L$, as these are part of the original contributions of the author.

Before moving on with the discussion, we also present another important property of the functional $\mathcal{E}$, which was proven in [70] (see also [119]): the Hessian of $\mathcal{E}$ at its minimizers is strictly positive above the trivial zero modes resulting from the invariance under translations and changes of phase. This further implies the validity of estimate (1.2.11) below, which is not stated explicitly in [70] but can be obtained by standard arguments as a consequence of the results therein contained (see, e.g., [35, Appendix A], [43]). There exists a constant $\tau > 0$, such that, for any L^2-normalized $f \in H^1(\mathbb{R}^3)$

$$\mathcal{E}(f) - \mathcal{E}(\psi_P) \geq \tau \operatorname{dist}^2_{H^1(\mathbb{R}^3)}\left(\mathcal{M}^{\mathcal{E}}, f\right) = \tau \inf_{y,\theta} \|\psi - e^{i\theta}\psi_P^y\|^2_{H^1(\mathbb{R}^3)}. \tag{1.2.11}$$

Again, we shall discuss in Section 1.2.4 the validity of (1.2.11) in the case of a bounded domain Ω or a torus $\mathbb{T}^3_L$, as also this is part of the original contributions of the author.

1.2.2 Leading order of E_α, Pekar Asymptotics

At this point, to verify the validity of the classical approximation in the strong coupling regime, we expect E_α to agree with E_P, at least to leading order in α (note that E_P does not depend on α). This is indeed the case, as it is possible to prove that, as $\alpha \to \infty$,

$$E_\alpha = E_P + o(1). \tag{1.2.12}$$

The expansion (1.2.12) is called Pekar asymptotics and was already formulated by Pekar in the 50s [95]. It is relatively simple to provide an upper bound for E_α that agrees with (1.2.12). In particular, it is sufficient to assume what is sometimes called Pekar ansatz, i.e. a decoupling between the electron and the phonons. Mathematically, this amounts to minimizing $\mathfrak{H}_\alpha$ over product states $\psi \otimes \Phi$, with $\psi \in L^2(\mathbb{R}^3)$ and $\Phi \in \mathcal{F}(L^2(\mathbb{R}^3))$. By a simple computation, one gets

$$\langle \psi \otimes \Phi | \mathfrak{H}_\alpha | \psi \otimes \Phi \rangle = \langle \psi | -\Delta | \psi \rangle + \langle \Phi | \mathbb{N} | \Phi \rangle - \int_{\mathbb{R}^3} |\psi(x)|^2 \langle \Phi | a(v_x) + a^\dagger(v_x) | \Phi \rangle \, dx. \tag{1.2.13}$$

For fixed ψ the optimal choice of Φ is given by the coherent state

$$\Phi = W(\alpha^2 \sigma_\psi) := e^{a^\dagger(\alpha^2\sigma_\psi) - a(\alpha^2\sigma_\psi)}\Omega, \tag{1.2.14}$$

where W denotes the Weyl operator and we recall that σ_ψ, defined in (1.2.6), is the optimal classical state of the phonon field for a fixed ψ and that $\Omega \in \mathfrak{h}_0 \subset \mathcal{F}(L^2(\mathbb{R}^3))$ is the vacuum. This choice of Ψ yields the desired upper bound

$$E_\alpha \leq \inf_{\psi\otimes\Phi} \langle \psi \otimes \Phi | \mathfrak{H}_\alpha | \psi \otimes \Phi \rangle = \inf_\psi \mathcal{E}(\psi) = E_P. \tag{1.2.15}$$

Looking at this computation in Q-space leads to a very nice, but again formal, interpretation. Indeed, if we recall expression (1.1.16) and that $\Phi \in \mathcal{F}(L^2(\mathbb{R}^3))$ can be interpreted as a probability distribution over classical states of the phonon field, then we see that (1.2.13) can equivalently written as

$$\langle \psi \otimes \Phi | \mathfrak{H}_\alpha | \psi \otimes \Phi \rangle = \langle \psi | -\Delta | \psi \rangle + \langle \Phi | \mathbb{N} | \Phi \rangle - \int_{\mathbb{R}^3} |\psi(x)|^2 V_{\alpha^{-2}\mathbb{E}_{|\Phi|^2}(\varphi)}(x) dx, \qquad (1.2.16)$$

where we denote by $\mathbb{E}_{|\Phi|^2}(\varphi)$ the expected classical field associated to the distribution $|\Phi|^2$. In words, this says that, as long as one assumes decoupling between the electron and the phonons, the electron is only affected (through a dipole potential) by the expected field of the distribution Φ. We can hence split the minimization in two: first minimizing $\mathbb{N}$ over states Φ with a given expected field $\alpha^2\bar{\varphi}$ and then minimizing over $\alpha^2\bar{\varphi}$. Since $\mathbb{N}$ is simply a rescaled harmonic oscillator in Q-space, its minimum, over states with fixed expected field $\alpha^2\bar{\varphi}$, equals $\|\bar{\varphi}\|_2^2$ and is achieved by a Gaussian centered at $\alpha^2\bar{\varphi}$, i.e. the coherent state $W(\alpha^2\bar{\varphi})$. This, equivalently to the previous computation, allows to conclude

$$\begin{aligned} E_\alpha &\leq \inf_{\psi\otimes\Phi} \langle \psi \otimes \Phi | \mathfrak{H}_\alpha | \psi \otimes \Phi \rangle = \inf_{\psi,\bar{\varphi}} \inf_{\substack{\psi\otimes\Phi \\ \mathbb{E}_{|\Phi|^2}(\varphi)=\alpha^2\bar{\varphi}}} \langle \psi \otimes \Phi | \mathfrak{H}_\alpha | \psi \otimes \Phi \rangle \\ &= \inf_{\psi,\bar{\varphi}} \left\langle \psi \otimes W(\alpha^2\bar{\varphi}) \middle| \mathfrak{H}_\alpha \middle| \psi \otimes W(\alpha^2\bar{\varphi}) \right\rangle = \inf_{\psi,\bar{\varphi}} \mathcal{G}(\psi, \bar{\varphi}) = E_P. \qquad (1.2.17) \end{aligned}$$

The situation is much more complicated for the lower bound needed to prove (1.2.12). It was only in the 80s, 30 years after Pekar's original conjecture, that this was first proved rigorously in [30]. Therein, Feynman's path integral formulation of the problem [37] is used (see [91, 92] for a rigorous definition of the Pekar process [111]). Later, this lower bound was proved also in [82], using a completely different approach that leads to the quantitative bound, as $\alpha \to \infty$,

$$E_\alpha \geq E_P - O(\alpha^{-1/5}). \qquad (1.2.18)$$

The approach used in [82] uses relatively simple operator techniques: the Hamiltonian is substituted with one to which an ultraviolet cutoff (for the phonons) and a localization (for the electron) are applied and the errors stemming from such substitution are precisely estimated using Lieb-Yamazaki bounds and IMS localization, respectively. Using the new effective Hamiltonian, it is possible, with some extra work, to make the $\mathbb{C}$-numbers substitution approach rigorous. This method is robust enough to allow generalizations and, in particular, it can be used to show that Pekar asymptotics is valid also in the case of a confined polaron.

With this, we conclude the discussion about the leading order of E_α as $\alpha \to \infty$, described by the Pekar asymptotics (1.2.12). This shows that indeed the system, or more precisely the phonon field, behaves classically in its strong coupling regime.

1.2.3 Second Order of E_α, Quantum Corrections

A natural question to ask here is whether the lower bound (1.2.18) is sharp or, more generally, what is the next order expansion of E_α as $\alpha \to \infty$. This is still an open problem, at least in the case of $\mathbb{R}^3$. Nevertheless, the next term in the expansion of E_α is conjectured to be $O(1)$ both in the mathematical literature (see [109]) and the physical literature (see [2, 3, 59, 114]), with the guess involving an explicit constant, as we shall see and justify below. Investigating this problem sheds more light on the precision and range of validity of the classical approximation and leads to a deeper understanding of the system. It is interesting, indeed, to see how the answer to this question needs to take the quantum nature of the phonon field into account again: it is only to leading order that it behaves classically, while the fluctuations around this limit are again governed by quantum mechanics.

We again begin with an heuristic computation. Going beyond the Pekar ansatz, which assumes decoupling between electron and phonons, we need to minimize $\mathfrak{H}_\alpha$ over states which factor in correlation. We can write any such state in Q-space as

$$\Psi = \psi(x, y_1, \dots, y_k, \dots)\Phi(y_1, \dots, y_k, \dots) = \psi(x, y)\Phi(y), \tag{1.2.19}$$

where we use for simplicity the notation y to denote the infinitely many variables of the phonons. Recalling the expression of $\mathfrak{H}_\alpha$ in Q-space (1.1.16) and plugging states of the form (1.2.19), we obtain

$$\langle \psi\Phi|\mathfrak{H}_\alpha|\psi\Phi\rangle = \langle \Phi|\mathbb{N} + \langle \psi|h_y|\psi\rangle|\Phi\rangle\,, \tag{1.2.20}$$

where $h_y = -\Delta + V_y$, as defined in (1.2.5). Therefore, to minimize $\mathfrak{H}_\alpha$, we take $\psi(x, y) = \psi_y(x)$, where we formally denote by ψ_φ the g.s. of h_φ (note that this does not always exist). Recalling the expression of $\mathbb{N}$ in Q-space (1.1.11) and the modified rescaled commutation relations (1.1.28) as well as the definition of the Pekar functional for the phonons $\mathcal{F}$ (1.2.8), this choice leads to

$$\begin{aligned}\inf_{\psi,\Phi}\ \langle \psi\Phi|\mathfrak{H}_\alpha|\psi\Phi\rangle &= \inf_{\Phi}\ \langle \Phi|\mathbb{N} + \inf\operatorname{spec} h_y|\Phi\rangle \\ &= \inf_{\Phi}\ \langle \Phi|-\frac{1}{4\alpha^4}\Delta_y + \|y\|_2^2 + \inf\operatorname{spec} h_y|\Phi\rangle - \sum_{j=1}^{\infty}\frac{1}{2\alpha^2} \\ &= \inf_{\Phi}\ \langle \Phi|-\frac{1}{4\alpha^4}\Delta_y + \mathcal{F}(y)|\Phi\rangle - \sum_{j=1}^{\infty}\frac{1}{2\alpha^2}.\end{aligned} \tag{1.2.21}$$

At this stage, this is only a formal expression, as in infinite dimensions the last term is simply infinite. Nevertheless, if we try to push this computation forward, we note that the scaling α^{-4} in front of the Laplacian suggests (one should show this rigorously) that only the y-s close to $\mathcal{M}^{\mathcal{F}}$, the set of minimizers of $\mathcal{F}$, play a role in this analysis. Recalling that Theorem 1.2.1 implies that $\mathcal{M}^{\mathcal{F}} = \{\varphi_P^z \mid z \in \mathbb{R}^3\}$, we can formally Taylor expand $\mathcal{F}$ around its minimizer φ_P (since the minimizer is not unique, this is another tricky part of this computation), obtaining

$$\inf_{\psi,\Phi}\ \langle \psi\Phi|\mathfrak{H}_\alpha|\psi\Phi\rangle \approx E_P + \inf_{\Phi}\ \langle \Phi|-\frac{1}{4\alpha^4}\Delta_y + \langle y-\varphi_P|D^2\mathcal{F}(\varphi_P)|y-\varphi_P\rangle|\Phi\rangle - \sum_{j=1}^{\infty}\frac{1}{2\alpha^2}. \tag{1.2.22}$$

At this point, since φ_P is the minimum of $\mathcal{F}$ and therefore $D^2\mathcal{F}(\varphi_P)$ is non-negative (one should rigorously take care of the eventual zero modes), it is possible to exactly minimize the expectation appearing above by plugging in the renormalized Gaussian

$$\Phi(y) = \frac{G(y)}{\|G\|}, \quad \text{where} \quad G(y) := \exp\left(-\alpha^2\,\langle y-\varphi_P|\sqrt{D^2\mathcal{F}(\varphi_P)}|y-\varphi_P\rangle\right), \tag{1.2.23}$$

the minimizer of a system of harmonic oscillators of frequencies given by the eigenvalues of $D^2\mathcal{F}(\varphi_P)$. This finally yields

$$\inf_{\psi,\Phi}\ \langle \psi\Phi|\mathfrak{H}_\alpha|\psi\Phi\rangle = E_P - \frac{1}{2\alpha^2}\operatorname{Tr}\Big(\mathbb{1} - \sqrt{D^2\mathcal{F}(\varphi_P)}\Big), \tag{1.2.24}$$

where the infinite sum appearing before has been reabsorbed in the trace. Note that the Hessian of $\mathcal{F}$ at φ_P can be computed using second order perturbation theory (see for example [41] for its computation in the case of a bounded domain), obtaining

$$D^2\mathcal{F}(\varphi_P) = \mathbb{1} - 4(-\Delta)^{-1/2}\psi_P \frac{Q}{h_{\varphi_P} - \mu_P}\psi_P(-\Delta)^{-1/2} =: \mathbb{1} - K, \tag{1.2.25}$$

where $\mu_P = \langle \psi_P | h_{\varphi_P} | \psi_P \rangle$ is the bottom of the spectrum of h_{φ_P} and $Q = \mathbb{1} - |\psi_P\rangle\langle\psi_P|$ (hence $\frac{Q}{h_{\varphi_P}-\mu_P}$ is simply the reduced resolvent of h_{φ_P}). This implies that the right hand side of (1.2.24) is finite and well defined, since the operator K can be shown to be trace class. Therefore, it makes sense to conjecture

$$E_\alpha = E_P - \frac{1}{2\alpha^2}\operatorname{Tr}\Big(\mathbb{1} - \sqrt{D^2\mathcal{F}(\varphi_P)}\Big) + o(\alpha^{-2}), \tag{1.2.26}$$

unveiling the second order term in the α-expansion of E_α, which appears to be of order α^{-2} and negative (clearly $K \geq 0$).

The previous computation allows to formulate conjecture (1.2.26), while at the same time singling out a strategy to prove it. In particular, the following points are formal and need rigorous justification:

(i) The computation cannot be carried out in infinite dimensions, as it immediately displays the infinite correction $\sum_{j=1}^{\infty} \frac{1}{2\alpha^2}$. On the other hand, we have seen above that it is possible to apply an ultraviolet cutoff (w.r.t. the phonons) to the Hamiltonian. This might allow to perform the previous computation in finite dimension and overcome this difficulty.

(ii) The lack of uniqueness of minimizers of $\mathcal{F}$ on $\mathbb{R}^3$ makes the Taylor expansion of $\mathcal{F}$ problematic. Therefore, one needs to expand $\mathcal{F}$ w.r.t. to the whole surface $\mathcal{M}^{\mathcal{F}}$ (which also includes finding a sensible way of doing it). Note that restricting to the case of a bounded domain Ω with Dirichlet boundary conditions breaks translation invariance and gives hope, at least under reasonable assumptions on Ω (e.g., convexity), to have uniqueness of minimizers.

(iii) In order to perform the Taylor expansion of $\mathcal{F}$, one needs to first understand how to split $L^2(\mathbb{R}^3)$ in a region close to $\mathcal{M}^{\mathcal{F}}$ and in one distant from it, and then to show that only the first contributes relevantly to E_α. For this purpose, it is necessary to prove a global lower bound on $\mathcal{F}$ that shows it grows rapidly enough moving away from $\mathcal{M}^{\mathcal{F}}$.

(iv) Finally, it is also necessary to study the properties of $D^2\mathcal{F}$ at its minimizers, dealing with its degenerate directions. Note that translation invariance, which holds on $\mathbb{R}^3$ and $\mathbb{T}^3_L$, implies that $D^2\mathcal{F}(\varphi_P)$ has at least three zero modes.

A first successful attempt to carry out this program is the content of [41], of which we here give a short overview as a final part of this section.

The case considered is the one of a polaron confined to a bounded domain Ω, exactly to overcome the difficulties explained in points (ii), (iii) and (iv). More precisely, it is assumed that Ω is nice enough to guarantee

(a) the validity of an analog of Theorem 1.2.1,

(b) the validity of an analog of estimate (1.2.11).

Note that the validity of both (a) and (b) has been verified by the author of this thesis, in collaboration with Robert Seiringer, in the case of Ω being a ball [32], as we explain in detail in Section 1.2.4, and is conjectured to hold under rather general assumptions on Ω (e.g., convexity). Being more precise, assumption (a) concerns the uniqueness of minimizers of the functional $\mathcal{E}_\Omega$, which is assumed to hold up to changes of phase only, and not up to translations (which are in any case not available on a bounded domain). Assumption (a) also guarantees that there exists a unique $\varphi_\Omega \in C^\infty(\Omega) \cap H_0^1(\Omega)$ minimizing $\mathcal{F}_\Omega$ and solves the difficulties explained in point (ii). A rather simple Lemma shows instead that assumption (b) also implies that for some $\kappa > 0$

$$\mathcal{F}(\varphi) - \mathcal{F}(\varphi_\Omega) \geq \langle \varphi - \varphi_\Omega | \mathbb{1} - (1 + \kappa(-\Delta_\Omega))^{-1/2} | \varphi - \varphi_\Omega \rangle . \tag{1.2.27}$$

This can be used to easily show that the Hessian of $\mathcal{F}$ is strictly positive, solving problem (iv). To solve problem (iii), instead, the authors apply IMS localization in Fock space, thus splitting $L^2(\mathbb{R}^3)$ in a region close to φ_Ω and one distant from it. Using again (1.2.27), together with quite some extra work, they manage to show that indeed the region away from the unique minimizer is negligible. Note that the fact that (1.2.27) is enough to solve point (iii) is a specific feature of the confined polaron, as the analog bound on $\mathbb{R}^3$ is not good enough because of the lack of compactness of $(-\Delta)^{-1/2}$. Finally, problem (i) is overcome in [41] by applying an ultraviolet cutoff to the Hamiltonian (w.r.t. the phonons). Note that, on a bounded domain, applying the cutoff instantly makes the number of phonon modes finite, by the spectral properties of $-\Delta_\Omega$ (this is not true on $\mathbb{R}^3$, indeed in [82] a further localization procedure has to be performed w.r.t. the electron, as we explained in Section 1.2.2). To quantify the error of the cutoff, the authors then use an approach which combines a triple Lieb-Yamazaki bound [83] and a Gross transformation [58, 94], already introduced in Section 1.1.2. Note that this approach is inspired by [82], but it is much more refined as the needed bounds on the error stemming from the ultraviolet cutoff are much stronger if one is interested in capturing the second order term in the expansion of E_α.

We conclude here our account of the problem (and previous literature related to) the computation of the ground state energy of the polaron in the strong coupling regime. It is in this background that the author made some of his original contributions, as we explain next.

1.2.4 Contributions by the Author

The study of problems related to the computation of the ground state energy of the polaron in its strong coupling regime, in particular to its second order expansion in α, is the main focus of this PhD thesis. In this area, the novel results proven by the author can be divided into two directions of research:

- Study of the properties of the functionals $\mathcal{E}_{\mathbb{T}^3_L}$ and $\mathcal{E}_{B_R}$, where for any $R > 0$

  $$B_R := \{(x_1, x_2, x_3) \in \mathbb{R}^3 \mid \sqrt{x_1^2 + x_2^2 + x_3^2} < R\}. \tag{1.2.28}$$

  In particular, the proof of analogous results to Theorem 1.2.1 and estimate (1.2.11). As discussed above, such results also allow to infer properties of the functionals $\mathcal{F}_\Omega$ and $\mathcal{F}_{\mathbb{T}^3_L}$, which are fundamental for a rigorous proof of the second order expansion of E_α.

- Extension of the results contained in [41] to the case of a torus $\mathbb{T}^3_L$. This can be seen as an intermediate step between the case of a bounded domain Ω with Dirichlet b.c. and the case of $\mathbb{R}^3$ (at present, still open): considering the problem on $\mathbb{T}^3_L$ reintroduces translational invariance and allows to understand how to treat the case of $\mathcal{M}^{\mathcal{F}}$ being a surface, at the same time keeping the problem on a compact domain.

Even if we are interested in understanding the same properties for both $\mathcal{E}_{B_R}$ and $\mathcal{E}_{\mathbb{T}^3_L}$, the two situations are very different. The first displays radial symmetry, which is a key ingredient of the proof of Theorem 1.2.1 and estimate (1.2.11) in the case of $\mathbb{R}^3$, and this allows to simply adapt the approach used on $\mathbb{R}^3$ to deal with boundary conditions. $\mathbb{T}^3_L$, instead, does not display radial symmetry and this calls for a novel approach: the key idea is to compare $\mathbb{T}^3_L$, for large L, with $\mathbb{R}^3$ and infer properties of $\mathcal{E}_{\mathbb{T}^3_L}$ by showing that it 'converges' to $\mathcal{E}$ in a suitable sense. In particular, this only allows to show our results for L sufficiently large, whereas we can prove our results for balls of any size.

The study of $\mathcal{E}_{B_R}$ is carried out in

- Dario Feliciangeli and Robert Seiringer. Uniqueness and nondegeneracy of minimizers of the Pekar functional on a ball. *SIAM Journal on Mathematical Analysis*, 52(1):605–622, 2020,

which is the content of Chapter 2. We prove the following two theorems.

Theorem 1.2.2 (Existence and Uniqueness of Minimizers of $\mathcal{E}_{B_R}$)**.** *For any $R > 0$, there exists a radial and decreasing minimizer $0 < \psi_R \in C^\infty(B_R) \cap H^1_0(B_R)$ such that*

$$\mathcal{E}_{B_R}(\psi_R) = E_{B_R} := \inf\{\mathcal{E}_{B_R}(\psi) : \psi \in H^1_0(B_R), \|\psi\|_2 = 1\}. \tag{1.2.29}$$

Moreover,

$$\mathcal{M}^{\mathcal{E}}_{B_R} := \{\psi \in H^1_0(B_R),\ \|\psi\|_2 = 1 \mid \mathcal{E}_{B_R}(\psi) = E_{B_R}\} = \{e^{i\theta}\psi_R \mid \theta \in [0, 2\pi)\} \tag{1.2.30}$$

Theorem 1.2.3 (Coercivity of $\mathcal{E}_{B_R}$)**.** *For any $R > 0$, there exists $K_R > 0$ such that, for any L^2-normalized $\psi \in H^1_0(B_R)$,*

$$\mathcal{E}_{B_R}(\psi) - E_{B_R} \geq K_R \min_{\theta\in[0,2\pi)} \int_{B_R} |\nabla(e^{i\theta}\psi_R - \psi)|^2 dx = K_R \operatorname{dist}^2_{\dot{H}^1_0(B_R)}(\psi, \mathcal{M}^{\mathcal{E}}_{B_R}). \tag{1.2.31}$$

Note that these two results coincide with the assumptions made in [41] (as explained in the previous Section) and complete the discussion about the second order expansion of E_α, at least in the case of Ω being a ball. We also emphasize that, as shown in [41], Theorems 1.2.2 and 1.2.3 imply analogous properties for $\mathcal{F}_{B_R}$, in particular the non-degeneracy of its Hessian and estimate (1.2.27). We conjecture the analog of Theorems 1.2.2 and 1.2.3 to hold on general domains Ω (under suitable assumptions, e.g., convexity) even if a new approach to prove them is needed (for lack of radial symmetry). Note that there exist cases of domains Ω for which the two results fail (see Chapter 2 for more details). The proofs of Theorem 1.2.2 and Theorem 1.2.3 follow closely the approaches used in [76] and [70], respectively. Modifications are needed, though, in order to deal with the boundary conditions. Both proofs rely heavily on radial symmetry and take advantage of Newton's shell Theorem, which can be used to deal with the non-locality of the Euler–Lagrange equation related to the minimization of $\mathcal{E}_{B_R}$.

Radial symmetry is fundamental also in our proof of Theorem 1.2.3. Indeed, this result is a standard consequence of the non-degeneracy of the Hessian of $\mathcal{E}_{B_R}$ at ψ_R (always understood up to the trivial zero mode given by invariance under changes of phase) and the latter is proven by splitting the space in spherical harmonics and analyzing each sector separately.

The study of $\mathcal{E}_{\mathbb{T}^3_L}$ and the extension of the results of [41] to the case of $\mathbb{T}^3_L$ are instead both carried out in

- Dario Feliciangeli and Robert Seiringer. The strongly coupled polaron on the torus: quantum corrections to the Pekar asymptotics. *arXiv preprint arXiv:2101.12566*, 2021,

which is the content of Chapter 3. In this work, we prove the following two results.

Theorem 1.2.4 (Properties of $\mathcal{E}_{\mathbb{T}^3_L}$). *There exist $L_1>0$ and a positive constant κ_1 independent of L, such that for $L>L_1$ there exists $0<\psi_L\in C^\infty(\mathbb{T}^3_L)$ such that*

$$\mathcal{E}_{\mathbb{T}^3_L}(\psi_L)=E_{\mathbb{T}^3_L}:=\inf\{\mathcal{E}_{\mathbb{T}^3_L}(\psi)\mid \psi\in L^2(\mathbb{T}^3_L),\ \|\psi\|_2=1\}. \tag{1.2.32}$$

Moreover

$$\mathcal{M}^{\mathcal{E}}_{\mathbb{T}^3_L}:=\{\psi\in L^2(\mathbb{T}^3_L),\ \|\psi\|_2=1\mid \mathcal{E}_{\mathbb{T}^3_L}(\psi)=E_{\mathbb{T}^3_L}\}=\{e^{i\theta}\psi_L^y\mid \theta\in[0,2\pi),\ y\in\mathbb{T}^3_L\}. \tag{1.2.33}$$

Finally for any L^2-normalized $f\in H^1(\mathbb{T}^3_L)$,

$$\mathcal{E}_{\mathbb{T}^3_L}(f)-E_{\mathbb{T}^3_L}\geq \kappa_1\inf_{y,\theta}\|e^{i\theta}\psi_L^y-f\|^2_{H^1(\mathbb{T}^3_L)}=\kappa_1\operatorname{dist}^2_{H^1}\left(\mathcal{M}^{\mathcal{E}}_{\mathbb{T}^3_L},f\right). \tag{1.2.34}$$

Again, Theorem 1.2.4 implies the validity of an analog result for the functional $\mathcal{F}_{\mathbb{T}^3_L}$ (see Corollary 3.2.1 in Chapter 3).

Theorem 1.2.5 (Second Order Expansion of E^L_α). *For any $L>L_1$, we denote by E^L_α the ground state energy of the strong coupling units Fröhlich Hamiltonian confined to $\mathbb{T}^3_L$ and define $\varphi_L:=2(\pi)^{1/2}(-\Delta_L)^{-1/2}|\psi_L|^2$. Then, as $\alpha\to\infty$*

$$E^L_\alpha=E_{\mathbb{T}^3_L}-\frac{1}{2\alpha^2}\operatorname{Tr}\left(\mathbb{1}-\sqrt{D^2\mathcal{F}_{\mathbb{T}^3_L}(\varphi_L)}\right)+o(\alpha^{-2}). \tag{1.2.35}$$

We can actually provide precise L-dependent bounds on the error term in expression(1.2.35) (see Theorem 3.2.2 in Chapter 3), which unfortunately are not good enough to allow for a straightforward generalization of our result to $\mathbb{R}^3$, or in other words do not allow to take the joint limit $L,\alpha\to\infty$. Note that the L_1 appearing in Theorem 1.2.5 is the same of Theorem 1.2.4, a simple manifestation of the importance of the properties of the classical Pekar functionals in the study of second order fluctuations of the ground state energy of the system. We can prove both Theorems 1.2.4 and 1.2.5 also in the regime of very small L, i.e. $L<L_0$ for an appropriate L_0. This regime is much less interesting though, since the unique minimizer of $\mathcal{F}_{\mathbb{T}^3_L}$ is the null function and this allows to directly use the approach of [41] (see also Remark 3.2.3 in Chapter 3).

We emphasize that both the proof of Theorem 1.2.4 and of Theorem 1.2.5 need a novel approach on $\mathbb{T}^3_L$, compared to previously known results, as we shall now illustrate.

As mentioned above, the proof of Theorem 1.2.4 in the previously known cases ($\mathbb{R}^3$ and B_R) relies on radial symmetry, not available for $\mathbb{T}^3_L$. The idea here is to compare $\mathcal{E}_{\mathbb{T}^3_L}$ with $\mathcal{E}$, for large L, and this is why the result is only valid for $L > L_1$. The first step is to show that $E_{\mathbb{T}^3_L} \to E_P$ as $L \to \infty$ and to show that all the states relevant to the minimization of $\mathcal{E}_{\mathbb{T}^3_L}$ localize, up to translations, around a suitable localization to $\mathbb{T}^3_L$ of ψ_P, the full space minimizer (see Proposition 3.3.1). The next step is concerned with the Hessian of $\mathcal{E}_{\mathbb{T}^3_L}$ at its minimizers, which again by comparison with $\mathcal{E}$ can be shown to be non-degenerate uniformly in L, up to trivial zero modes (see Proposition 3.3.2). Combining these two results allows to show uniqueness up to translations of minimizers, for $L > L_1$, and finally standard arguments can be used to show local and global coercivity.

The proof of Theorem 1.2.5, instead, follows quite closely the proof of the analog Theorem for Ω contained in [41], but with a fundamental difference: on $\mathbb{T}^3_L$, for $L > L_1$ the set of minimizers of $\mathcal{F}_{\mathbb{T}^3_L}$ is actually a three-dimensional surface. This is related to point (ii) at the end of Section 1.2.3, the second problem listed in relation to to the formal computation leading to the conjecture for the second order expansion of E_α. Like in [41], IMS localization is performed in Fock space in order to separate the two regions close and distant to $\mathcal{M}^{\mathcal{F}}_{\mathbb{T}^3_L}$, but in light of the structure of $\mathcal{M}^{\mathcal{F}}_{\mathbb{T}^3_L}$ this turns out to be a localization to the tubular neighborhood of a surface, rather than the localization to a ball centered at φ_Ω. A totally new approach is needed to deal with this situation: first, we need to carry out a precise study of the surface $\mathcal{M}^{\mathcal{F}}_{\mathbb{T}^3_L}$ and its neighborhoods (see Lemma 3.3.11), then we introduce a diffeomorphism 3.4.1, which we call Gross coordinates (since it is inspired by [59]) and use it to straighten the tubular neighborhoods of $\mathcal{M}^{\mathcal{F}}_{\mathbb{T}^3_L}$ and treat them as if they were tubular neighborhoods of a flat torus. Note that this is carried out in dimension $N \to \infty$, where N is the number of phonon modes unaffected by the $\mathbb{T}^3_L$-analog of the ultraviolet cutoff mentioned above and already used in [41]. We also note that, on $\mathbb{T}^3_L$, the IMS localization has to be performed w.r.t. to a weighted and α-dependent norm. Indeed, using the norm $\|f\|_*^2 := \langle f|(-\Delta_{\mathbb{T}^3_L}+1)^{-1/2}|f\rangle$, the one that identifies the region where it is possible to perform the Taylor expansion of $\mathcal{F}_{\mathbb{T}^3_L}$ and also the one used in [41], is not enough to control the error term resulting from the region distant to $\mathcal{M}^{\mathcal{F}}_{\mathbb{T}^3_L}$.

In conclusion, the contributions of the author in the context of the computation of the second order expansion of the ground state energy of a polaron serve both as a justification of previously known results and as a step forward in the understanding of the system in both its classical and quantum nature. Indeed, [32] verifies the validity of the assumptions made in [41] and allows to completely settle the problem at least in the case of Ω being a ball, while [33], besides proving new properties about the functional $\mathcal{E}_{\mathbb{T}^3_L}$ and $\mathcal{F}_{\mathbb{T}^3_L}$, is the first known result that manages to compute the g.s. energy of the polaron to second order in α in a translational invariant setting and represents a stepping stone for any approach that aims to do the same on $\mathbb{R}^3$: at present, the main open problem in this context.

1.3 Effective Dynamics of the Polaron at Strong Coupling

We discuss here the dynamics of the polaron, which are driven by the Schrödinger equation introduced in (1.1.22). As anticipated above, in the strong coupling regime, it is well-described by a system of coupled non-linear effective equations, called Landau–Pekar (LP) equations (see, e.g., [66, 8, 27]). For initial conditions $(\psi_0, \varphi_0) \in L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)$, these are defined by

$$\begin{aligned} i\partial_t \psi_t &= h_{\varphi_t} \psi_t, \\ i\alpha^2 \partial_t \varphi_t &= \varphi_t + \sigma_{\psi_t}, \end{aligned} \tag{1.3.1}$$

where h_φ, V_φ and σ_ψ are defined in (1.2.5) and (1.2.6). These equations already consider the situation in which the phonons are treated classically. They display, through the different α-dependence in the equations driving the electron and the phonon evolutions, a clear separation of time scales (sometimes called adiabatic decoupling [113]): as $\alpha \to \infty$, the electron tends to be the fast variable of the system and the phonon field the slow one. Note that the electron is subject to a simple Schrödinger equation, which features the dipole potential generated by the time-evolving dipole field φ_t. The classical Pekar functional $\mathcal{G}$, introduced in (1.2.3), represents also the classical energy functional corresponding to (1.3.1) and is therefore conserved along solutions (see [38], Lemma 2.1).

In recent years, several rigorous studies of these equations have been carried out, aimed at understanding both their relation to the full quantum Schödinger equation and their own properties.

1.3.1 Effectiveness of Landau–Pekar Equations

It is possible to show that, for initial conditions of the form

$$\psi_0 \otimes W(\alpha^2 \varphi_0)\Omega \tag{1.3.2}$$

where W is defined in (1.2.14) and Ω is the vacuum, the quantum dynamics driven by (1.1.22), or more precisely the Schrödinger equation related to $\mathfrak{H}_\alpha$, is approximated by the Landau–Pekar equations with initial condition (ψ_0, φ_0). A multitude of results have been derived in this context (see [40, 38, 39, 56, 73, 87]), varying in the time-range of validity of the Landau–Pekar description and the assumptions on the initial states (ψ_0, φ_0). In particular, all these results concern times $t \ll \alpha^2$. Recently, it was shown in [74] that in order to obtain a norm approximation valid for times of order α^2, one needs to implement correlations among phonons, which are captured by a suitable Bogoliubov dynamics acting on the Fock space of the phonons only. In fact, considering initial data satisfying

$$\varphi_0 \in L^2(\mathbb{R}^3), \quad \inf \operatorname{spec} h_{\varphi_0} < 0, \tag{1.3.3}$$

[74, Theorem I.3] proves that there exist constants $C, T > 0$ (depending on φ_0) such that

$$\| e^{-i\mathfrak{H}_\alpha t} \psi_{\varphi_0} \otimes W(\alpha^2 \varphi_0)\Omega - e^{-i\int_0^t ds\, \omega(s)} \psi_t \otimes W(\alpha^2 \varphi_t)\Upsilon_t \|_{L^2(\mathbb{R}^3)\otimes\mathcal{F}} \le C\alpha^{-1} \quad \text{for all} \quad |t| \le T\alpha^2, \tag{1.3.4}$$

where ψ_{φ_0} denotes the ground state of h_{φ_0} (which exists by assumption (1.3.3)), $\omega(s) = \alpha^2 \operatorname{Im}\langle \varphi_s, \partial_s \varphi_s \rangle + \|\varphi_s\|_2^2$, (ψ_t, φ_t) is the solution of the LP equations with initial condition $(\psi_{\varphi_0}, \varphi_0)$ and Υ_t is the solution of the dynamics of a suitable Bogoliubov Hamiltonian on $\mathcal{F}$ (see [74, Definition I.2] for a precise definition). We emphasize that the restriction to times $|t| \le T\alpha^2$ results from the need of a spectral gap of h_{φ_t} of order one (compare with [74, Remark I.4]), which under the sole assumption (1.3.3) is guaranteed only for $|t| \le T\alpha^2$ (see [73, Lemma II.1]).

1.3.2 Adiabatic Theorem

The separation of time scales, between the electron and the phonons, is an immediately interesting property displayed by the LP equations. It suggests the validity of an adiabatic theorem in the large α regime, rigorously capturing the intuitive picture according to which, for initial conditions of the form $(\psi_{\varphi_0}, \varphi_0)$, the phonon field φ_t evolves slowly (on times of order α^2) while the extremely fast electron (which moves on times of order 1) instantaneously arrange its motion to follow the evolving ground state of h_{φ_t}. A similar result was first proven in [38, 39], in one dimension, and later established in three dimensions in [73]. Again under assumption (1.3.3) and denoting by (ψ_t, φ_t) the solution of the Landau–Pekar equations (1.3.1) with initial data $(\psi_{\varphi_0}, \varphi_0)$, [73, Thm. II.1 & Rem. II.3] proves that there exist constants $C, T > 0$ (depending on φ_0) such that

$$\|\psi_t - e^{-i\int_0^t ds \inf \operatorname{spec} h_{\varphi_s}} \psi_{\varphi_t}\|_2^2 \leq C\alpha^{-4} \quad \text{for all} \quad |t| \leq T\alpha^2, \tag{1.3.5}$$

where ψ_{φ_t} denotes the unique positive and normalized ground state of h_{φ_t} and. Also here, the restriction on $|t|$ in (4.1.9) is due to the need of ensuring that the spectral gap of the effective Hamiltonian h_{φ_t} does not become too small for initial data satisfying (1.3.3), which is only proven (in [73, Lemma II.1]) for times $|t| \leq T\alpha^2$.

1.3.3 Contributions by the Author

The contributions of the author in this context are contained in

- Dario Feliciangeli, Simone Rademacher, and Robert Seiringer. Persistence of the spectral gap for the Landau–Pekar equations. *Letters in Mathematical Physics*, 111(1):1–19, 2021,

which is the content of Chapter 4. This work is concerned with finding a set of initial data (ψ_0, φ_0) for the Landau–Pekar equations such that the spectral gap of the evolving effective Hamiltonian h_{φ_t} stays open for all times. In light of the discussion in the previous two sections, for such initial states it is possible to extend the validity of (1.3.4) and (1.3.5) to times larger than $T\alpha^2$, as this restriction was solely due to the need of ensuring that the spectral gap of the evolved Hamiltonian would not close.

We here sketch the strategy used to find such states, which consists in exploiting the analytical properties of the classical Pekar functionals $\mathcal{G}$, $\mathcal{E}$ and $\mathcal{F}$, together with the conservation of $\mathcal{G}$ along solution of the Landau–Pekar equations. Starting from the coercivity bounds (1.2.11) known for $\mathcal{E}$, we first show in Lemma 4.2.7 that there exists $\tau > 0$ such that

$$\mathcal{F}(\varphi) - E_P \geq \tau \operatorname{dist}^2_{L^2}(\mathcal{M}^{\mathcal{F}}, \varphi), \quad \forall \varphi \in L^2(\mathbb{R}^3). \tag{1.3.6}$$

Note that, because of the L^2-norm appearing in the RHS, this bound is different from the coercivity bounds for $\mathcal{F}$ we introduced and used in Section 1.2 (both (1.2.27) and its full space counterpart). Combining (1.3.6) with the conservation of $\mathcal{G}$, it is then easy to see that for any $\varepsilon > 0$ there exists δ_ε such that, if the initial conditions (ψ_0, φ_0) satisfy

$$\mathcal{G}(\psi_0, \varphi_0) < E_P + \delta_\varepsilon, \tag{1.3.7}$$

then the corresponding solution (ψ_t, φ_t) of (1.3.1) satisfies

$$\operatorname{dist}_{L^2}(\varphi_t, \mathcal{M}^{\mathcal{F}}) < \varepsilon, \quad \forall t \in \mathbb{R}. \tag{1.3.8}$$

Using that $\mathcal{M}^{\mathcal{F}} = \{\varphi_P^y \mid y \in \mathbb{R}^3\}$ and that the spectral gap of $h_{\varphi_P^y}$ is open and independent of y, together with the stability of the spectral gap of h_φ under L^2-perturbations, we can finally show (see Theorem 4.1.1) that for initial conditions (ψ_0, φ_0) satisfying (1.3.7) with δ_ε sufficiently small, the spectral gap of h_{φ_t} never closes. For such states, we can hence extend the validity of (1.3.4) and (1.3.5) to larger times (see Corollary 4.1.2 and Corollary 4.1.1, respectively), going beyond the somewhat artificial restriction $|t| \le T\alpha^2$.

A natural question to ask here, which at present does not have an answer, is whether the restriction (1.3.7) is sharp in order to ensure that h_{φ_t} possess a spectral gap of order 1 for all times. In other words, our result is purely 'geometrical' and does not take into account the LP equations at all. Might it be that the equations intrinsically tend to preserve the spectral gap of h_{φ_0} and that, therefore, assuming (1.3.7) is not needed?

1.4 Effective Mass of the Polaron at Strong Coupling

The last property of the polaron with which this work is concerned is its effective mass. The very first observation to make is that the model does not display explicitly a notion of mass and, therefore, it is first necessary to find a meaningful way of defining it. One way of doing this is to exploit the fact that the Fröhlich Hamiltonian H_α is translation-invariant and hence commutes with the total momentum operator

$$P = -i\nabla_x + P_f, \quad P_f = \int_{\mathbb{R}^3} k a_k^\dagger a_k \, dk. \tag{1.4.1}$$

This allows to write H_α in its fiber decomposition as

$$H_\alpha = \int_{\mathbb{R}^3}^{\oplus} dp H_\alpha^p, \tag{1.4.2}$$

where H_α^p formally denotes the restriction of H_α to states with total momentum p. Defining $E_\alpha(p) := \inf \operatorname{spec} H_\alpha^p$, one can then define implicitly the effective mass of the polaron as

$$E_\alpha(p) = E_\alpha(0) + \frac{p^2}{2m} + o(|p|^2), \quad \text{as } p \to 0, \tag{1.4.3}$$

or explicitly as

$$m := \left(2 \lim_{p \to 0} \frac{E_\alpha(p) - E_\alpha(0)}{p^2} \right)^{-1}. \tag{1.4.4}$$

Another equivalent (as shown in [80]) way of defining the mass of the polaron is to compare, as $\lambda \to 0$, the ground state energy of

$$H_{\alpha,\lambda} := H_\alpha + \lambda^2 W(\lambda x), \tag{1.4.5}$$

to the ground state energy of the Schrödinger operator $-\Delta/m + \lambda^2 W(\lambda x)$.

The Physics literature contains several formal computations of m (see [66, 37, 111, 27]), which lead to conjecture that

$$m = \frac{2}{3} \|\nabla \varphi_P\|_2^2 \alpha^4 + o(\alpha^4), \quad \text{as } \alpha \to \infty. \tag{1.4.6}$$

Nevertheless, the only rigorous result concerning this question which is possible to find in the mathematical literature is contained in [81], where the authors manage prove an explicit upper bound on $E_\alpha(p) - E_\alpha(0)$, obtaining

$$\lim_{\alpha\to\infty} m = \infty. \tag{1.4.7}$$

Recalling the physical picture described by the Fröhlich model, it makes sense that the effective mass of the polaron diverges as $\alpha \to \infty$. Indeed, in suggestive physical terms, one could say that the electron is slowed down, progressively more strongly as $\alpha \to \infty$, by the cloud of phonon excitations that it induces.

1.4.1 Contributions by the Author

The contributions of the author in this context are contained in

- Dario Feliciangeli, Simone Rademacher, and Robert Seiringer. Effective mass of the polaron via Landau-Pekar equations. *arXiv preprint arXiv:2107.03720*, 2021,

which is the content of Chapter 5. In this work, we consider a different approach and a different definition of the effective mass of the system. Instead of looking at the mass in the full quantum setting, we prefer to set ourselves in the classical approximation of the dynamics of the polaron: the Landau–Pekar equations. Hence, we set out to understand if the mass actually shows up in these equations (which, a priori, is not clear) and if its computation allows to verify (1.4.6), at least on a classical level.

Since in this case it is not possible to define m via the energy-momentum relation $E(p)$, we investigate how the energy of the system changes in relation to its velocity, instead. Indeed, since we are dealing with an evolution equation, it makes sense to try to define a notion of position, and consequently velocity, of the system at time t. For the electron the situation is simple, as the state ψ_t can already be considered as a probability distribution over positions. Therefore, we define

$$X_{\mathsf{el}}(t) := \langle \psi_t | x | \psi_t \rangle , \quad V_{\mathsf{el}}(t) := \frac{d}{dt} X_{\mathsf{el}}(t) = 2 \langle \psi_t | -i\nabla_x | \psi_t \rangle . \tag{1.4.8}$$

For the phonons the situation is more complicated, since φ_t does not encode any notion of position by itself. Nevertheless, we can turn to ideas already discussed in Section 1.3.3 to find a way of defining the position of the phonon field. By the coercivity of $\mathcal{F}$, the conservation of $\mathcal{G}$ and the local properties of $\mathcal{M}^{\mathcal{F}}$ (see Lemma 5.2.1), there exists $\delta > 0$ such that, if $\mathcal{G}(\psi_0, \varphi_0) < \delta$, then φ_t admits an unique L^2-projection $\varphi_P^{y(t)}$ onto $\mathcal{M}^{\mathcal{F}}$ for all times (recall that $\mathcal{M}^{\mathcal{F}} = \{\varphi_P^y \mid y \in \mathbb{R}^3\}$) and moreover $y(t)$ is a differentiable function. We can hence use the unique projection to define, admittedly in a quite implicit fashion, the position and the velocity of the phonon at time t as

$$X_{\mathsf{ph}}(t) := y(t), \quad V_{\mathsf{ph}}(t) := \frac{d}{dt} X_{\mathsf{ph}}(t) = \dot{y}(t). \tag{1.4.9}$$

At this point, we can derive an expression for the energy of the system in terms of its velocity by minimizing the energy functional related to the LP equations, i.e. $\mathcal{G}$, over initial states (ψ_0, φ_0) with initial instantaneous velocity v (compare with (5.2.16) for the precise definition of the set of initial states with velocity v). This leads, as shown in Theorem 5.2.1, to

$$E(v) = E_P + \frac{1}{2}\left(\frac{2}{3}\|\nabla\varphi_P\|_2^2\alpha^4 + \frac{1}{2}\right)v^2 + O(v^3), \quad \text{as } v \to 0. \tag{1.4.10}$$

This expression implicitly defines m and allows to conclude

$$m = \frac{2}{3}\|\nabla\varphi_P\|_2^2\alpha^4 + \frac{1}{2}, \tag{1.4.11}$$

showing that m satisfies (1.4.6) and even providing a guess for the second order expansion in α of m, which we now proceed to justify (compare with Section 5.4.1). For $\alpha = 0$, the LP equations degenerate into the so-called Choquard equation, only affecting the electron. The existence of explicit traveling waves solutions for the Choquard equation, i.e. solutions of the form

$$(\psi_t) = (e^{-ie_v t}(\psi_0)^{vt}), \quad v \in \mathbb{R}^3, \tag{1.4.12}$$

allow to derive an energy-velocity relation and obtain $m = 1/2$ for $\alpha = 0$. We see this as a justification of (1.4.11), since taking the limit $\alpha \to 0$ in (1.4.11) also yields $m = 1/2$. Note that this approach for the definition of m is not available for any $\alpha > 0$, as we conjecture travelling waves solutions to not exist for $\alpha \neq 0$. Nevertheless, formally assuming their existence also for $\alpha > 0$, one arrives again at (1.4.11).

1.5 Appendix: Non-Commutative Entropic Optimal Transport

We finally say a few words about Appendix A, which considers a completely different framework compared to the other results discussed in this thesis. It consists of the work

- Dario Feliciangeli, Augusto Gerolin, and Lorenzo Portinale. A non-commutative entropic optimal transport approach to quantum composite systems at positive temperature. *arXiv preprint arXiv:2106.11217*, 2021.

The objects under study are composite and finite dimensional quantum systems at positive temperature. In particular, we investigate the problem of computing their ground state energy conditionally to the knowledge of the states of all their subsystems.

More precisely, we consider a composite system $\mathfrak{h} = \mathfrak{h}_1 \otimes \cdots \otimes \mathfrak{h}_N$, composed by N subsystems $\{\mathfrak{h}_j\}_{j=1}^N$ each of which is a finte dimensional Hilbert space. We denote by H the Hamiltonian to which the whole system is subject and suppose that $H = H_0 + H_{\mathsf{int}}$, where H_0 is the non-interacting part of the Hamiltonian, i.e. $H_0 = \bigoplus_{j=1}^N H_j := H_1 \otimes \mathbb{1} \cdots \otimes \mathbb{1} + \cdots + \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes H_N$ with H_j acting on $\mathfrak{h}_j$, and H_{int} is its interacting part. We also suppose to have knowledge of the states $\boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_N)$ of the N subsystems, where each γ_j is a density matrix over $\mathfrak{h}_j$. Hence, we consider the problem of minimizing the energy of the system at temperature $\varepsilon > 0$, i.e.

$$\begin{aligned}\inf_{\Gamma \mapsto \boldsymbol{\gamma}} \{\mathrm{Tr}(H\Gamma) + \varepsilon S(\Gamma)\} &= \sum_{j=1}^N \mathrm{Tr}(H_j\gamma_j) + \mathfrak{F}^\varepsilon(\boldsymbol{\gamma}) \\ &:= \sum_{j=1}^N \mathrm{Tr}(H_j\gamma_j) + \inf_{\Gamma \mapsto \boldsymbol{\gamma}} \{\mathrm{Tr}(H_{\mathsf{int}}\Gamma) + \varepsilon S(\Gamma)\}, \end{aligned} \tag{1.5.1}$$

where the shorthand notation $\Gamma \mapsto \boldsymbol{\gamma}$ denotes the set of density matrices over $\mathfrak{h}$ with j-th partial trace equal to γ_j, and $S(\Gamma) := \mathrm{Tr}(\Gamma\log(\Gamma))$ is the opposite of Von Neumann entropy of Γ (note that we adopt the mathematical sign convention).

Our approach for the study of $\mathfrak{F}^\varepsilon(\gamma)$ borrows ideas from optimal transport and convex analysis, and takes the following observation as a starting point: the minimization appearing in $\mathfrak{F}^\varepsilon$ can be cast as a non-commutative entropic optimal transport problem. Indeed, one looks for an optimal non-commutative coupling Γ, with fixed non-commutative marginals (i.e. partial traces) γ, which minimizes the sum of a transport cost (given by $\mathrm{Tr}(H_{\mathsf{int}}\Gamma)$) and an entropic term. In light of this interpretation, setting the quantum problem at positive temperature ε corresponds to consider an entropic optimal transport problem with parameter ε.

The main contributions of this work consist in

- Theorem A.2.1, which represents a duality result for the functional $\mathfrak{F}^\varepsilon$. Theorem A.2.1 also includes the characterization of the optimizers of $\mathfrak{F}^\varepsilon$ (and of its dual functional).
- The introduction of a non-commutative Sinkhorn algorithm, which can be used to compute the aforementioned optimizers. We also prove convergence and robustness of this algorithm in Theorem A.2.2.
- The generalization of Theorem A.2.1 to the case of bosonic or fermionic systems, stated in Theorem A.2.3. This also allows to give an interesting variational characterization of the Pauli exclusion principle (see Proposition A.2.2).

Our results are based on a novel, noncommutative notion of (H, ε)-transform, which takes inspiration from the recent contribution of Di Marino and Gerolin [29] in the classical setting.

CHAPTER 2

Uniqueness and Non-degeneracy of Minimizers of the Pekar Functional on a Ball

This Chapter contains the work

- Dario Feliciangeli and Robert Seiringer. Uniqueness and nondegeneracy of minimizers of the Pekar functional on a ball. *SIAM Journal on Mathematical Analysis*, 52(1):605–622, 2020.

Abstract

We consider the Pekar functional on a ball in $\mathbb{R}^3$. We prove uniqueness of minimizers, and a quadratic lower bound in terms of the distance to the minimizer. The latter follows from non-degeneracy of the Hessian at the minimum.

2.1 Statement of the Problem and Main Results

The Pekar functional arises as a classical approximation of the ground state energy of the Fröhlich polaron model. Works of Donsker and Varadhan [30] and Lieb and Thomas [82] show that this approximation is correct, up to lower order corrections, in the strong coupling limit. Motivated by [41], where quantum corrections to the classical approximation were studied in the case of a polaron confined to a bounded subset of $\mathbb{R}^3$, we consider here the Pekar functional on a ball. Our goal is to extend the results of [76] and [70], where the problem is treated on $\mathbb{R}^3$, to this case. In particular, we refer to the existence and uniqueness of minimizers (proved in [76]) and to the coercivity around these minimizers (proved in [70]).

Let B_R denote the open ball of radius R centered at the origin. We will consider Dirichlet boundary conditions on B_R, which corresponds to working with functions $\phi \in H_0^1(B_R)$. The Pekar functional is

$$\mathcal{E}_R(\phi) = \int_{B_R} |\nabla \phi|^2 dx - 4\pi \int_{B_R} \int_{B_R} (-\Delta_{B_R})^{-1}(x,y) |\phi(x)|^2 |\phi(y)|^2 dx dy \,, \tag{2.1.1}$$

where $(-\Delta_{B_R})^{-1}(x,y)$ denotes the integral kernel of the inverse of the Dirichlet Laplacian on B_R. Explicitly,

$$(-\Delta_{B_R})^{-1}(x,y) = \frac{1}{4\pi}\left(\frac{1}{|x-y|} - \frac{1}{\left|\frac{|y|}{R}x - \frac{R}{|y|}y\right|}\right). \tag{2.1.2}$$

For completeness, we note that $(-\Delta_{B_R})^{-1}$ is *symmetric* and *positivity improving*, i.e. $(-\Delta_{B_R})^{-1}(x,y) = (-\Delta_{B_R})^{-1}(y,x) > 0$ for all $x, y \in B_R$.

Our main results are as follows:

Theorem 2.1.1. *For any $R > 0$, there exists a minimizer $0 \le \phi_R \in C^\infty(B_R) \cap H_0^1(B_R)$ such that*

$$\mathcal{E}_R(\phi_R) = E_R := \inf\{\mathcal{E}_R(\phi) : \phi \in H_0^1(B_R), \|\phi\|_2 = 1\}. \tag{2.1.3}$$

Moreover, ϕ_R is the unique positive minimizer, it is strictly positive, radial and decreasing. Any other minimizer of $\mathcal{E}_R$ differs from ϕ_R by multiplication by a constant phase.

Theorem 2.1.2. *For any $R > 0$, there exists a $K_R > 0$ such that the coercivity estimate*

$$\mathcal{E}_R(\phi) \ge \mathcal{E}_R(\phi_R) + K_R \min_{\theta\in[0,2\pi)} \int_{B_R} |\nabla(e^{i\theta}\phi_R - \phi)|^2 dx. \tag{2.1.4}$$

holds for any L^2-normalized $\phi \in H_0^1(B_R)$.

The study of this problem is motivated by the recent work [41], where lower order corrections to the ground state energy of the Fröhlich polaron model in the strong coupling limit are investigated. In particular, in [41], Theorem 2.1.1 and, in a slightly weaker form, Theorem 2.1.2 are taken as assumptions and are conjectured to hold for a large class of domains (e.g. convex domains). The goal of our work is to show that, at least in the case of balls, these assumptions hold true.

Remark 2.1.1. *Our results apply equally if we consider instead of $\mathcal{E}_R$ the Pekar functional on the full space $\mathbb{R}^3$ restricted to $H_0^1(B_R)$. This amounts to considering, for $\phi \in H_0^1(B_R)$ with $\|\phi\|_2 = 1$, the functional*

$$\tilde{\mathcal{E}}_R(\phi) = \int_{B_R} |\nabla\phi|^2 dx - \int_{B_R}\int_{B_R} \frac{|\phi(x)|^2|\phi(y)|^2}{|x-y|} dx dy\,. \tag{2.1.5}$$

The necessary modifications in the proofs will be explained in Remark 2.4.3.

Remark 2.1.2. *In the context of nonlinear Schrödinger equations with* local *nonlinearities the non-degeneracy of linearizations is a well known fact (see [120], [17]). Our model does not fall into this category since the linearization we have to deal with has a* non-local *nature. Nevertheless, using similar techniques as the ones used in [70] and [119], the radial symmetry of the problem still allows to conclude non-degeneracy. Uniqueness and non-degeneracy of ground states has also been addressed in a similar setting in [103] (with modifications to the interaction term) and in [122] (with modifications to the power of the non-linearity). In both latter references the problem is set on $\mathbb{R}^3$.*

2.2 Existence and Properties of Minimizers

We start by showing that minimizers exist. This can be done with standard techniques; the proof is actually easier on balls (because of compactness) than it is on the whole space. It will be convenient to introduce the notation

$$T_R(\phi) = \int_{B_R} |\nabla\phi|^2 dx, \qquad W_R(\phi) = 4\pi \int_{B_R}\int_{B_R} (-\Delta_{B_R})^{-1}(x,y)|\phi(x)|^2|\phi(y)|^2 dxdy\,. \tag{2.2.1}$$

Proposition 2.2.1. *For any $R > 0$, there exists an L^2-normalized $\phi_R \in H_0^1(B_R)$ such that $\mathcal{E}_R(\phi_R) = E_R$.*

Proof. Let $\phi \in H_0^1(B_R)$. By the Hardy–Littlewood–Sobolev, Hölder and Sobolev inequalities,

$$W_R(\phi) \leq \int_{B_R}\int_{B_R} \frac{|\phi(x)|^2|\phi(y)|^2}{|x-y|} dxdy \leq C\|\phi^2\|_{6/5}^2 \leq C\|\phi\|_6\|\phi\|_2^3 \leq C\|\nabla\phi\|_2\|\phi\|_2^3 \tag{2.2.2}$$

for suitable constants C (which may take different values at different appearances). Hence

$$\mathcal{E}_R(\phi) = T_R(\phi) - W_R(\phi) \geq \tfrac{1}{2}\|\nabla\phi\|_2^2 - C\|\phi\|_2^6\,. \tag{2.2.3}$$

We conclude that the functional is bounded from below for L^2-normalized functions, and that any minimizing sequence is bounded in $H_0^1(B_R)$. The Rellich–Kondrachov and Banach–Alaoglu Theorems allow us to conclude that any minimizing sequence ϕ_n has a subsequence that converges to some ϕ_R, strongly in $L^p(B_R)$ for every $p \in [1,6)$ and weakly in $H_0^1(B_R)$. Hence we have $\|\phi_R\|_2 = 1$ and, by lower semicontinuity of the norm w.r.t. weak convergence, $T_R(\phi_R) \leq \liminf_{n\to\infty} T_R(\phi_n)$. Moreover, with $\rho_n := |\phi_n|^2$ and $\rho := |\phi_R|^2$ we have

$$\begin{aligned} |W_R(\phi_n) - W_R(\phi_R)| &= 4\pi \left| \langle \rho_n | -\Delta_{B_R}^{-1} | \rho_n \rangle - \langle \rho | -\Delta_{B_R}^{-1} | \rho \rangle \right| \\ &= 4\pi |\langle \rho_n - \rho | -\Delta_{B_R}^{-1} | \rho_n + \rho \rangle| \leq C_R \|\rho_n - \rho\|_2 \|\rho_n + \rho\|_2 \to 0. \end{aligned} \tag{2.2.4}$$

Here, we used that $-\Delta_{B_R}^{-1}$ is a bounded operator (actually compact) on $L^2(B_R)$ and that $\rho_n \to \rho$ in L^2. Putting these pieces together, we conclude that ϕ_R is a minimizer, since

$$\mathcal{E}_R(\phi_R) \leq \liminf_{n\to\infty} \mathcal{E}_R(\phi_n) = E_R, \quad \phi_R \in H_0^1(B_R) \quad \text{and} \quad \|\phi_R\|_{L^2(B_R)} = 1\,. \tag{2.2.5}$$

□

Remark 2.2.1. *We point out that this proof extends* verbatim *to any bounded domain, the fact that we are working on B_R does not play any role. This is not true for the uniqueness statements that will come in the next sections, however.*

Having established existence, we proceed to investigate properties of minimizers.

Lemma 2.2.1. *Let $\phi \in H_0^1(B_R)$, $\|\phi\|_2 = 1$ and $\mathcal{E}_R(\phi) = E_R$. Then ϕ satisfies the equation*

$$(-\Delta - e_\phi - 2V_\phi)\,\phi = 0 \tag{2.2.6}$$

on B_R, with

$$e_\phi := T_R(\phi) - 2W_R(\phi) \tag{2.2.7}$$

and

$$V_\phi(x) := 4\pi \int_{B_R} (-\Delta_{B_R})^{-1}(x,y)|\phi(y)|^2 dy > 0. \tag{2.2.8}$$

Moreover, $\phi \in C^\infty(B_R)$ and if $\phi \geq 0$ then $\phi > 0$ on B_R.

Proof. Eq. (2.2.6) is the Euler–Lagrange equation associated to our minimization problem and its derivation is standard. The strict positivity of V_ϕ follows immediately by the fact that $(-\Delta_{B_R})^{-1}$ is positivity improving and since ϕ is L^2-normalized.

Since $\phi \in H_0^1(B_R)$, $|\phi|^2$ is in L^2 (by Sobolev embeddings). Moreover, the function $y \mapsto (-\Delta_{B_R})^{-1}(x,y)$ is bounded in $L^2(B_R)$ uniformly in x. Indeed, by the explicit form of $(-\Delta_{B_R})^{-1}(x,y)$ (given in (2.1.2)) and by its positivity, we have, for any $x \in B_R$

$$\int_{B_R} |(-\Delta_{B_R})^{-1}(x,y)|^2 dy < \frac{1}{(4\pi)^2}\int_{B_R} \frac{1}{|x-y|^2}dy \leq \frac{1}{(4\pi)^2}\int_{B_R}\frac{1}{|y|^2}dy = \frac{R}{4\pi}. \tag{2.2.9}$$

Therefore, we can conclude that $V_\phi \in L^\infty(B_R)$. Since ϕ solves (2.2.6) and is in $H_0^1(B_R)$, it satisfies

$$\phi(x) = \int_{B_R} (-\Delta_{B_R} + \lambda)^{-1}(\lambda + e_\phi + 2V_\phi(y))\phi(y)dy \tag{2.2.10}$$

for any $\lambda > -\inf \mathrm{spec}(-\Delta_{B_R})$, and by bootstrapping we can conclude that $\phi \in C^\infty(B_R)$. Finally, suppose $\phi \geq 0$. Choosing $\lambda > -e_\phi$ and exploiting the fact that $(-\Delta_{B_R}+\lambda)^{-1}$ is positivity improving, (2.2.10) implies that $\phi > 0$. □

Next we shall exploit the radial symmetry of the problem. Similarly to [76], we will make use of the tool of symmetric decreasing rearrangement [78, Chapter 3]. For any measurable positive function f, we will denote its symmetric decreasing rearrangement as f^*. If f is complex-valued, we will denote $f^* = |f|^*$. We recall the following Theorem, known as Talenti's Inequality [112]. In the strict form stated here, it is proved in [4, Theorem 3] (see also [64] and [65]). The result in [4, Theorem 3] is actually more general, but for simplicity we only state the version needed for our purposes.

Theorem A (Talenti's Inequality). *Let $0 \leq f \in L^2(B_R)$, and let $u, v \in H_0^1(B_R)$ solve*

$$\begin{cases} -\Delta u = f & x \in B_R, \\ u = 0 & x \in \partial B_R, \end{cases} \quad \text{and} \quad \begin{cases} -\Delta v = f^* & x \in B_R, \\ v = 0 & x \in \partial B_R. \end{cases} \tag{2.2.11}$$

Then $u^* \leq v$ a.e. in B_R. If additionally $u^*(x_0) = v(x_0)$ for some x_0 with $|x_0| = t \in (0,R)$, then $u(x) = v(x)$ and $f(x) = f^*(x)$ for all x with $t \leq |x| \leq R$.

With these tools in hand, we can show the following key Proposition, which will be essential to prove uniqueness of minimizers.

Proposition 2.2.2. *Let $\phi \in H_0^1(B_R)$ be a minimizer of $\mathcal{E}_R$. Then $|\phi| = \phi^*$ and there exists $\theta \in [0, 2\pi)$ such that $\phi = e^{i\theta}|\phi|$.*

Proof. Clearly, for any $\psi \in H_0^1(B_R)$, $W_R(\psi) = W_R(|\psi|)$, and it is easy to see ([78, Theorem 7.8]) that $T_R(\psi) \geq T_R(|\psi|)$. Hence, $\mathcal{E}_R(\psi) \geq \mathcal{E}_R(|\psi|)$. To proceed, we exploit the properties of symmetric decreasing rearrangements. The Pólya–Szegő inequality [78, Lem. 7.17] states that

$$T_R(|\psi|) \geq T_R(\psi^*). \tag{2.2.12}$$

We claim that also

$$W_R(|\psi|) \leq W_R(\psi^*), \tag{2.2.13}$$

with equality if and only if $|\psi| = \psi^*$. To see this we define

$$u(x) := \int_{B_R} (-\Delta_{B_R})^{-1}(x,y)|\psi(y)|^2 dy \quad \text{and} \quad v(x) := \int_{B_R} (-\Delta_{B_R})^{-1}(x,y)\psi^*(y)^2 dy. \tag{2.2.14}$$

These functions satisfy (2.2.11) with $f(x) = |\psi(x)|^2$. By Theorem A, we conclude that $u^* \leq v$. Applying first this estimate and then the Hardy–Littlewood rearrangement inequality [78, Thm. 3.4], we obtain

$$\begin{aligned} W_R(\psi^*) = 4\pi \int_{B_R} \psi^*(x)^2 v(x) dx &\geq 4\pi \int_{B_R} \psi^*(x)^2 u^*(x) dx \\ &\geq 4\pi \int_{B_R} |\psi(x)|^2 u(x) dx = W_R(|\psi|). \end{aligned} \tag{2.2.15}$$

To have equality in (2.2.15), we must have $v = u^*$ on the support of ψ^*, which contains a non-empty ball centered at the origin. Hence the second part of Theorem A implies that $v = u$ and thus $|\psi| = \psi^*$ on B_R, as claimed. For any $\psi \in H_0^1(B_R)$, we conclude that $\mathcal{E}_R(\psi) \geq \mathcal{E}_R(\psi^*)$, with equality if and only if $|\psi| = \psi^*$.

If now we take ϕ to be a minimizer, we then immediately obtain $|\phi| = \phi^*$. Moreover, by the previous Lemma, $|\phi| \in C^\infty(B_R)$ and $|\phi| > 0$. It remains to show that $\phi = e^{i\theta}|\phi|$. This follows from the fact that both ϕ and $|\phi|$ are eigenfunctions of the Schrödinger operator $-\Delta - 2V_\phi$. Since the latter function is strictly positive, e_ϕ must be the ground state energy of this operator, and is a simple eigenvalue. □

2.3 Uniqueness of Minimizers

In the previous section we have shown that any minimizer, up to a multiplication by a constant phase, must be real, strictly positive, C^∞ and radial. To show uniqueness of minimizers it is then sufficient to show uniqueness among functions with these properties. The big advantage of this restriction, as already utilized in [76], is that the Euler–Lagrange equation for minimizers can be written in the following convenient form.

Remark 2.3.1. *Throughout this paper, we shall make a convenient abuse of notation, and write equivalently $\phi(x)$ or $\phi(r)$ if ϕ is a radial function and $x \in \mathbb{R}^3$ with $|x| = r$.*

Lemma 2.3.1. *Let $\phi \in H_0^1(B_R)$ be a radial function with $\|\phi\|_2 = 1$. Then ϕ satisfies Eq.* (2.2.6) *if and only if ϕ satisfies*

$$\left[-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + 2U_\phi(r)\right]\phi(r) = \nu_\phi \phi(r)\,, \tag{2.3.1}$$

where

- $U_\phi(r) := \int_0^r K(r,s)|\phi(s)|^2 ds$, *with* $K(r,s) = 4\pi s^2(\frac{1}{s} - \frac{1}{r}) \geq 0$ *for* $s \leq r$,
- $\nu_\phi = e_\phi + 2I(\phi) - \frac{2}{R} > 0$, *with* $I(\phi) := \int_{B_R} \frac{|\phi(x)|^2}{|x|} dx$.

Proof. The proof of this Lemma is just a straightforward application of Newton's Theorem [78, Thm. 9.7] to the nonlocal term V_ϕ. Indeed, with $r = |x|$ we have

$$\begin{aligned} V_\phi(x) &= \int_{B_R} \frac{|\phi(y)|^2}{|x-y|} dy - \int_{B_R} \frac{|\phi(y)|^2}{\left|\frac{|y|}{R}x - \frac{R}{|y|}y\right|} dy \\ &= \frac{1}{r}\int_{B_r} |\phi(y)|^2 dy + \int_{B_R \setminus B_r} \frac{|\phi(y)|^2}{|y|} dy - \frac{1}{R} \\ &= -U_\phi(r) + I(\phi) - \frac{1}{R}. \end{aligned} \tag{2.3.2}$$

Recalling the original form of the Euler–Lagrange equation (2.2.6), this identity immediately implies our claim. To show $\nu_\phi > 0$ one just needs to integrate the equation against ϕ and use the positivity of U_ϕ and of $-\Delta_{B_R}$. □

It is important to note that the nonlocal term $U_\phi(x)$ only depends, at a fixed x, on the values of ϕ on $B_{|x|}$ and *not* on the whole ball B_R. By using ODE techniques, as in [76, 70] (see also [115]), this will allow us to conclude uniqueness of solutions.

Proposition 2.3.1 (Uniqueness of minimizers)**.** *For any $R > 0$, there exists a unique positive and L^2-normalized minimizer of $\mathcal{E}_R$.*

Proof. From Lemma 2.2.1 and Proposition 2.2.2 we deduce that any positive minimizer is in $C^\infty(B_R)$, is radially decreasing and strictly positive. Moreover, by the previous Lemma, it satisfies (2.3.1). Suppose that ϕ_1 and ϕ_2 are two distinct positive L^2-normalized minimizers. We distinguish two cases: ν_{ϕ_1} and ν_{ϕ_2} can either be equal (first case) or not (second case).

First case: Note that $\phi_i'(0) = 0$ for $i \in \{1, 2\}$, since ϕ_i is smooth and radial. If $\phi_1(0) = \phi_2(0)$ it follows from standard fixed point arguments (explained for completeness in Section 2.5) that $\phi_1 = \phi_2$ on B_R. W.l.o.g. we can hence suppose that $\phi_1(0) > \phi_2(0)$. By integrating the Euler–Lagrange equation using that $\phi_i'(0) = 0$, we find

$$\left(\frac{\phi_1}{\phi_2}\right)'(r) = \frac{2}{r^2\phi_2^2(r)} \int_0^r s^2 \phi_1(s)\phi_2(s)\left[U_{\phi_1}(s) - U_{\phi_2}(s)\right] ds. \tag{2.3.3}$$

Exploiting the fact that $U_\phi(s)$ only depends on the values of ϕ in $[0, s)$, and it does so *monotonically*, we conclude that if $\phi_1 > \phi_2$ on $[0, t)$ for some $t > 0$, then $(\phi_1/\phi_2)'(t) > 0$. This readily implies that $\phi_1 > \phi_2$ on B_R, which is a contradiction to our assumption that both functions are L^2-normalized.

Second case: W.l.o.g. we assume that $\nu_{\phi_1} > \nu_{\phi_2} > 0$. Let $\lambda = \sqrt{\nu_{\phi_1}/\nu_{\phi_2}} > 1$ and consider the function $\tilde{\phi}_2(x) := \lambda^2\phi_2(\lambda x)$ defined on $B_{R/\lambda} \subset B_R$. Its L^2-norm equals $\sqrt{\lambda} > 1$ and it satisfies

$$\left[-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + 2U_{\tilde{\phi}_2}(r)\right]\tilde{\phi}_2(r) = \lambda^2\nu_{\phi_2}\tilde{\phi}_2(r) = \nu_{\phi_1}\tilde{\phi}_2(r) \tag{2.3.4}$$

on $B_{R/\lambda}$. Hence ϕ_1 and $\tilde{\phi}_2$ satisfy the equation with same eigenvalue on $B_{R/\lambda}$ and we have reduced the problem to the first case. In particular, we have that either $\phi_1 > \tilde{\phi}_2$ or $\phi_1 < \tilde{\phi}_2$ or $\phi_1 = \tilde{\phi}_2$ on the whole of $B_{R/\lambda}$. Each of these possibilities yields a contradiction since $\tilde{\phi}_2$ has L^2-norm strictly larger than ϕ_1 and is supported on a smaller ball. □

In combination with Prop. 2.2.2, Prop. 2.3.1 proves Thm. 2.1.1.

The unique positive minimizer will henceforth be denoted by ϕ_R. It is natural to expect that, as $R \to \infty$, it converges to a minimizer of the problem on the full space $\mathbb{R}^3$. This is indeed the case, as detailed in Section 2.6.

While the proof of existence of minimizers extends to general domains in $\mathbb{R}^3$, as discussed in Remark 2.2.1, the proof of uniqueness relies heavily on symmetric decreasing rearrangement and hence cannot be easily generalized. Extending the uniqueness result to more general domains is hence an open problem. As the following counterexample shows, uniqueness can actually fail on particular domains. Nevertheless, we believe that uniqueness holds *generically*, in the sense that if Ω is any domain for which different minimizers exist, then a generic perturbation of Ω should still lead to a unique minimizer (up to phase). We conjecture that convexity of Ω is a sufficient condition to ensure uniqueness.

Remark 2.3.2. *Consider two disjoint balls of the same size in $\mathbb{R}^3$, $B_1 := B_R(x_1)$ and $B_2 := B_R(x_2)$, with $|x_1 - x_2| > 2R$. Let $\Omega = B_1 \cup B_2$ and consider the Pekar functional defined on Ω:*

$$\mathcal{E}_\Omega(\phi) = \int_\Omega |\nabla\phi|^2 dx - 4\pi \int_\Omega \int_\Omega (-\Delta_\Omega)^{-1}(x,y)|\phi(x)|^2|\phi(y)|^2 dxdy = T_\Omega(\phi) - W_\Omega(\phi). \tag{2.3.5}$$

Here $(-\Delta_\Omega)^{-1}(x,y)$ denotes the integral kernel of the inverse Dirichlet Laplacian on Ω. Any L^2-normalized $\phi \in H_0^1(\Omega)$ can be written as $\phi = \sqrt{t}\phi_1 + \sqrt{1-t}\phi_2$, for some $t \in [0,1]$ and L^2-normalized $\phi_1 \in H_0^1(B_1)$, $\phi_2 \in H_0^1(B_2)$. For general functions f_1, f_2,

$$\begin{aligned}&\langle tf_1 + (1-t)f_2 | -\Delta_\Omega^{-1} | tf_1 + (1-t)f_2\rangle \\ &= t\langle f_1|-\Delta_\Omega^{-1}|f_1\rangle + (1-t)\langle f_2|-\Delta_\Omega^{-1}|f_2\rangle - t(1-t)\langle f_1 - f_2|-\Delta_\Omega^{-1}|f_1 - f_2\rangle .\end{aligned} \tag{2.3.6}$$

By the positivity of $-\Delta_\Omega^{-1}$ as an operator, the last term is strictly negative unless $t \in \{0,1\}$ or $f_1 = f_2$. In other words, $\langle\cdot|-\Delta_\Omega^{-1}|\cdot\rangle$ is strictly convex, which holds true for general Ω, in fact. In particular

$$\begin{aligned}\mathcal{E}_\Omega(\phi) &= t\int_{B_1} |\nabla\phi_1|^2 dx + (1-t)\int_{B_2} |\nabla\phi_2|^2 dx - W_\Omega\left(\sqrt{t}\phi_1 + \sqrt{1-t}\phi_2\right) \\ &\geq t\mathcal{E}_{B_1}(\phi_1) + (1-t)\mathcal{E}_{B_2}(\phi_2) \geq E_R\end{aligned} \tag{2.3.7}$$

and the first inequality is strict unless $t = 0$ or $t = 1$. We conclude that any minimizer of $\mathcal{E}_\Omega$ is obtained by translating a minimizer of $\mathcal{E}_R$ by x_1 or *x_2. In particular, uniqueness up to phase does not hold on Ω.*

The fact that Ω has two distinct connected components is not essential in our argument. The lack of uniqueness would still hold, by continuity, if B_1 and B_2 were connected by a sufficiently narrow corridor, respecting the symmetry between the two balls. On the other hand, a generic *perturbation of Ω (or of Ω connected by a corridor) would restore uniqueness up to phase of minimizers, since it would break the symmetry.*

2.4 Study of the Hessian

Recall that for given $R > 0$, ϕ_R denotes the unique L^2-normalized positive minimizer of $\mathcal{E}_R$ on B_R. In this section we study the Hessian of $\mathcal{E}_R$ at ϕ_R, following ideas in [70] (see also

[119]). Let ϕ be any function in $H_0^1(B_R)$. A straightforward computation shows that

$$\mathcal{E}_R\left(\frac{\phi_R+\varepsilon\phi}{\|\phi_R+\varepsilon\phi\|_2}\right)=\mathcal{E}_R(\phi_R)+\varepsilon^2 H_R(\phi)+O(\varepsilon^3) \tag{2.4.1}$$

as $\varepsilon\to 0$, where

$$H_R(\phi)=\ \langle \mathrm{Im}(\phi)|L_-|\mathrm{Im}(\phi)\rangle +\ \langle \mathrm{Re}(\phi)|QL_+Q|\mathrm{Re}(\phi)\rangle\,, \tag{2.4.2}$$

$Q=\mathbb{1}-|\phi_R\rangle\langle\phi_R|$, and the operators $L_\pm$ are given by

$$L_-:=-\Delta_{B_R}-2V_{\phi_R}-e_{\phi_R}\ ,\quad L_+=L_--4X \tag{2.4.3}$$

with

$$(Xf)(x):=4\pi\phi_R(x)\int_{B_R}(-\Delta_{B_R})^{-1}(x,y)\phi_R(y)f(y)dy\,. \tag{2.4.4}$$

We recall that $e_{\phi_R}=T_R(\phi_R)-2W_R(\phi_R)$. Moreover V_ϕ is defined in (2.2.8). Since ϕ_R is smooth, it is not difficult to see that both V_{ϕ_R} and X are bounded operators. In particular, the domain of $L_\pm$ equals the domain of Δ_{B_R}, namely $H^2(B_R)\cap H_0^1(B_R)$. Using (2.1.2), we find it convenient to decompose X as $X=X_1-X_2$ with

$$(X_1f)(x):=\phi_R(x)\int_{B_R}\frac{\phi_R(y)f(y)}{|x-y|}dy\ ,\quad (X_2f)(x):=\phi_R(x)\int_{B_R}\frac{\phi_R(y)f(y)}{\left|\frac{|y|}{R}x-\frac{R}{|y|}y\right|}dy\,. \tag{2.4.5}$$

Note that $\phi_R\in\ker L_-$ by the Euler–Lagrange equation (2.2.6). Since $Q\phi_R=0$, clearly also $\phi_R\in\ker QL_+Q$. Our aim is to show that 0 is a simple eigenvalue for both QL_+Q and L_-. This will imply the strict positivity of the Hessian on $\operatorname{ran}Q$. Indeed, by minimality of ϕ_R, both operators are non-negative and, since the domain under consideration is bounded, have compact resolvents and discrete spectrum.

The simplicity of 0 as an eigenvalue of L_- follows from the fact that L_- is a Schrödinger operator with $\inf\operatorname{spec}L_-=0$ (since the corresponding eigenfunction ϕ_R is positive). Note that the non-triviality of $\ker L_-$ is a consequence of the $U(1)$-symmetry of $\mathcal{E}_R$ leading to uniqueness *up to phase* of the minimizer only. Indeed, purely imaginary perturbations of ϕ_R by functions in $\operatorname{span}\{\phi_R\}$ correspond to phase rotations of ϕ_R.

The analysis of $\ker QL_+Q$ is more tricky. The presence of the projection Q does not allow the use of standard arguments to show simplicity of the least eigenvalue based on positivity. It will be essential to utilize that L_+ commutes with rotations. We recall that

$$L^2(B_R)=\bigoplus_{l=0}^{\infty}\mathcal{H}_l, \tag{2.4.6}$$

where $\mathcal{H}_l:=L^2([0,R],r^2dr)\otimes\mathcal{Y}_l$, $\mathcal{Y}_l=\operatorname{span}\{Y_{lm}\}_{m=-l}^{l}$ is the $(2l+1)$-dimensional eigenspace corresponding to the eigenvalue $l(l+1)$ of the negative spherical Laplacian on $L^2(\mathbb{S}^2)$ and Y_{lm} is the m-th spherical harmonic of angular momentum l. The fact that L_+ commutes with rotations implies that L_+ acts invariantly on each $\mathcal{H}_l$, i.e., it can be decomposed as

$$L_+=\bigoplus_{l=0}^{\infty}L_+|_{\mathcal{H}_l}=:\bigoplus_{l=0}^{\infty}L_+^{(l)}\,. \tag{2.4.7}$$

Since ϕ_R is radial, also Q leaves each $\mathcal{H}_l$ invariant (in particular $Q|_{\mathcal{H}_l} = \mathbb{1}$ if $l \geq 1$), hence

$$QL_+Q = \bigoplus_{l=0}^{\infty} (QL_+Q)|_{\mathcal{H}_l} = \left(QL_+^{(0)}Q\right) \oplus \left(\bigoplus_{l=1}^{\infty} L_+^{(l)}\right). \tag{2.4.8}$$

Identifying the kernel of QL_+Q is equivalent to identifying the kernels of $QL_+^{(0)}Q$ and of $L_+^{(l)}$ for $l \geq 1$. We start with the study of $QL_+^{(0)}Q$, the only operator in which Q still appears, complicating the analysis. The operators $L_+^{(l)}$, in which Q does not appear, will be studied with more standard arguments below.

Proposition 2.4.1.

$$\ker\left(QL_+^{(0)}Q\right) = \ker Q = \operatorname{span}\{\phi_R\}. \tag{2.4.9}$$

Proof. Since $\ker(QL_+^{(0)}) \cap \operatorname{ran} Q = \{0\}$ implies $\ker QL_+^{(0)}Q = \ker Q$, our strategy will be to show that $\ker(QL_+^{(0)})$ does not contain any non-null functions that are in $\operatorname{ran} Q$. Since all operators are real (i.e., commute with complex conjugation), it is sufficient to consider real-valued functions. We consider a $f \in \operatorname{dom} L_+^{(0)}$ (which in particular implies $f \in \mathcal{H}_0$, i.e., f radial) and observe that, by Newton's Theorem,

$$(L_+f)(r) = (L_+f)(r) - \sigma(f)\phi_R(r), \tag{2.4.10}$$

with

$$\begin{aligned} (L_+f)(r) &:= (L_-f)(r) + 4\phi_R(r)\int_{B_r}\left(\frac{1}{|y|} - \frac{1}{r}\right)\phi_R(y)f(y)dy, \\ \sigma(f) &:= 4\int_{B_R}\left(\frac{1}{|y|} - \frac{1}{R}\right)\phi_R(y)f(y)dy\,. \end{aligned} \tag{2.4.11}$$

Any $f \in \operatorname{dom} L_+^{(0)}$ is in $\ker(QL_+^{(0)})$ if and only $L_+f = \lambda\phi_R$ for some $\lambda \in \mathbb{R}$ and, by (2.4.10), this is true if and only if

$$L_+f = \mu\phi_R \text{ for some } \mu \in \mathbb{R}. \tag{2.4.12}$$

The operator L_+ can be naturally defined on the extended domain $H^2(B_R)$ (without Dirichlet boundary conditions at R) and it will be convenient to do so in the following. From the above discussion we infer that $f \in \ker(QL_+^{(0)})$ must be of the form $f = v + c\varphi$, with $c \in \mathbb{R}$, v a solution of $L_+v = 0$ and φ being a *particular* solution of (2.4.12), with $\mu \neq 0$. While f needs to satisfy Dirichlet boundary conditions, i.e., $f \in H_0^1(B_R)$, this need not be the case for v and φ separately, however. In the following, we will exhibit a particular solution φ that is *radial*, hence we are only interested in radial solutions of $L_+v = 0$.

We begin by studying the radial solutions of $L_+v = 0$. A bootstrapping argument shows that any such v must be in $C^\infty(B_R)$. Moreover, by Newton's Theorem, v satisfies

$$v''(r) + \frac{2}{r}v'(r) = a(r)v(r) + b(r), \tag{2.4.13}$$

where

$$a(r) := -2V_{\phi_R}(r) - e_{\phi_R}\,, \quad b(r) := 4\phi_R(r)\int_{B_r}\left(\frac{1}{|y|} - \frac{1}{r}\right)\phi_R(y)v(y)dy\,. \tag{2.4.14}$$

By the regularity of v, we have $v'(0) = 0$. Arguing as in the proof of Lemma 2.5.1, we see that the equation possesses no non-trivial solution that vanishes at the origin.

Recall that ϕ_R satisfies

$$\phi_R''(r) + \frac{2}{r}\phi_R'(r) = a(r)\phi_R(r)\,. \tag{2.4.15}$$

By applying the same computations as in the proof of Thm. 2.3.1, using $v'(0) = \phi_R'(0) = 0$, we obtain

$$\left(\frac{v}{\phi_R}\right)'(r) = \frac{1}{r^2\phi_R^2(r)}\int_0^r s^2 b(s)\phi_R(s)ds\,. \tag{2.4.16}$$

Note that $b(r) \geq 0$ if $v \geq 0$ in $[0, r)$. Assuming that $v(0) > \phi_R(0)$ this implies that $v > \phi_R$ on B_R. In other words, any non-trivial radial solution of $L_+ v = 0$ has a multiple which is strictly larger than ϕ_R on B_R. In particular any non-trivial radial solution must have constant sign.

Consider now the radial function $\varphi(r) := 2\phi_R(r) + r\phi_R'(r)$. We observe that $\varphi \notin \operatorname{ran} Q$, since $\langle\phi_R|\varphi\rangle = 1/2$ as an argument using integration by parts shows. A straightforward computation shows that $L_+\varphi = \lambda\phi_R$ for some $\lambda \in \mathbb{R}$, which implies that also $L_+\varphi = \mu\phi_R$ for some $\mu \in \mathbb{R}$. We claim that $\mu \neq 0$, which is an immediate consequence of our previous findings about radial solutions of $L_+ v = 0$. Indeed, $\varphi(0) > 0$ whereas $\varphi(R) < 0$ (a proof of this last statement is given in Lemma 2.5.2 in Section 2.5), hence φ does not have constant sign and cannot be in $\ker L_+$. We conclude that φ is a particular solution of (2.4.12) and this implies, by the previous discussion, that any $f \in \ker(QL_+^{(0)})$ must be of the form $f = v + c\varphi$, for some $v \in \ker L_+$ and some $c \in \mathbb{R}$. The case $v \equiv 0$ immediately yields $f = 0$, since φ does not satisfy the boundary condition $f(R) = 0$. All the other solutions v have constant sign, thus the boundary condition $f(R) = 0$ is satisfied if and only if c has the same sign of v. In particular,

$$\langle\phi_R|f\rangle = \langle\phi_R|v\rangle + \frac{c}{2} \neq 0 \tag{2.4.17}$$

unless $f = 0$, i.e., $f \in \operatorname{ran} Q$ if and only if $f = 0$. We conclude that $\ker QL_+^{(0)} \cap \operatorname{ran} Q = \{0\}$, as claimed. □

We now proceed with the study of $\ker L_+^{(l)}$ for $l \geq 1$. We first investigate the explicit expressions of these operators. We note that the action of L_+ is not only invariant on $\mathcal{H}_l = L^2([0, R], r^2 dr) \otimes \mathcal{Y}_l$, but it also acts as the identity on the second factor. Hence we can identify the operators $L_+^{(l)}$ with operators acting on $L^2([0, R], r^2 dr)$ only, which we will denote by the same symbol for simplicity. That is, if $\phi \in \mathcal{H}_l$ is of the form $\phi(r\omega) = \sum_{m=-l}^{m=l}\phi_m(r)Y_{ml}(\omega)$ for $\omega \in \mathbb{S}^2$, then

$$L_+\phi = L_+^{(l)}\phi = \sum_{m=-l}^{m=l}(L_+^{(l)}\phi_m)Y_{ml}\,, \tag{2.4.18}$$

where he operators $L_+^{(l)}$ are defined on $L^2([0, R], r^2 dr)$ by

$$L_-^{(l)} = -\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{l(l+1)}{r^2} - e_{\phi_R} - 2V_{\phi_R} \tag{2.4.19}$$

and $L_+^{(l)} = L_-^{(l)} - 4X^{(l)}$ with $X^{(l)} = X_1^{(l)} - X_2^{(l)}$, where

$$\begin{aligned}(X_1^{(l)}\phi)(r) &= \frac{4\pi}{2l+1}\phi_R(r)\int_0^R \phi(s)\phi_R(s)s^2\frac{\min\{r,s\}^l}{\max\{r,s\}^{l+1}}ds,\\ (X_2^{(l)}\phi)(r) &= \frac{4\pi}{2l+1}\phi_R(r)\int_0^R \phi(s)\phi_R(s)s^2\frac{(rs)^l}{R^{2l+1}}ds.\end{aligned} \tag{2.4.20}$$

This follows from a straightforward computation, using the *multipole expansion* (see, for example [23])

$$\frac{1}{|x-y|} = 4\pi \sum_{k=0}^{\infty} \sum_{n=-k}^{k} \frac{1}{2k+1} \frac{\min\{|x|,|y|\}^k}{\max\{|x|,|y|\}^{k+1}} Y_{kn}(\omega_x) Y^*_{kn}(\omega_y)\,. \tag{2.4.21}$$

Let us define the operator $\tilde{L}_+ := L_- - 4X_1$, and the corresponding restriction to $\mathcal{H}_l$, $\tilde{L}_+^{(l)} := L_-^{(l)} - 4X_1^{(l)}$.

Lemma 2.4.1. *For $l \geq 1$ the operators $L_+^{(l)}$ and $\tilde{L}_+^{(l)}$ satisfy the Perron–Frobenius property, i.e., their least eigenvalue is* simple *and there exists a corresponding eigenfunction which is* strictly *positive on $(0,R)$. This eigenfunction is in $C^\infty((0,R))$ and has strictly negative (left) derivative at $r = R$.*

Proof. We will give the proof for the operators $L_+^{(l)}$; it will be important that $X^{(l)} = X_1^{(l)} - X_2^{(l)}$ is positivity improving, which can be checked easily using the explicit form (2.4.20). The proof for $\tilde{L}_+^{(l)}$ works in exactly the same way, using simply that $X_1^{(l)}$ is positivity improving instead.

It will be convenient to introduce the unitary and positive transformation

$$U : L^2([0,R], r^2 dr) \to L^2([0,R], dr) \quad \text{with} \quad (Uf)(r) = rf(r) \tag{2.4.22}$$

which satisfies

$$\begin{aligned} UL_+^{(l)}U^{-1} &= -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + V, \\ V &:= -e_{\phi_R} - 2V_{\phi_R} - 4UX^{(l)}U^{-1}. \end{aligned} \tag{2.4.23}$$

Since U is positive, it is equivalent to show the Perron–Frobenius property for $UL_+^{(l)}U^{-1}$.

Since V is bounded, the operators $UL_+^{(l)}U^{-1}$ have compact resolvent and eigenfunctions corresponding to the least eigenvalue certainly exist. By bootstrapping, we conclude that they are $C^\infty((0,R))$. Moreover, if $\phi \geq 0$ is such an eigenfunction, then $\phi > 0$ on $(0,R)$. Indeed, if we suppose that ϕ is not strictly positive, then there exists an $r_0 \in (0,R)$ such that $\phi(r_0) = 0$. Evaluating the Euler–Lagrange equation at r_0 we find, using that U is positive and $X^{(l)}$ is positivity improving,

$$-\phi''(r_0) = 4(UX^{(l)}U^{-1}\phi)(r_0) > 0. \tag{2.4.24}$$

This is clearly a contradiction since ϕ attains a minimum in r_0. From this, we can conclude by standard arguments that the Perron–Frobenius property holds.

Finally, we need to show that $\phi'(R) < 0$ if ϕ is the positive ground state function. We already know that $\phi(R) = 0$ and $\phi'(R) \leq 0$ (since ϕ is positive). If by contradiction $\phi'(R) = 0$ standard uniqueness arguments along the lines of Lemma 2.5.2 imply that $\phi \equiv 0$. Note also that this property is preserved by U since $\phi(R) = 0$. □

Remark 2.4.1. *From this Lemma and the fact that $X_2^{(l)}$ is positivity improving we conclude that for each $l \geq 1$ we have $\inf\operatorname{spec} L_+^{(l)} > \inf\operatorname{spec} \tilde{L}_+^{(l)}$. Thus, in order to show that $\ker L_+^{(l)} = \{0\}$ for $l \geq 1$, it is sufficient to show $\inf\operatorname{spec} \tilde{L}_+^{(l)} \geq 0$ for $l \geq 1$. It is actually even possible to show $\inf\operatorname{spec} \tilde{L}_+^{(l)} > 0$ for $l \geq 1$, which is the content of the next Proposition. This is going to be relevant for Remark 2.4.3 at the end of this section.*

Proposition 2.4.2. *For any $l > 1$, we have*

$$\inf \operatorname{spec} \tilde{L}_+^{(l)} > \inf \operatorname{spec} \tilde{L}_+^{(1)} > 0. \tag{2.4.25}$$

In particular, $\ker L_+^{(l)} = \{0\} = \ker \tilde{L}_+^{(l)}$ *for all* $l \geq 1$.

Proof. For $i \in \{1, 2, 3\}$, we have $\frac{\partial}{\partial x_i}\phi_R(x) \in \mathcal{H}_1$, with

$$\frac{\partial}{\partial x_i}\phi_R(x) = \phi_R'(r)\frac{x_i}{r} = \sum_{m=-1}^{1} c_m^i \phi_R'(r) Y_{1m}(\omega) \tag{2.4.26}$$

for suitable c_m^i. Since $\phi_R'(R) < 0$, this function is not in the domain of $\tilde{L}_+^{(1)}$. As in the proof of Prop. 2.4.1, we can however consider the extension of $\tilde{L}_+^{(1)}$ to $H^2(B_R) \cap \mathcal{H}_l$ (ignoring the Dirichlet boundary condition). A straightforward computation shows that

$$\tilde{L}_+^{(1)}\phi_R' = 0 \tag{2.4.27}$$

i.e., ϕ_R' is in the kernel of the extended operator.

Let ϕ denote the unique positive ground state of the original, unextended $\tilde{L}_+^{(1)}$, with ground state energy $\tilde{e}_1$. The function ϕ is strictly positive on $(0, R)$ and satisfies $\phi'(R) < 0$. Integrating by parts, we have

$$\begin{aligned} 0 = \left\langle \phi \middle| \tilde{L}_+^{(1)}\phi_R' \right\rangle = \left\langle \tilde{L}_+^{(1)}\phi \middle| \phi_R' \right\rangle + \phi'(R)\phi_R'(R)R^2 - \phi(R)\phi_R''(R)R^2 = \\ = \tilde{e}_1 \left\langle \phi | \phi_R' \right\rangle + \phi'(R)\phi_R'(R)R^2. \end{aligned} \tag{2.4.28}$$

In particular, we conclude that

$$\tilde{e}_1 = -\frac{\phi'(R)\phi_R'(R)R^2}{\langle \phi | \phi_R' \rangle} > 0\,, \tag{2.4.29}$$

which is the second inequality in (2.4.25). For the first inequality, observe that if $0 < \phi \in L^2([0, R], r^2 dr)$ and $l \geq 2$,

$$\begin{aligned} (\tilde{L}_+^{(l)}\phi)(r) - (\tilde{L}_+^{(1)}\phi)(r) = \left(\frac{l(l+1)}{r^2} - \frac{2}{r^2}\right)\phi(r) \\ + 4\pi\phi_R(r)\int_0^R \phi(s)\phi_R(s)s^2 \left(\frac{\min\{r,s\}}{3\max\{r,s\}^2} - \frac{\min\{r,s\}^l}{(2l+1)\max\{r,s\}^{l+1}}\right) ds > 0. \end{aligned} \tag{2.4.30}$$

By Lemma 2.4.1, the ground state ϕ_l of $\tilde{L}_+^{(l)}$ is strictly positive. Thus

$$\inf \operatorname{spec} \tilde{L}_+^{(l)} = \langle \phi_l | \tilde{L}_+^{(l)} | \phi_l \rangle_{L^2([0,R], r^2 dr)} > \langle \phi_l | \tilde{L}_+^{(1)} | \phi_l \rangle_{L^2([0,R], r^2 dr)} \geq \tilde{e}_1 > 0, \tag{2.4.31}$$

which completes the proof. □

With the aid of Propositions 2.4.1 and 2.4.2, we can now give the proof of Theorem 2.1.2. The proof follows closely [41, Appendix A], with some minor modifications due to the fact that our statement is slightly stronger than the one in [41]. We emphasize that the hard part of the proof was establishing the triviality of the kernel of QL_+Q (which enters as an assumption in [41]), the remaining part uses only fairly standard arguments.

Proof of Theorem 2.1.2. We shall actually prove the following slightly stronger inequality: For any L^2-normalized $\phi \in H_0^1(B_R)$ with $\langle \phi | \phi_R \rangle \geq 0$,

$$\mathcal{E}_R(\phi) \geq \mathcal{E}_R(\phi_R) + K_R \int_{B_R} |\nabla(\phi_R - \phi)|^2 dx \tag{2.4.32}$$

for some $K_R > 0$ (independent of ϕ). Because of the invariance of $\mathcal{E}_R(\phi)$ under multiplication of ϕ by a complex phase, (2.4.32) readily implies (2.1.4).

To show (2.4.32) we shall proceed in two steps, one to ensure that the estimate holds *locally* and one to ensure that it holds *globally*.

Step 1: In this step we show that (2.4.32) holds locally. Let $\phi \in H_0^1(B_R)$ with $\|\phi\|_2 = 1$ and $\langle \phi | \phi_R \rangle \geq 0$. Denoting $\delta = \phi - \phi_R$ and expanding $\mathcal{E}_R$ around ϕ_R, we have

$$\begin{aligned}\mathcal{E}_R(\phi) &= \mathcal{E}_R(\phi_R + \delta) \\ &= \mathcal{E}_R(\phi_R) + \langle \operatorname{Im}\delta | L_- | \operatorname{Im}\delta \rangle + \langle \operatorname{Re}\delta | L_+ | \operatorname{Re}\delta \rangle + O(\|\delta\|^3_{H^1(B_R)})\end{aligned} \tag{2.4.33}$$

for small $\|\delta\|^3_{H^1(B_R)}$, with $L_\pm$ defined in (3.3.69). Recall that $L_- = QL_-Q$ for $Q = \mathbb{1} - |\phi_R\rangle\langle\phi_R|$, and that $L_+ = L_- - 4X$.

In order to utilize the previous results, we would need QXQ in place of X. To estimate the difference, observe that, since both ϕ_R and ϕ have L^2-norm equal to 1, we have

$$\begin{aligned}&\|\delta\|_2^2 = 2 - 2\langle \phi_R | \phi \rangle, \\ &(\mathbb{1} - Q)\operatorname{Re}\delta = \phi_R \langle \phi_R | \delta \rangle = \phi_R(\langle \phi_R | \phi \rangle - 1) = -\phi_R \frac{\|\delta\|_2^2}{2}.\end{aligned} \tag{2.4.34}$$

This readily implies that

$$\langle \operatorname{Re}\delta | X | \operatorname{Re}\delta \rangle = \langle \operatorname{Re}\delta | QXQ | \operatorname{Re}\delta \rangle + O(\|\delta\|^3_{H^1(B_R)}). \tag{2.4.35}$$

In particular, we have

$$\mathcal{E}_R(\phi) = \mathcal{E}_R(\phi_R) + \langle \operatorname{Im}\delta | L_- | \operatorname{Im}\delta \rangle + \langle Q\operatorname{Re}\delta | L_+ | Q\operatorname{Re}\delta \rangle + O(\|\delta\|^3_{H^1(B_R)}). \tag{2.4.36}$$

As argued in the beginning of this section, we have $L_- \geq \kappa_- Q$ for some $\kappa_- > 0$. Moreover, Propositions 2.4.1 and 2.4.2 imply that $QL_+Q \geq \kappa_+ Q$ for some $\kappa_+ > 0$. With $\kappa = \min\{\kappa_-, \kappa_+\} > 0$, we thus have

$$\begin{aligned}&\langle \operatorname{Im}\delta | L_- | \operatorname{Im}\delta \rangle + \langle Q\operatorname{Re}\delta | L_+ | Q\operatorname{Re}\delta \rangle \\ &\geq \kappa(\|Q\operatorname{Im}\delta\|_2^2 + \|Q\operatorname{Re}\delta\|_2^2) = \kappa\|Q\delta\|_2^2.\end{aligned} \tag{2.4.37}$$

The assumption $\langle \phi | \phi_R \rangle \geq 0$ implies that

$$\|Q\delta\|_2^2 = \|\delta\|_2^2 - \langle \delta | \phi_R \rangle^2 = \|\delta\|_2^2 \left(1 - \tfrac{1}{4}\|\delta\|_2^2\right) \geq \tfrac{1}{2}\|\delta\|_2^2 \tag{2.4.38}$$

and hence

$$\langle \operatorname{Im}\delta | L_- | \operatorname{Im}\delta \rangle + \langle \operatorname{Re}\delta | QL_+Q | \operatorname{Re}\delta \rangle \geq \frac{\kappa}{2}\|\delta\|_2^2. \tag{2.4.39}$$

Next we want to improve this lower bound by including the full H^1-norm of δ. We can do this by exploiting the explicit form of L_+ and L_-. Indeed, by the boundedness of V_{ϕ_R},

$$L_- \geq -\Delta - C. \tag{2.4.40}$$

Using the smoothness of ϕ_R, it not difficult to see that also

$$QL_+Q \geq -\Delta - C\,. \tag{2.4.41}$$

In particular,

$$\langle \mathrm{Im}\,\delta | L_- | \mathrm{Im}\,\delta\rangle + \langle \mathrm{Re}\,\delta | QL_+Q | \mathrm{Re}\,\delta\rangle \geq \langle \delta | -\Delta - C | \delta\rangle = \|\nabla\delta\|_2^2 - C\|\delta\|_2^2. \tag{2.4.42}$$

By interpolating between (2.4.39) and (2.4.42), we have

$$\langle \mathrm{Im}\,\delta | L_- | \mathrm{Im}\,\delta\rangle + \langle \mathrm{Re}\,\delta | QL_+Q | \mathrm{Re}\,\delta\rangle \geq \left[\frac{\kappa(1-\alpha)}{2} - C\alpha\right] \|\delta\|_2^2 + \alpha\|\nabla\delta\|_2^2 \tag{2.4.43}$$

for any $0 \leq \alpha \leq 1$. By choosing $\alpha = \frac{\kappa}{2+\kappa+2C}$ and substituting in (2.4.36), we obtain

$$\mathcal{E}_R(\phi) \geq \mathcal{E}_R(\phi_R) + \frac{\kappa}{2+\kappa+2C}\|\nabla\delta\|_2^2 + O(\|\delta\|^3_{H^1(B_R)}). \tag{2.4.44}$$

In particular, there exist $c > 0$ and $K > 0$ such that, if $\|\delta\|_{H^1(B_R)} \leq c$, then

$$\mathcal{E}_R(\phi) \geq \mathcal{E}_R(\phi_R) + K\|\nabla(\phi - \phi_R)\|_2^2\,. \tag{2.4.45}$$

In words, we have shown that the desired coercivity estimate holds locally, in the sense that it holds whenever the H^1-norm of δ is sufficiently small.

Step 2: Suppose by contradiction that we cannot find a K_R such that (2.4.32) holds globally on $H_0^1(B_R)$. Then there exist $\phi_n \in H_0^1(B_R)$ with $\|\phi_n\|_2 = 1$ and $\langle \phi_n | \phi_R\rangle \geq 0$ such that

$$\mathcal{E}_R(\phi_n) \leq \mathcal{E}_R(\phi_R) + \frac{1}{n}\|\nabla(\phi_R - \phi_n)\|_2^2 \tag{2.4.46}$$

for any $n \in \mathbb{N}$. At the same time, we recall that by the estimate (2.2.3), we have

$$\mathcal{E}_R(\phi_n) \geq \frac{1}{2}\|\nabla\phi_n\|_2^2 - C. \tag{2.4.47}$$

By combining the two inequalities, we see that ϕ_n is bounded in $H^1(B_R)$. Thus, also $\|\nabla(\phi_R - \phi_n)\|_2^2$ is bounded, which implies that $\mathcal{E}_R(\phi_n) \to \mathcal{E}_R(\phi_R)$, i.e., ϕ_n is a minimizing sequence. Therefore, up to subsequences, ϕ_n is converging in H^1 to a minimizer, i.e., to $e^{i\theta}\phi_R$ for some $\theta \in [0, 2\pi)$, by the compactness properties exploited in the proof of Theorem 2.2.1. (There, only L^2-convergence and weak H^1-convergence are proved, but the strong H^1-convergence follows immediately from the convergence of the individual parts of the functional.) The assumption $\langle \phi_n | \phi_R\rangle \geq 0$ implies that $\|\phi_n - \phi_R\|_2 \leq \|\phi_n - e^{i\theta}\phi_R\|_2 \to 0$, which in turn implies that $\theta = 0$. Thus, we find a contradiction since $\phi_n \to \phi_R$ in H^1 and we can use the local result of step 1. □

Remark 2.4.2. *As explained in Remark 2.3.2, uniqueness of minimizers may fail on general domains, which implies that also* (2.1.4) *fails in this case. We still believe the bound to hold* locally *even if uniqueness fails, however. In other words, the Hessian at the minimizer(s) should be non-degenerate, in which case step* 1 *in the previous proof still applies. Uniqueness of minimizers enters only in step* 2*.*

Remark 2.4.3. *As a final remark, we point out that all the results in this paper can be obtained also if considering, instead of the Pekar functional* (2.1.1) *on a ball, the Pekar functional on the full space, restricted to functions in* $H_0^1(B_R)$ *(extended by* 0 *outside* B_R*), i.e., the functional* (2.1.5). *Indeed, existence of minimizers can be shown exactly as in Section 3, as well as regularity of minimizers. To show that minimizers must be radial, one needs to use the strong form of the Riesz inequality proved in [76] instead of Talenti's inequality. Note that on radial functions the two functionals* $\mathcal{E}_R$ *and* $\tilde{\mathcal{E}}_R$ *differ only by a constant* $1/R$ *(by Newton's Theorem), i.e., if* $\phi \in H_0^1(B_R)$ *is radial and* L^2*-normalized then*

$$\mathcal{E}_R(\phi) = \tilde{\mathcal{E}}_R(\phi) + \frac{1}{R}. \tag{2.4.48}$$

In particular, the two functionals have the same minimizers.

The non-degeneracy results for the Hessian can also be extended to $\tilde{\mathcal{E}}_R$. *If we denote by* $\tilde{H}_R$ *the Hessian of* $\tilde{\mathcal{E}}_R$ *at* ϕ_R*, we have*

$$\tilde{H}_R(\phi) = \langle \operatorname{Im}\phi | L_- | \operatorname{Im}\phi \rangle + \langle Q \operatorname{Re}\phi | \tilde{L}_+ | Q \operatorname{Re}\phi \rangle . \tag{2.4.49}$$

Here, $Q = \mathbb{1} - |\phi_R\rangle\langle\phi_R|$ *as above,* $L_\pm$ *is defined in* (3.3.69), *and* $\tilde{L}_+ = L_+ - 4X_2 = L_- - 4X_1$ *with* $X_{1,2}$ *defined in* (2.4.5). *The decomposition* (2.4.49) *implies that the study of imaginary perturbations can be carried out as above. For real perturbations, we can again decompose the Hessian w.r.t. spherical harmonics, and carry out the analysis in each angular momentum sector separately. For* $l = 0$*, i.e., for radial functions, we can argue exactly as in the proof of Proposition 2.4.1, since the modification of the interaction kernel only affects the term* σ *in* (2.4.11), *leaving the operator* L_+ *unchanged. For* $l \geq 1$*, we have actually already shown above that* $\tilde{L}_+ > 0$ *on* $\mathcal{H}_l$. *Also the proof of Theorem 2.1.2 carries over to the modified interaction kernel without change. We thus conclude that Theorems 2.1.1 and 2.1.2 are also valid, as stated, for the functional* $\tilde{\mathcal{E}}_R$.

2.5 Appendix A: Uniqueness Properties for the Radial Euler–Lagrange Equation

In this section we show two Lemmas dealing with the radial Euler–Lagrange equation (2.3.1). The first one proves uniqueness of solutions with the same boundary conditions at $r = 0$. We recall that $U_\phi = 4\pi \int_0^r s^2(\frac{1}{s} - \frac{1}{r})|\phi(s)|^2 ds$. We take the eigenvalue $\nu_\phi = 1$ for simplicity, which can be achieved by a suitable rescaling.

Lemma 2.5.1. *Let* $v_1, v_2 \in C^2([0,T])$ *be two solutions of*

$$\begin{cases} -v''(r) - \frac{2}{r}v'(r) + 2U_v(r)v(r) = v(r) \qquad r \in [0,T] \\ v(0) = a, \\ v'(0) = 0 \end{cases} \tag{2.5.1}$$

for some $a \in \mathbb{R}$ *and* $T > 0$. *Then* $v_1 = v_2$ *in* $[0,T]$.

Proof. Let $\sigma_i(r) := rv_i(r)$. Then $\sigma_i'(r) = v_i(r) + rv_i'(r)$ and $\sigma_i'' = 2U_{v_i}\sigma_i - \sigma_i$. By applying Taylor's formula with remainder in integral form, and denoting $I_r := [0,r]$, we have

$$\begin{aligned}|\sigma_1(r) - \sigma_2(r)| &\leq \left|\int_0^r \left[\sigma_1(s)(2U_{v_1}(s)-1) - \sigma_2(s)(2U_{v_2}(s)-1)\right](r-s)ds\right| \\ &\leq \int_0^r (r-s)|\sigma_1(s)-\sigma_2(s)|ds + 2\int_0^r (r-s)|\sigma_1(s)U_{v_1}(s) - \sigma_2(s)U_{v_2}(s)|ds \\ &\leq r^2\left[\|\sigma_1-\sigma_2\|_{L^\infty(I_r)}(\tfrac{1}{2} + \|U_{v_1}\|_{L^\infty(I_r)}) + \|\sigma_2\|_{L^\infty(I_r)}\|U_{v_1} - U_{v_2}\|_{L^\infty(I_r)}\right]. \end{aligned} \tag{2.5.2}$$

Boundedness of $v_{1,2}$ implies that $\|U_{v_1}\|_{L^\infty(I_r)} \leq Cr^2$ and $\|\sigma_2\|_{L^\infty(I_r)} \leq Cr$ for suitable constants C. Elementary computations also show that $\|U_{v_1} - U_{v_2}\|_{L^\infty(I_r)} \leq Cr\|\sigma_1 - \sigma_2\|_{L^\infty(I_r)}$. In particular, from (2.5.2) we conclude that

$$\|\sigma_1 - \sigma_2\|_{L^\infty(I_r)} \leq r^2(\tfrac{1}{2} + Cr^2)\|\sigma_1 - \sigma_2\|_{L^\infty(I_r)}. \tag{2.5.3}$$

Thus, $\sigma_1 = \sigma_2$ on I_δ whenever $\delta^2(\frac{1}{2} + C\delta^2) < 1$, and we have local uniqueness of solutions for (3.3.6). The same computations can be carried out *mutatis mutandis* by considering an arbitrary starting point instead of 0. In particular, we can go from local uniqueness to global uniqueness by iteration of the argument: if the two functions only coincide in a *maximal* interval $[0, T^*]$ with $T^* < T$ (note that by continuity they necessarily coincide on a closed interval) then we get a contradiction by applying the argument with starting point T^*. □

The second Lemma is concerned with uniqueness of solutions with the same boundary conditions at $r = R$. In particular, we want to show that if a function vanishes at R, its derivative there must be non-zero, unless the function is identically zero. The proof proceeds along the same lines as above, but is slightly simpler since it suffices to consider here the case where the potential is fixed to be U_{ϕ_R}, with ϕ_R the unique minimizer of the Pekar functional, i.e., we only consider the linearized equation.

Lemma 2.5.2. *The derivative of ϕ_R satisfies*

$$\lim_{r\nearrow R} \phi_R'(r) = c \quad \textit{for some} \quad c < 0. \tag{2.5.4}$$

Proof. Integrating Eq. (2.3.1) using that $\phi_R'(0) = 0$, we have

$$\phi_R'(r) = \frac{1}{r^2}\int_0^r s^2\left(2U_{\phi_R}(s) - \nu_{\phi_R}\right)\phi_R(s)ds. \tag{2.5.5}$$

From this we deduce that the limit in (2.5.4) exists and is finite, and by the monotonicity of ϕ_R it must be non-positive. Suppose that $\phi_R'(R) = 0$ and consider the function $\sigma(r) := r\phi_R(r)$, which then satisfies

$$\begin{cases} \sigma'' = \left(2U_{\phi_R} - \nu_{\phi_R}\right)\sigma & \text{in } [0,R] \\ \sigma(R) = 0, \\ \sigma'(R) = 0. \end{cases} \tag{2.5.6}$$

Using Taylor expansion (w.r.t. R) with remainder in integral form, we have

$$\sigma(r) = \int_r^R (s-r)\sigma''(s)ds = \int_r^R (s-r)\left(2U_{\phi_R}(s) - \nu_{\phi_R}\right)\sigma(s)ds. \tag{2.5.7}$$

Since U_{ϕ_R} is bounded,

$$|\sigma(r)| \leq C(R-r)^2\|\sigma\|_{L^\infty([r,R])}, \tag{2.5.8}$$

which implies that $\sigma \equiv 0$ on $[\bar{r}, R]$ if $\bar{r}$ is such that $C(R-\bar{r})^2 < 1$. This is a contradiction since $\phi_R > 0$ on B_R. □

2.6 Appendix B: Convergence Results

In this section we shall show that the Pekar minimizer ϕ_R and its energy E_R converge to the corresponding full space quantities as $R \to \infty$. Recall that we have shown above that, for each $R > 0$, there exists a unique positive minimizer ϕ_R of $\mathcal{E}_R$ (for L^2-normalized functions in $H^1_0(B_R)$). On the other hand, it was shown in [76] that there exists a unique positive and radial Ψ minimizing the full space Pekar functional

$$\mathcal{E}(\phi) = \int_{\mathbb{R}^3} |\nabla \phi|^2 dx - \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|\phi(x)|^2|\phi(y)|^2}{|x-y|} dxdy =: T(\phi) - W(\phi). \tag{2.6.1}$$

(for L^2-normalized functions in $H^1(\mathbb{R}^3)$). Our goal is to show that $\phi_R \to \Psi$ (in $H^1(\mathbb{R}^3)$-norm, as well as pointwise) as $R \to \infty$, and that $E_R \to E_\infty := \mathcal{E}(\Psi)$. We start with the latter.

Proposition 2.6.1. $\lim_{R\to\infty} E_R = E_\infty$

Proof. We start by approximating Ψ with functions in $H^1_0(B_R)$. Consider the sequence of cutoff functions

$$\eta_R(x) = \begin{cases} 1 & x \in B_{R/2}, \\ \frac{2(R-|x|)}{R} & x \in B_R \setminus B_{R/2}, \\ 0 & x \in B_R^c. \end{cases} \tag{2.6.2}$$

We claim that $\Psi_R := \eta_R \Psi \to \Psi$ in $H^1(\mathbb{R}^3)$ and that $\mathcal{E}_R(\Psi_R) \to \mathcal{E}(\Psi) = E_\infty$. The L^2-convergence of Ψ_R to Ψ is immediate. Moreover,

$$\begin{aligned} \int_{\mathbb{R}^3} |\nabla(\Psi_R - \Psi)|^2 dx &\leq 2\int_{\mathbb{R}^3} |(\eta_R - 1)\nabla\Psi|^2 dx + 2\int_{\mathbb{R}^3} |\Psi \nabla \eta_R|^2 dx \\ &\leq 2\int_{B^c_{R/2}} |\nabla \Psi|^2 dx + \frac{8}{R^2}\int_{B_R \setminus B_{R/2}} |\Psi|^2 dx \to 0 \end{aligned} \tag{2.6.3}$$

as $R \to \infty$, showing the H^1-convergence. To show $\mathcal{E}_R(\Psi_R) \to \mathcal{E}(\Psi)$, we first observe that H^1-convergence implies the convergence of the L^2-norms of the gradients and hence that $T_R(\Psi_R) \to T(\Psi)$. Moreover, from Newton's Theorem and the fact that the functions Ψ_R are radial, we get

$$W_R(\Psi_R) = W(\Psi_R) + \frac{1}{R}\|\Psi_R\|_2^4. \tag{2.6.4}$$

We can then apply dominated convergence to show $W(\Psi_R) \to W(\Psi)$ and conclude that our claim holds.

It is now straightforward to conclude convergence of the minima. Indeed, using that $\|\Psi_R\|_2 < \|\Psi\|_2 = 1$, we have

$$E_\infty \leftarrow \mathcal{E}_R(\Psi_R) = \|\Psi_R\|_2^2 \left(T_R(\Psi_R/\|\Psi_R\|_2) - \|\Psi_R\|_2^2 W_R(\Psi_R/\|\Psi_R\|_2)\right) \geq \|\Psi_R\|_2^2 E_R. \tag{2.6.5}$$

On the other hand,

$$E_R = \mathcal{E}_R(\phi_R) \geq \mathcal{E}(\phi_R) \geq E_\infty. \tag{2.6.6}$$

Therefore, necessarily $E_R \to E_\infty$. □

From the the previous Proposition, we readily deduce that ϕ_R is a minimizing sequence for the full space Pekar functional (2.6.1). We can then proceed as in the proof of [76, Theorem 7] to conclude that ϕ_R is converging to Ψ pointwise, weakly in $H^1(\mathbb{R}^3)$ and strongly in $L^2(\mathbb{R}^3)$.

This latter statement implies also the convergence of the interaction energies, and since we have already proven the convergence of the full energies in Prop. 2.6.1, we conclude that also $\|\nabla\phi_R\|_2 \to \|\nabla\Psi\|_2$. In combination with weak H^1-convergence, this implies strong H^1-convergence, and thus completes the proof of the convergence of the minimizers.

Remark 2.6.1. *It is also possible to frame this discussion in the language of Γ-convergence of the functionals $\mathcal{E}_R$ to $\mathcal{E}$ w.r.t. the $H^1(\mathbb{R}^3)$-norm. The corresponding liminf inequalities are readily shown to hold, and it is possible to recast the cutoff argument to construct recovery sequences for any $\Phi \in H^1(\mathbb{R}^3)$ (which requires a little extra work for non-radial functions). In order to deduce the convergence of minimizers, one still needs to employ the methods in [76] in order to conclude equi-mild-coercivity of the functionals, however.*

CHAPTER 3

The Strongly Coupled Polaron on the Torus: Quantum Corrections to Pekar Asymptotics

This Chapter contains the work

- Dario Feliciangeli and Robert Seiringer. The strongly coupled polaron on the torus: quantum corrections to the Pekar asymptotics. *arXiv preprint arXiv:2101.12566*, 2021.

Abstract

We investigate the Fröhlich polaron model on a three-dimensional torus, and give a proof of the second-order quantum corrections to its ground-state energy in the strong-coupling limit. Compared to previous work in the confined case, the translational symmetry (and its breaking in the Pekar approximation) makes the analysis substantially more challenging.

3.1 Introduction

The underlying physical system we are interested in studying is that of a charged particle (e.g., an electron) interacting with the quantized optical modes of a polar crystal (called phonons). In this situation, the electron excites the phonons by inducing a polarization field, which, in turn, interacts with the electron. In the case of a 'large polaron' (i.e., when the De Broglie wave-length of the electron is much larger than the lattice spacing in the medium), this system is described by the Fröhlich Hamiltonian [47], which represents a simple and well-studied model of non-relativistic quantum field theory (see [1, 44, 52, 89, 109, 111] for properties, results and further references).

A key parameter that appears in the problem is the coupling constant, usually denoted by α. We study the strong coupling regime of the model, i.e., its asymptotic behavior as $\alpha \to \infty$. In this limit, the ground state energy of the Fröhlich Hamiltonian agrees to leading order with the prediction of the Pekar approximation [95], which assumes a classical behavior for the phonon field. This was first proved in [30], using a path integral approach (see also [91] and [92], for recent work on the polaron process [111]). Later, the result was improved in [82], by providing explicit bounds on the leading order correction term.

The object of our study is, precisely, the main correction to the classical (Pekar) approximation of the polaron model, i.e., the leading error term in the aforementioned asymptotics for the ground state energy. Such correction is expected to be of order $O(\alpha^{-2})$ smaller than the leading term, and arises from the quantum fluctuations about the classical limit [3]. This claim was first verified rigorously in [41], where both the electron and the phonon field are confined to a bounded domain (of linear size adjusted to the natural length scale set by the Pekar ansatz) with Dirichlet boundary conditions. Such restriction breaks translation invariance and simplifies the structure of the Pekar problem in comparison with the unconfined case, guaranteeing, at least in the case of the domain being a ball [32], uniqueness up to phase of the Pekar minimizers and non-degeneracy of the Hessian of the Pekar functional. We build upon the strategy developed in [41] to treat the ultraviolet singularity of the model, which in turn relies on multiple application of the Lieb–Yamazaki commutator method [83] and a subsequent use of Nelson's Gross transformation [58, 94].

The key novelty of the present work is to deal with a translation invariant setting. We investigate the quantum correction to the Pekar approximation of the polaron model on a torus, and prove the validity of the predictions in [3] also in this setting. As a first step, we analyze the structure of the set of minimizers of the corresponding Pekar functional, proving uniqueness of minimizers up to symmetries, which was so far known to hold only in the unconfined case [76, 70] and on balls with Dirichlet boundary conditions [32]. The translation invariance leads to a degeneracy of the Hessian of the Pekar functional and corresponding zero modes, substantially complicating the analysis of the quantum fluctuations. In order to 'flatten' the surface of minimizers, we introduce a convenient diffeomorphism inspired by formal computations in [59], which effectively allows us to decouple the zero modes.

3.2 Setting and Main Results

3.2.1 The Model

We consider a 3-dimensional flat torus of side length $L > 0$. We denote by Δ_L the Laplacian on $\mathbb{T}^3_L$ and by $\Delta_L^{-1}(x,y)$ the integral kernel of its 'inverse', which we define by

$$\begin{cases} \Delta_L \left[\Delta_L^{-1}(\,\cdot\,,y)\right] = \delta_y \\ \fint_{\mathbb{T}^3_L} \Delta_L^{-1}(x,y)dx = 0. \end{cases} \tag{3.2.1}$$

An explicit formula for $\Delta_L^{-1}(x,y)$ is given by

$$-\Delta_L^{-1}(x,y) = \sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{|k|^2}\frac{e^{ik\cdot(x-y)}}{L^3}, \tag{3.2.2}$$

which, for any $x \in \mathbb{T}^3_L$, yields an L^2 function of y, its Fourier coefficients being in ℓ^2. Analogously we define Δ_L^{-s} for any $s > 0$. In the following, we identify $\mathbb{T}^3_L$ with the box $[-L/2, L/2]^3 \subset \mathbb{R}^3$, and the Laplacian with the corresponding one on $[-L/2, L/2]^3$ with periodic boundary conditions.

Let

$$v_L(y) := -\Delta_L^{-1/2}(0,y) = \sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{|k|}\frac{e^{-ik\cdot y}}{L^3}, \tag{3.2.3}$$

and $v_L^x(y) := v_L(y-x)$. The Fröhlich Hamiltonian [47] for the polaron is given by

$$\begin{aligned}\mathbb{H}_L &:= -\Delta_L \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{N} - a(v_L^x) - a^\dagger(v_L^x) \\ &= -\Delta_L \otimes \mathbb{1} + \mathbb{1} \otimes \sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3} a_k^\dagger a_k - \frac{1}{L^{3/2}} \sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{|k|}\left(a_k e^{ik\cdot x} + a_k^\dagger e^{-ik\cdot x}\right),\end{aligned} \tag{3.2.4}$$

acting on $L^2(\mathbb{T}_L^3) \otimes \mathcal{F}(L^2(\mathbb{T}_L^3))$, where $\mathcal{F}(L^2(\mathbb{T}_L^3))$ denotes the bosonic Fock space over $L^2(\mathbb{T}_L^3)$. The number operator, denoted by $\mathbb{N}$, accounts for the field energy, whereas $-\Delta_L$ accounts for the electron kinetic energy. The creation and annihilation operators for a plane wave of momentum k are denoted by $a_k^\dagger$ and a_k, respectively, and they are assumed to satisfy the rescaled canonical commutation relations

$$[a_k, a_j^\dagger] = \alpha^{-2}\delta_{k,j}. \tag{3.2.5}$$

In light of (3.2.5), $\mathbb{N}$ has spectrum $\sigma(\mathbb{N}) = \alpha^{-2}\{0,1,2,\dots\}$. We note that the definition (3.2.4) is somewhat formal, since $v_L \notin L^2(\mathbb{T}_L^3)$. It is nevertheless possible to define $\mathbb{H}_L$ via the associated quadratic form, and to find a suitable domain on which it is self-adjoint and bounded from below (see [57], or Remark 3.4.1 in Section 3.4 below).

We shall investigate the ground state energy of $\mathbb{H}_L$, for fixed L and $\alpha \to \infty$.

Remark 3.2.1. *By rescaling all lengths by α, $\mathbb{H}_L$ is unitarily equivalent to the operator $\alpha^{-2}\widetilde{\mathbb{H}}_L$, where $\widetilde{\mathbb{H}}_L$ can be written compactly as*

$$\widetilde{\mathbb{H}}_L = -\Delta_{\alpha^{-1}L} - \sqrt{\alpha}\left[\tilde{a}(v_{\alpha^{-1}L}^x) + \tilde{a}^\dagger(v_{\alpha^{-1}L}^x)\right] + \widetilde{\mathbb{N}}, \tag{3.2.6}$$

with the creation and annihilation operators $\tilde{a}^\dagger$ and $\tilde{a}$ now satisfying the (un-scaled) canonical commutation relations $[\tilde{a}(f), \tilde{a}^\dagger(g)] = \langle f|g\rangle$, and $\widetilde{\mathbb{N}}$ the corresponding number operator. Large α hence corresponds to the strong-coupling limit of a polaron confined to a torus of side length $L\alpha^{-1}$. We find it more convenient to work in the variables defined in (3.2.4)*, however.*

Remark 3.2.2. *The Fröhlich polaron model is typically considered without confinement, i.e., as a model on $L^2(\mathbb{R}^3) \otimes \mathcal{F}(L^2(\mathbb{R}^3))$ with electron-phonon coupling function given by $(-\Delta_{\mathbb{R}^3})^{-1/2}(x,y) = (2/\pi)^{1/2}|x-y|^{-2}$. In the confined case studied in [41], $\mathbb{R}^3$ was replaced by a bounded domain Ω, and thus the electron-phonon coupling function was given by $(-\Delta_\Omega)^{-1/2}(x,y)$, where $-\Delta_\Omega$ denotes the Dirichlet Laplacian on Ω. The latter setting, similarly to ours, has the advantage of guaranteeing compactness for the corresponding inverse Laplacian, which is a key technical ingredient both for [41] and our main results. In addition, for generic domains Ω the Pekar functional has a unique minimizer up to phase (which is proved in [32] for Ω a ball, and enters the analysis in [41] for general Ω as an assumption). Compared with [41], setting the problem on the torus (or on $\mathbb{R}^3$) introduces the extra difficulty of having to deal with translation invariance and a whole continuum of Pekar minimizers. Hence the present work can be seen as a first step in the direction of generalizing the results of [41] to the case of $\mathbb{R}^3$.*

3.2.2 Pekar Functional(s)

For $\psi \in H^1(\mathbb{T}_L^3)$, $\|\psi\|_2 = 1$, and $\varphi \in L^2_{\mathbb{R}}(\mathbb{T}_L^3)$, we introduce the classical energy functional corresponding to (3.2.4) as

$$\mathcal{G}_L(\psi,\varphi) := \langle\psi|h_\varphi|\psi\rangle + \|\varphi\|_2^2, \tag{3.2.7}$$

where h_φ is the Schrödinger operator

$$h_\varphi := -\Delta_L + V_\varphi, \quad V_\varphi := 2\Delta_L^{-1/2}\varphi. \tag{3.2.8}$$

We define the Pekar energy as

$$e_L := \min_{\psi,\varphi} \mathcal{G}_L(\psi,\varphi). \tag{3.2.9}$$

In the case of $\mathbb{R}^3$, it was shown in [30] and [82] that the infimum of the spectrum of the Fröhlich Hamiltonian converges to the minimum of the corresponding classical energy functional as $\alpha \to \infty$. In [41], it was shown that the same holds for the model confined to a bounded domain with Dirichlet boundary conditions and the subleading correction in this asymptotics was computed. Our goal is to extend the results of [41] to the case of $\mathbb{T}^3_L$.

We define the two functionals

$$\mathcal{E}_L(\psi) := \min_{\varphi} \mathcal{G}_L(\psi,\varphi), \quad \mathcal{F}_L(\varphi) := \min_{\psi} \mathcal{G}_L(\psi,\varphi), \tag{3.2.10}$$

and their respective sets of minimizers

$$\mathcal{M}^{\mathcal{E}}_L := \left\{\psi \in H^1(\mathbb{T}^3_L) \,|\, \|\psi\|_2 = 1,\ \mathcal{E}_L(\psi) = e_L\right\}, \tag{3.2.11}$$

$$\mathcal{M}^{\mathcal{F}}_L := \{\varphi \in L^2_{\mathbb{R}}(\mathbb{T}^3_L) \mid \mathcal{F}_L(\varphi) = e_L\}. \tag{3.2.12}$$

Clearly, $\mathcal{E}_L$ is invariant under translations and changes of phase and $\mathcal{F}_L$ is invariant under translations. It is thus useful to introduce the notation

$$\Theta_L(\psi) := \{e^{i\theta}\psi^y(\,\cdot\,) := e^{i\theta}\psi(\,\cdot\, - y) \mid \theta \in [0,2\pi),\, y \in \mathbb{T}^3_L\}, \tag{3.2.13}$$

$$\Omega_L(\varphi) = \{\varphi^y \mid y \in \mathbb{T}^3_L\}, \tag{3.2.14}$$

for $\psi \in H^1(\mathbb{T}^3_L)$ and $\varphi \in L^2_{\mathbb{R}}(\mathbb{T}^3_L)$, respectively.

Our first result, Theorem 3.2.1 (or, more precisely, Corollary 3.2.1) is a fundamental ingredient to prove our main result, Theorem 3.2.2. It concerns the uniqueness of minimizers of $\mathcal{E}_L$ up to symmetries and shows the validity of a quadratic lower bound for $\mathcal{E}_L$ in terms of the H^1-distance from the surface of minimizers. We shall prove these properties for sufficiently large L.

Theorem 3.2.1 (Uniqueness of Minimizers and Coercivity for $\mathcal{E}_L$)**.** *There exist $L_1 > 0$ and a positive constant κ_1 independent of L, such that for $L > L_1$ there exists $0 < \psi_L \in C^\infty(\mathbb{T}^3_L)$ such that*

$$e_L < 0, \quad \mathcal{M}^{\mathcal{E}}_L = \Theta_L(\psi_L). \tag{3.2.15}$$

Moreover $\psi_L^y \neq \psi_L$ for any $0 \neq y \in \mathbb{T}^3_L$ and, for any L^2-normalized $f \in H^1(\mathbb{T}^3_L)$,

$$\mathcal{E}_L(f) - e_L \geq \kappa_1 \operatorname{dist}^2_{H^1}\left(\mathcal{M}^{\mathcal{E}}_L, f\right). \tag{3.2.16}$$

These properties of $\mathcal{E}_L$ translate easily to analogous properties for the functional $\mathcal{F}_L$, as stated in the following corollary.

Corollary 3.2.1 (Uniqueness of Minimizers and Coercivity for $\mathcal{F}_L$)**.** *For $L > L_1$ (where L_1 is the same as in Theorem 3.2.1) there exists $\varphi_L \in C^\infty(\mathbb{T}^3_L)$ such that*

$$\mathcal{M}^{\mathcal{F}}_L = \Omega_L(\varphi_L). \tag{3.2.17}$$

Moreover, with ψ_L as in Theorem 3.2.1, we have

$$\varphi_L = \sigma_{\psi_L} := (-\Delta_L)^{-1/2}|\psi_L|^2, \quad \psi_L = \textit{unique positive g.s. of } h_{\varphi_L}. \tag{3.2.18}$$

Finally, there exists $\kappa' > 0$ independent of L such that, for all $\varphi \in L^2(\mathbb{T}^3_L)$,

$$\mathcal{F}_L(\varphi) - e_L \geq \min_{y \in \mathbb{T}^3_L} \langle \varphi - \varphi^y_L | \mathbb{1} - (\mathbb{1} + \kappa'(-\Delta_L)^{1/2})^{-1} | \varphi - \varphi^y_L \rangle + \left| L^{-3/2} \int_{\mathbb{T}^3_L} \varphi \right|^2, \tag{3.2.19}$$

and this implies

$$\mathcal{F}_L(\varphi) - e_L \geq \tau_L \operatorname{dist}^2_{L^2}(\mathcal{M}^{\mathcal{F}}_L, \varphi) \tag{3.2.20}$$

with $\tau_L := \frac{\kappa'(2\pi/L)^2}{1+\kappa'(2\pi/L)^2}$.

In the case of $\mathbb{R}^3$, similar results are known to hold. In particular, the analogue of (3.2.15) was shown in [76] and the analogue of (3.2.16) follows from the results in [70]. In the case of a bounded domain with Dirichlet boundary conditions, an equivalent formulation of Theorem 3.2.1 was taken as working assumption in [41]. In the case of a ball in $\mathbb{R}^3$ with Dirichlet boundary conditions, the analogue of Theorem 3.2.1 was proved in [32]. In both the case of $\mathbb{R}^3$ and of balls, rotational symmetry plays a key role in the proof of these results. Rotational symmetry is not present in our setting, hence a different approach is required. Our method of proof of Theorem 3.2.1 relies on a comparison of the models on $\mathbb{T}^3_L$ and $\mathbb{R}^3$, for large L. As a consequence, our analysis does not yield quantitative estimates on L_1.

To state our main result, which also holds in the case $L > L_1$, we need to introduce the Hessian of the functional $\mathcal{F}_L$ at its unique (up to translations) minimizer φ_L,

$$\lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2} \left(\mathcal{F}_L(\varphi_L + \varepsilon\phi) - e_L \right) =: \langle \phi | H^{\mathcal{F}_L}_{\varphi_L} | \phi \rangle \quad \forall \phi \in L^2_{\mathbb{R}}(\mathbb{T}^3_L). \tag{3.2.21}$$

An explicit computation gives (see Proposition 3.3.4)

$$H^{\mathcal{F}_L}_{\varphi_L} = \mathbb{1} - 4(-\Delta_L)^{-1/2} \psi_L \frac{Q_{\psi_L}}{h_{\varphi_L} - \inf \operatorname{spec} h_{\varphi_L}} \psi_L (-\Delta_L)^{-1/2}, \tag{3.2.22}$$

where h_{φ_L} is defined in (3.2.8), ψ_L is interpreted as a multiplication operator and $Q_{\psi_L} := \mathbb{1} - |\psi_L\rangle\langle\psi_L|$. Clearly, by minimality of φ_L, $H^{\mathcal{F}_L}_{\varphi_L} \geq 0$, and it is also easy to see that $H^{\mathcal{F}_L}_{\varphi_L} \leq 1$. We shall show that $H^{\mathcal{F}_L}_{\varphi_L}$ has a three-dimensional kernel, given by $\operatorname{span}\{\nabla \varphi_L\}$, corresponding to the invariance under translations of the functional. Note that we could define the Hessian of $\mathcal{F}_L$ at any other minimizer φ^y_L, obtaining a unitarily equivalent operator $H^{\mathcal{F}_L}_{\varphi^y_L}$.

3.2.3 Main Result

Recall the definition (3.2.9) for the Pekar energy e_L as well as (3.2.22) for the Hessian of $\mathcal{F}_L$ at its minimizers, for $L > L_1$. Our main result is as follows.

Theorem 3.2.2. *For any $L > L_1$, as $\alpha \to \infty$*

$$\inf \operatorname{spec} \mathbb{H}_L = e_L - \frac{1}{2\alpha^2} \operatorname{Tr}\left(\mathbb{1} - \sqrt{H^{\mathcal{F}_L}_{\varphi_L}}\right) + o(\alpha^{-2}). \tag{3.2.23}$$

More precisely, the bounds

$$-C_L \alpha^{-1/7} \leq \alpha^2 \inf \operatorname{spec} \mathbb{H}_L - \alpha^2 e_L + \frac{1}{2} \operatorname{Tr}\left(\mathbb{1} - \sqrt{H^{\mathcal{F}_L}_{\varphi_L}}\right) \leq C_L \alpha^{-2/11} \tag{3.2.24}$$

hold for some $C_L > 0$ and α sufficiently large.

The trace appearing in (3.2.23) and (3.2.24) is over $L^2(\mathbb{T}^3_L)$. Note that, since $H^{\mathcal{F}_L}_{\varphi_L} \leq 1$, the coefficient of α^{-2} in (3.2.23) is negative.

In the case of bounded domains with Dirichlet boundary conditions, an analogue of Theorem 3.2.2 was proven in [41] (where logarithmic corrections appear in the bounds that correspond to (3.2.24) as a consequence of technical complications due to the boundary). Showing the validity of an analogous result on $\mathbb{R}^3$ still remains an open problem, however. Indeed, the constant C_L appearing in the lower bound in (3.2.24) diverges as $L \to \infty$. On the other hand, our method of proof used in Section 3.4.1 to show the upper bound in (3.2.24) does apply, with little modifications, to the full space case. In any case, both the upper and lower bound are expected to hold in the case of $\mathbb{R}^3$ as well [3, 59, 41, 109].

Compared to the results obtained in [41], Theorem 3.2.2 deals with the additional complication of the invariance under translations of the problem, which implies that the set of minimizers of $\mathcal{F}_L$ is a three-dimensional manifold. This substantially complicates the proof of the lower bound in (3.2.24), as we shall see in Section 3.4.3. In particular, we need to perform a precise local study around the manifold of minimizers $\Omega_L(\varphi_L)$, which we carry out by introducing a suitable diffeomorphism (inspired by [59]).

Remark 3.2.3 (Small L Regime)**.** *As we show in Lemma 3.3.2, there exists $L_0 > 0$ such that the analogue of Theorem 3.2.1 for $L < L_0$ can be proven with a few-line-argument. In this case, $\mathcal{E}_L$ is simply non-negative and is therefore minimized by the constant function. In particular, $e_L = 0$ and $\varphi_L = 0$.*

Also an analogue of Theorem 3.2.2 can be proven in the regime $L < L_0$, i.e., it is possible to show that for $L < L_0$ there exists $C_L > 0$ such that

$$-C_L \alpha^{-1/7} \leq \alpha^2 \inf \operatorname{spec} \mathbb{H}_L + \frac{1}{2} \sum_{0 \neq k \in \frac{2\pi}{L}\mathbb{Z}^3} \left(1 - \sqrt{1 - \frac{4}{L^3 |k|^4}}\right) \leq C_L \alpha^{-2/11} \tag{3.2.25}$$

for large α. In this case (unlike the regime $L > L_1$ where the set of minimizers $\mathcal{M}^{\mathcal{F}}_L$ is a three-dimensional manifold) $\mathcal{M}^{\mathcal{F}}_L$ only consists of the 0 function, and this allows to follow essentially the same arguments of [41] (with only small modifications, which are also needed in the regime $L > L_1$ and hence are discussed in this paper). We shall therefore not carry out the details of this analysis here.

Whether uniqueness of Pekar minimizers up to symmetries holds for all *$L > 0$ (i.e., also in the regime $L_0 \leq L \leq L_1$) remains an open problem.*

Throughout the paper, we use the word *universal* to describe any constant (which is generally denoted by C) or property that is independent of all the parameters involved and in particular independent of L, for $L \geq L_0$ (for some fixed $L_0 > 0$). Also, we write $a \lesssim b$ whenever $a \leq Cb$ for some universal and positive C. We write C_L whenever a constant depends on L but is otherwise universal with respect to all other parameters. Finally, we write $a \lesssim_L b$ whenever $a \leq C_L b$ for some positive C_L.

3.2.4 Structure of the Paper

In Section 3.3 we study the properties of the Pekar functionals $\mathcal{E}_L$ and $\mathcal{F}_L$, showing the validity of Theorem 3.2.1, Corollary 3.2.1, as well as some other important properties of $\mathcal{F}_L$. In Section 3.4 we prove Theorem 3.2.2.

3.3 Properties of the Pekar Functionals

In this section we derive important properties of the functionals $\mathcal{E}_L$ and $\mathcal{F}_L$, introduced in (3.2.10). In Section 3.3.1, we show the validity of Theorem 3.2.1, relying on the comparison of the models on $\mathbb{T}^3_L$ and $\mathbb{R}^3$ for large L. In Section 3.3.2, we study the functional $\mathcal{F}_L$. In particular, we prove Corollary 3.2.1 and compute the Hessian of $\mathcal{F}_L$ at its minimizers.

Given a function $f \in L^2(\mathbb{T}^3_L)$ and $k \in \frac{2\pi}{L}\mathbb{Z}^3$, we denote by f_k the k-th Fourier coefficient of f. We also denote

$$\hat{f} := f - L^{-3} \int_{\mathbb{T}^3_L} f. \tag{3.3.1}$$

We shall use the following definition of *fractional Sobolev semi-norms* for functions $f \in L^2(\mathbb{T}^3_L)$, $0 \neq s \in \mathbb{R}$:

$$\|f\|^2_{\mathring{H}^s(\mathbb{T}^3_L)} = \langle f|(-\Delta_L)^s|f\rangle = \sum_{0\neq k \in \frac{2\pi}{L}\mathbb{Z}^3} |k|^{2s}|f_k|^2. \tag{3.3.2}$$

3.3.1 Study of $\mathcal{E}_L$

An important role in this analysis is played by the full-space Pekar functional, of which we recall the definition: let $\psi \in H^1(\mathbb{R}^3)$ be an $L^2(\mathbb{R}^3)$-normalized function, then

$$\mathcal{E}(\psi) := \int_{\mathbb{R}^3} |\nabla\psi(x)|^2 dx - \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \rho_\psi(x)(-\Delta_{\mathbb{R}^3})^{-1}(x,y)\rho_\psi(y)dxdy =: T(\psi) - W(\psi), \tag{3.3.3}$$

where $\rho_\psi := |\psi|^2$ and $(-\Delta_{\mathbb{R}^3})^{-1}(x,y) = (4\pi)^{-1}|x-y|^{-1}$. By a simple completion of the square, it is straightforward to see that $\mathcal{E}_L$, defined in (3.2.10), can also be written as

$$\mathcal{E}_L(\psi) = \int_{\mathbb{T}^3_L} |\nabla\psi(x)|^2 dx - \int_{\mathbb{T}^3_L}\int_{\mathbb{T}^3_L} \rho_\psi(x)(-\Delta_L)^{-1}(x,y)\rho_\psi(y)dxdy =: T_L(\psi) - W_L(\psi), \tag{3.3.4}$$

for any L^2-normalized $\psi \in H^1(\mathbb{T}^3_L)$. To compare the two, we need the following Lemma.

Lemma 3.3.1. *There exists a universal constant C such that*

$$\sup_{x,y\in\mathbb{T}^3_L} \left|(-\Delta_L^{-1}(x,y) - (4\pi)^{-1}(\mathrm{dist}_{\mathbb{T}^3_L}(x,y))^{-1}\right| \leq \frac{C}{L}. \tag{3.3.5}$$

Proof. We define $F_L(x) := -\Delta_L^{-1}(x,0)$ and $F(x) = (4\pi)^{-1}|x|^{-1}$ and observe that our statement is equivalent to showing that

$$\|F_L - F\|_{L^\infty([-L/2,L/2]^3)} \leq \frac{C}{L}. \tag{3.3.6}$$

By definition, we have $F_L(x) = \frac{1}{L}F_1(\frac{x}{L})$. Hence, (3.3.6) is equivalent to

$$\|F_1 - F\|_{L^\infty([-1/2,1/2]^3)} \leq C. \tag{3.3.7}$$

Again by definition, $F_1 - F$ is harmonic (distributionally and hence also classically) on $(\mathbb{R}^3 \setminus \{\mathbb{Z}^3\}) \cup \{0\}$ (when F_1, and only F_1, is extended to the whole space by periodicity). Thus we conclude that $F_1 - F$ is in $C^\infty((-1,1)^3)$ and, in particular, bounded on $[-1/2,1/2]^3$. $\square$

The previous discussion, combined with Lemma 3.3.1, suggests that $\mathcal{E}_L$ formally converges to $\mathcal{E}$ as $L \to \infty$. As we shall see, this convergence can be made rigorous, and allows to infer properties of $\mathcal{E}_L$ by comparing it to $\mathcal{E}$, in the large L regime.

We recall here the main known results about the full-space Pekar functional. As shown in [76], $\mathcal{E}$ admits a *unique* positive and radially decreasing minimizer Ψ which is also smooth, the set of minimizers of $\mathcal{E}$ coincides with

$$\Theta(\Psi) := \{e^{i\theta}\Psi^y \mid \theta \in [0,2\pi),\ y \in \mathbb{R}^3\}, \tag{3.3.8}$$

and Ψ satisfies the Euler–Lagrange equation

$$(-\Delta_{\mathbb{R}^3} + V_{\sigma_\Psi} - \mu_\Psi)\Psi = 0, \tag{3.3.9}$$

with

$$V_{\sigma_\Psi} = 2\Delta_{\mathbb{R}^3}^{-1}|\Psi|^2, \quad \mu_\Psi = T(\Psi) - 2W(\Psi). \tag{3.3.10}$$

We denote by e_∞ the infimum of $\mathcal{E}$ over L^2-normalized functions in $H^1(\mathbb{R}^3)$, i.e.,

$$e_\infty := \mathcal{E}(\Psi). \tag{3.3.11}$$

Furthermore, as was shown in [70], the Hessian of $\mathcal{E}$ at its minimizers is strictly positive above the trivial zero modes resulting from the invariance under translations and changes of phase. This implies the validity of the following Theorem, which is not stated explicitly in [70] but can be obtained by standard arguments (see, e.g., [35, Appendix A], [43]) as a consequence of the results therein contained.

Theorem B. *There exists a constant $C > 0$, such that, for any L^2-normalized $f \in H^1(\mathbb{R}^3)$*

$$\mathcal{E}(f) - e_\infty \geq C\,\mathrm{dist}^2_{H^1}(\Theta(\Psi), f). \tag{3.3.12}$$

We now dwell on the study of the properties of $\mathcal{E}_L$. In Section 3.3.1 we derive an important preliminary result, namely Proposition 3.3.1. It formalizes in a mathematical useful way the concept of $\mathcal{E}_L$ converging to $\mathcal{E}$. In Section 3.3.1, we study the Hessian of $\mathcal{E}_L$, showing that it converges (in the sense of Proposition 3.3.2) to the Hessian of $\mathcal{E}$ and therefore is strictly positive above its trivial zero modes for large L. Finally, in Section 3.3.1 we use the results obtained in Sections 3.3.1 and 3.3.1 to show the validity of Theorem 3.2.1.

We remark that our approach differs from the one used on $\mathbb{R}^3$ and on balls to show, for the related $\mathcal{E}$-functional, uniqueness of minimizers and strict positivity of the Hessian (see [76] and [70] for the case of $\mathbb{R}^3$ and [32] for the case of balls). In those cases, rotational symmetry allows to first show uniqueness of minimizers and then helps to derive the positivity of the Hessian at the minimizers. We take somewhat the opposite road: comparing $\mathcal{E}_L$ to $\mathcal{E}$, we first show that minimizers (even if not unique) all localize around the full-space minimizers (see Proposition 3.3.1) and that the Hessian at each minimizer is universally strictly positive (see Proposition 3.3.2) for large L. We then use these two properties to derive, as a final step, uniqueness of minimizers.

Preliminary Results

The next Lemma proves the existence of minimizers for any $L > 0$. Moreover, it shows that there exists $L_0 > 0$ such that, for $L < L_0$, $\mathcal{E}_L$ is strictly positive on any non-constant L^2-normalized function, as already mentioned in Remark 3.2.3.

Lemma 3.3.2. *For any $L > 0$, e_L in (3.2.9) is attained, and there exists a universal constant $C > 0$ such that $e_L > -C$. Moreover, there exists $L_0 > 0$ such that, for $L < L_0$, $\mathcal{E}_L(\psi) > 0$ for any non-constant L^2-normalized ψ.*

Proof. We consider any L^2-normalized $\psi \in H^1(\mathbb{T}^3_L)$ and begin by observing that in terms of the Fourier coefficients we have

$$W_L(\psi) = \sum_{0\neq k \in \frac{2\pi}{L}\mathbb{Z}^3} \frac{|(\rho_\psi)_k|^2}{|k|^2}, \tag{3.3.13}$$

$$(\rho_\psi)_k = \sum_{j \in \frac{2\pi}{L}\mathbb{Z}^3} \frac{\bar{\psi}_j \psi_{j+k}}{L^{3/2}} = (\rho_{\hat{\psi}})_k + \frac{\bar{\psi}_0 \psi_k}{L^{3/2}} + \frac{\bar{\psi}_{-k}\psi_0}{L^{3/2}}. \tag{3.3.14}$$

By Parseval's identity $|\psi_0| \leq 1$ and thus, using the Cauchy–Schwarz inequality, we can deduce that

$$|(\rho_\psi)_k|^2 \leq \begin{cases} L^{-3}, \\ 3|(\rho_{\hat{\psi}})_k|^2 + \frac{3}{L^3}(|\psi_k|^2 + |\psi_{-k}|^2). \end{cases} \tag{3.3.15}$$

Therefore

$$\begin{aligned} W_L(\psi) &\leq 3\left(\sum_{0\neq k \in \frac{2\pi}{L}\mathbb{Z}^3} \frac{|(\rho_{\hat{\psi}})_k|^2}{|k|^2}\right) + \frac{6}{L^3}\left(\sum_{0\neq k \in \frac{2\pi}{L}\mathbb{Z}^3} \frac{|\psi_k|^2}{|k|^2}\right) \\ &\leq 3W_L(\hat{\psi}) + \frac{6}{(2\pi)^2 L}\|\hat{\psi}\|^2_{L^2(\mathbb{T}^3_L)}. \end{aligned} \tag{3.3.16}$$

We can bound both terms on the r.h.s. in two different ways, one which is good for small L and one which is good for all the other L. Indeed, by applying estimate (3.3.15) and using the Poincaré-Sobolev inequality (see [78], chapter 8) on the zero-mean function $\hat{\psi}$, we get

$$\begin{aligned} W_L(\hat{\psi}) &\leq \left(\sum_{0\neq k \in \frac{2\pi}{L}\mathbb{Z}^3} \frac{|(\rho_{\hat{\psi}})_k|^2}{|k|^4}\right)^{1/2} \left(\sum_{0\neq k \in \frac{2\pi}{L}\mathbb{Z}^3} |(\rho_{\hat{\psi}})_k|^2\right)^{1/2} \lesssim L^2 \|(\rho_{\hat{\psi}})_k\|_{l^\infty} \|\hat{\psi}\|^2_{L^4(\mathbb{T}^3_L)} \\ &\lesssim L^{1/2}\|\hat{\psi}\|^2_{L^4(\mathbb{T}^3_L)} \lesssim L\|\hat{\psi}\|^2_{L^6(\mathbb{T}^3_L)} \lesssim LT_L(\hat{\psi}) = LT_L(\psi). \end{aligned} \tag{3.3.17}$$

Moreover,

$$L^{-1}\|\hat{\psi}\|^2_{L^2(\mathbb{T}^3_L)} \lesssim LT_L(\hat{\psi}) = LT_L(\psi). \tag{3.3.18}$$

Therefore, we can conclude that

$$W_L(\psi) \lesssim LT_L(\psi) \quad \Rightarrow \quad \mathcal{E}_L(\psi) \geq (1-CL)T_L(\psi). \tag{3.3.19}$$

Thus, for $L < L_0 := C^{-1}$, either $\psi \equiv \text{const.}$ and $\mathcal{E}_L(\psi) = 0$ or $\mathcal{E}_L(\psi) \gtrsim T_L(\psi) > 0$. Moreover, this also implies

$$\mathcal{E}_L(\psi) \gtrsim T_L(\psi) \geq \frac{(2\pi)^2}{2L_0^2}\|\hat{\psi}\|_2^2 + \frac{1}{2}T_L(\psi) \gtrsim \operatorname{dist}^2_{H^1}\left(\Theta_L\left(\frac{1}{L^{3/2}}\right), \psi\right), \tag{3.3.20}$$

which is the analogue of (3.2.16) from Theorem 3.2.1 in the case $L < L_0$.

We now proceed to study the more interesting regime $L \geq L_0$. By Lemma 3.3.1, splitting $\operatorname{dist}^{-1}_{\mathbb{T}^3_L}(x, \cdot)$ into an $L^{3/2}$ part and the remaining L^∞ part (whose norms can be chosen to be proportional to ε and ε^{-1}, respectively, for any $\varepsilon > 0$), and by applying again the Poincaré-Sobolev inequality, we obtain

$$W_L(\hat{\psi}) \leq \int_{\mathbb{T}^3_L \times \mathbb{T}^3_L} \frac{\rho_{\hat{\psi}}(x)\rho_{\hat{\psi}}(y)}{4\pi \operatorname{dist}_{\mathbb{T}^3_L}(x,y)} dx dy + \frac{C}{L} \lesssim \varepsilon \|\hat{\psi}\|^2_{L^6(\mathbb{T}^3_L)} + \varepsilon^{-1} + 1 \leq \frac{T_L(\psi)}{6} + C. \tag{3.3.21}$$

Moreover, since $L \geq L_0$, trivially $L^{-1}\|\hat{\psi}\|^2_{L^2(\mathbb{T}^3_L)} \lesssim 1$ and we can conclude that for any L^2-normalized $\psi \in H^1(\mathbb{T}^3_L)$

$$W_L(\psi) \leq \frac{T_L(\psi)}{2} + C \quad \Rightarrow \quad \mathcal{E}_L(\psi) \geq \frac{T_L(\psi)}{2} - C. \tag{3.3.22}$$

From this we can infer that $e_L \geq -C$ for any L. To show existence of minimizers, we observe that by (3.3.22) any minimizing sequence ψ_n on $\mathbb{T}^3_L$ must be bounded in $H^1(\mathbb{T}^3_L)$. Therefore, there exists a subsequence (which we still denote by ψ_n for simplicity) that converges weakly in $H^1(\mathbb{T}^3_L)$ and strongly in $L^p(\mathbb{T}^3_L)$, for any $1 \leq p < 6$ to some ψ (by the Banach-Alaoglu Theorem and the Rellich-Kondrachov embedding Theorem). The limit function ψ is L^2-normalized and

$$T_L(\psi) \leq \liminf_{n\to\infty} T_L(\psi_n) \tag{3.3.23}$$

by weak lower semicontinuity of the norm. Using the L^4-convergence of ψ_n to ψ and the fact that $\|\cdot\|_{\mathring{H}^{-1}(\mathbb{T}^3_L)} \lesssim L\|\cdot\|_{L^2(\mathbb{T}^3_L)}$, we finally obtain

$$\begin{aligned} |W_L(\psi_n) - W_L(\psi)| &= \left(\|\rho_\psi\|_{\mathring{H}^{-1}(\mathbb{T}^3_L)} + \|\rho_{\psi_n}\|_{\mathring{H}^{-1}(\mathbb{T}^3_L)}\right)\left|\|\rho_\psi\|_{\mathring{H}^{-1}(\mathbb{T}^3_L)} - \|\rho_{\psi_n}\|_{\mathring{H}^{-1}(\mathbb{T}^3_L)}\right| \\ &\lesssim L\|\rho_{\psi_n} - \rho_\psi\|_{\mathring{H}^{-1}(\mathbb{T}^3_L)} \lesssim L^2\|\rho_{\psi_n} - \rho_\psi\|_{L^2(\mathbb{T}^3_L)} \\ &\leq L^2\|\psi_n - \psi\|_{L^4(\mathbb{T}^3_L)}\left(\|\psi_n\|_{L^4(\mathbb{T}^3_L)} + \|\psi\|_{L^4(\mathbb{T}^3_L)}\right) \to 0. \end{aligned} \tag{3.3.24}$$

This implies that

$$\mathcal{E}_L(\psi) \leq \liminf_{n\to\infty} \mathcal{E}_L(\psi_n) = e_L, \tag{3.3.25}$$

and thus that ψ is a minimizer. Note that, since $\mathcal{E}_L(\psi_n) \to e_L = \mathcal{E}_L(\psi)$ by definition of ψ_n and, as shown, $W_L(\psi_n) \to W_L(\psi)$, it also holds

$$T_L(\psi_n) = \mathcal{E}_L(\psi_n) + W_L(\psi_n) \to \mathcal{E}_L(\psi) + W_L(\psi) = T_L(\psi) \tag{3.3.26}$$

which implies that ψ_n actually converges to ψ strongly in $H^1(\mathbb{T}^3_L)$. □

Once we have shown existence of minimizers, we need to investigate more carefully their properties. Some of them are derived in the following Lemma. Recall that

$$V_\psi = 2\Delta_L^{-1/2}\psi, \quad \sigma_\psi = -\Delta_L^{-1/2}|\psi|^2, \tag{3.3.27}$$

and that, as stated above, we call any property universal which does not depend on $L \geq L_0$.

Lemma 3.3.3. *Let $\psi \in \mathcal{M}_L^{\mathcal{E}}$ (as defined in (3.2.11)). Then ψ satisfies the following Euler-Lagrange equation*

$$(-\Delta_L + V_{\sigma_\psi} - \mu_\psi^L)\psi = 0, \quad \textit{with} \quad \mu_\psi^L = T_L(\psi) - 2W_L(\psi). \tag{3.3.28}$$

Moreover, $\psi \in C^\infty(\mathbb{T}_L^3)$, is universally bounded in $H^2(\mathbb{T}_L^3)$ (and therefore in $L^\infty(\mathbb{T}_L^3)$), has constant phase and never vanishes. Finally, any L^2-normalized sequence $f_n \in H^1(\mathbb{T}_{L_n}^3)$ such that $\mathcal{E}_{L_n}(f_n)$ is universally bounded, is universally bounded in $H^1(\mathbb{T}_{L_n}^3)$.

Proof. The fact that sequences $f_n \in H^1(\mathbb{T}_{L_n}^3)$ of L^2-normalized functions for which $\mathcal{E}_{L_n}$ is universally bounded are universally bounded in $H^1(\mathbb{T}_{L_n}^3)$ follows trivially from estimate (3.3.22). This immediately yields a universal bound on the H^1-norm of minimizers.

The Euler–Lagrange equation (3.3.28) for the problem is derived by standard computations omitted here. By Lemma 3.3.1 and by splitting $(\mathrm{dist}_{\mathbb{T}_L^3}(0,\,\cdot\,))^{-1}$ in its $L^{3/2}$ and L^∞ parts, we have

$$|V_{\sigma_\psi}(x)| \leq 2\int_{\mathbb{T}_L^3} \frac{1}{\mathrm{dist}_{\mathbb{T}_L^3}(x,y)}|\psi(y)|^2 dy + \frac{C}{L} \lesssim \left(\|\psi\|_{L^6(\mathbb{T}_L^3)}^2 + 1\right) \lesssim \left(T_L(\psi) + 1\right). \tag{3.3.29}$$

Therefore, by the universal H^1-boundedness of minimizers, V_{σ_ψ} is universally bounded in $L^\infty(\mathbb{T}_L^3)$, for any $\psi \in \mathcal{M}_L^{\mathcal{E}}$. This immediately allows to conclude universal $\mathring{H}^2$ (and hence H^2) bounds for functions in $\mathcal{M}_L^{\mathcal{E}}$, using the Euler–Lagrange equation (3.3.28), Lemma 3.3.2 and the universal H^1-boundedness of minimizers, which guarantee that

$$0 \geq \mu_\psi^L = 2\mathcal{E}_L(\psi) - T_L(\psi) \geq -C.$$

Since $L \geq L_0$, universal H^2-boundedness also implies universal L^∞-boundedness of minimizers by the Sobolev inequality.

For any $L > 0$, any $\psi \in \mathcal{M}_L^{\mathcal{E}}$ satisfies (3.3.28), is in $H^1(\mathbb{T}_L^3)$ and is such that $V_{\sigma_\psi} \in L^\infty(\mathbb{T}_L^3)$. Therefore ψ also satisfies, for any $\lambda > 0$

$$\psi = (-\Delta_L + \lambda)^{-1}(-V_{\sigma_\psi} + \mu_\psi^L + \lambda)\psi. \tag{3.3.30}$$

In particular, by a bootstrap argument we can conclude that $\psi \in C^\infty(\mathbb{T}_L^3)$. Moreover, picking $\lambda > -\mu_\psi^L + \|V_{\sigma_\psi}\|_{L^\infty(\mathbb{T}_L^3)}$ and using that $(-\Delta_L + \lambda)^{-1}$ is positivity improving, we can also conclude that if $\psi \geq 0$ then $\psi > 0$. By the convexity properties of the kinetic energy (see [78], Theorem 7.8), we have that $T_L(|\psi|) \leq T_L(\psi)$ which implies that if $\psi \in \mathcal{M}_L^{\mathcal{E}}$ then $T_L(\psi) = T_L(|\psi|)$ and also $|\psi| \in \mathcal{M}_L^{\mathcal{E}}$. Hence both ψ and $|\psi|$ are eigenfunctions of the least and *simple* (by positivity of one of the eigenfunctions) eigenvalue $\mu_\psi^L = \mu_{|\psi|}^L$ of the Schrödinger operator $-\Delta_L + V_{\sigma_\psi}$, which allows us to infer that ψ has constant phase and never vanishes. ☐

We now proceed to develop the tools that will allow to show the validity of Theorem 3.2.1. We begin with a simple Lemma.

Lemma 3.3.4. *For $\psi \in H^1(\mathbb{T}^3_L)$,*

$$\|\rho_\psi\|_{\mathring{H}^{1/8}(\mathbb{T}^3_L)} \lesssim \|\psi\|^2_{H^1(\mathbb{T}^3_L)}. \tag{3.3.31}$$

Proof. We have

$$\begin{aligned}
\|\rho_\psi\|^2_{\mathring{H}^{1/8}(\mathbb{T}^3_L)} &= |\langle \nabla\rho_\psi | \nabla(\Delta_L^{-7/8}\rho_\psi)\rangle| \\
&= 2\left|\int_{\mathbb{T}^3_L} |\psi(x)|\nabla(|\psi(x)|)\cdot\nabla_x\left(\sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3}\frac{(\rho_\psi)_k}{|k|^{7/4}}\frac{e^{ik\cdot x}}{L^{3/2}}\right)dx\right| \\
&= \left|\sum_{i=1}^3\int_{\mathbb{T}^3_L}|\psi(x)|\partial_i\left(|\psi(x)|\right)\sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3}\frac{k_i(\rho_\psi)_k}{|k|^{7/4}}\frac{e^{ik\cdot x}}{L^{3/2}}dx\right|.
\end{aligned} \tag{3.3.32}$$

We define

$$g_i(x) := \sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3}\frac{k_i(\rho_\psi)_k}{|k|^{7/4}}\frac{e^{ik\cdot x}}{L^{3/2}}, \tag{3.3.33}$$

and observe that $(g_i)_0 = 0$ and $|(g_i)_k| = \frac{|k_i(\rho_\psi)_k|}{|k|^{7/4}} \leq \frac{|(\rho_\psi)_k|}{|k|^{3/4}}$ for $k \neq 0$. These estimates on the Fourier coefficients of g_i imply that, for $i = 1, 2, 3$,

$$\|g_i\|^2_{\mathring{H}^{3/4}(\mathbb{T}^3_L)} = \sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3}|k|^{3/2}|(g_i)_k|^2 \leq \sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3}|(\rho_\psi)_k|^2 \leq \|\psi\|^4_{L^4(\mathbb{T}^3_L)}. \tag{3.3.34}$$

Moreover, using the fractional Sobolev embeddings (see, for example, [10]) and that g_i has zero mean, we have

$$\|g_i\|_{L^4(\mathbb{T}^3_L)} \lesssim \|g_i\|_{\mathring{H}^{3/4}(\mathbb{T}^3_L)} \leq \|\psi\|^2_{L^4(\mathbb{T}^3_L)}. \tag{3.3.35}$$

Applying these results to (3.3.32) and using Hölder's inequality two times, the Poincaré-Sobolev inequality and the convexity properties of the kinetic energy (see [78], Theorem 7.8), we conclude

$$\begin{aligned}
\|\rho_\psi\|^2_{\mathring{H}^{1/8}(\mathbb{T}^3_L)} &\lesssim \|\psi\|_{L^4(\mathbb{T}^3_L)}\|g_i^{1/8}\|_{L^4(\mathbb{T}^3_L)}\|\nabla(|\psi|)\|_{L^2(\mathbb{T}^3_L)} \leq \|\psi\|^3_{L^4(\mathbb{T}^3_L)}\|\psi\|_{\mathring{H}^1(\mathbb{T}^3_L)} \\
&\leq \|\psi\|^{3/4}_{L^2(\mathbb{T}^3_L)}\|\psi\|^{9/4}_{L^6(\mathbb{T}^3_L)}\|\psi\|_{\mathring{H}^1(\mathbb{T}^3_L)} \lesssim \|\psi\|^4_{H^1(\mathbb{T}^3_L)}.
\end{aligned} \tag{3.3.36}$$

□

Our next goal is to show that $e_L \to e_\infty$ as $L \to \infty$, and that in the large L regime the states that are relevant for the minimization of $\mathcal{E}_L$ are necessarily close to the full space minimizer (or any of its translates). This is a key ingredient for the discussion carried out in the following sections, and is stated in a precise way in the next proposition. The coercivity results obtained in [70] are of fundamental importance here as they guarantee that, at least for the full space model, low energy states are close to minimizers.

We recall that the full-space Pekar functional, defined in (3.3.3), admits a unique positive and radial minimizer Ψ which is also smooth (see (3.3.8)), and we introduce the notation

$$\Psi_L := \Psi\chi_{[-L/2,L/2]^3}. \tag{3.3.37}$$

Note that $\Psi_L \in H^1(\mathbb{T}^3_L)$, by radiality and regularity of Ψ.

Proposition 3.3.1. *We have*

$$\lim_{L\to\infty} e_L = e_\infty. \tag{3.3.38}$$

Moreover, for any $\varepsilon > 0$ there exist L_ε and δ_ε such that for any $L > L_\varepsilon$ and any L^2-normalized $\psi \in H^1(\mathbb{T}^3_L)$ with $\mathcal{E}_L(\psi) - e_L < \delta_\varepsilon$,

$$\operatorname{dist}_{H^1}(\Theta_L(\psi), \Psi_L) \leq \varepsilon, \quad |\mu^L_\psi - \mu_\Psi| \leq \varepsilon, \tag{3.3.39}$$

where $\Theta_L(\psi)$, Ψ_L, μ^L_ψ and μ_Ψ are defined in (3.2.13), (3.3.37), (3.3.28) *and* (3.3.10)*, respectively.*

Proof. We first show that $\limsup_{L\to\infty} e_L \leq e_\infty$ by using Ψ_L as a trial state for $\mathcal{E}_L$. Observe that $\|\Psi_L\|_{L^2(\mathbb{T}^3_L)} \to 1$ and $T_L(\Psi_L) \to T(\Psi)$ as $L \to \infty$. To estimate the difference of the interaction terms we note that $\Psi_L(\Psi - \Psi_L) = 0$ and therefore

$$|W_L(\Psi_L) - W(\Psi)| \leq |W_L(\Psi_L) - W(\Psi_L)| + W(\Psi - \Psi_L) + 2\left\langle (\Psi - \Psi_L)^2 \middle| \Delta^{-1}_{\mathbb{R}^3} \Psi_L^2 \right\rangle. \tag{3.3.40}$$

By dominated convergence, the last two terms converge to zero as $L \to \infty$. On the other hand, by Lemma 3.3.1 and since Ψ is normalized

$$|W_L(\Psi_L) - W(\Psi_L)| \leq \frac{C}{L} + \frac{1}{4\pi} \int_{[-L/2,L/2]^6} \Psi_L(x)^2 \Psi_L(y)^2 \left| \frac{1}{\operatorname{dist}_{\mathbb{T}^3_L}(x,y)} - \frac{1}{|x-y|} \right| dxdy. \tag{3.3.41}$$

Moreover, since $\operatorname{dist}_{\mathbb{T}^3_L}(x,y) = |x-y|$ for $x, y \in [-L/4, L/4]^3$ and using the symmetry and the positivity of the integral kernel and the fact that $\operatorname{dist}_{\mathbb{T}^3_L}(x,y) \leq |x-y|$, we get

$$\begin{aligned} &\int_{[-L/2,L/2]^6} \Psi_L(x)^2 \Psi_L(y)^2 \left| \frac{1}{\operatorname{dist}_{\mathbb{T}^3_L}(x,y)} - \frac{1}{|x-y|} \right| dxdy \\ &\leq 2 \int_{[-L/2,L/2]^3} \Psi_L^2(x) \left(\int_{[-L/2,L/2]^3} \frac{(\Psi_L - \Psi_{L/2})^2(y)}{\operatorname{dist}_{\mathbb{T}^3_L}(x,y)} dy \right) dx. \end{aligned} \tag{3.3.42}$$

Finally, by splitting $\operatorname{dist}^{-1}_{\mathbb{T}^3_L}(x,\cdot)$ in its L^∞ and L^1 parts and using that Ψ is normalized, we can bound the r.h.s. of (3.3.42) by $\left(C_1\|\Psi_L - \Psi_{L/2}\|_2^2 + C_2\|\Psi_L - \Psi_{L/2}\|_\infty^2\right)$, which vanishes as $L \to \infty$, since $\Psi(x) \xrightarrow{|x|\to\infty} 0$. Putting the pieces together, we conclude

$$|W_L(\Psi_L) - W(\Psi_L)| = o_L(1). \tag{3.3.43}$$

This shows our first claim, since

$$e_L \leq \mathcal{E}_L(\Psi_L/\|\Psi_L\|_2) = \frac{1}{\|\Psi_L\|_2^2}\left(T_L(\Psi_L) - \frac{1}{\|\Psi_L\|_2^2} W_L(\Psi_L)\right) \to e_\infty. \tag{3.3.44}$$

We now proceed to show that

$$\liminf_{L\to\infty} e_L \geq e_\infty \tag{3.3.45}$$

and the validity of (3.3.39) using IMS localization. We shall show that for any L^2-normalized sequence $\psi_n \in H^1(\mathbb{T}^3_{L_n})$ with $L_n \to \infty$ such that

$$\mathcal{E}_{L_n}(\psi_n) - e_{L_n} \to 0, \tag{3.3.46}$$

we have

$$\liminf_{n\to\infty} \mathcal{E}_{L_n}(\psi_n) \geq e_\infty, \quad \lim_{n\to\infty} \mathrm{dist}_{H^1}\left(\Theta_{L_n}(\psi_n), \Psi_{L_n}\right) = 0, \quad \lim_{n\to\infty} |\mu^{L_n}_{\psi_n} - \mu_\Psi| = 0, \tag{3.3.47}$$

which implies the claim of the proposition.

Pick $\eta \in C^\infty(\mathbb{R}^3)$ with supp$(\eta) \subset B_1$ and $\|\eta\|_2 = 1$. We denote by η_R the rescaled copy of η supported on B_R with L^2-norm equal to 1. As long as $R \leq L/2$, $\eta_R \in C^\infty(\mathbb{T}^3_L)$ and we then consider the translates η^y_R for any $y \in \mathbb{T}^3_L$. Given $\psi \in H^1(\mathbb{T}^3_L)$, we also define

$$\psi^y_R := \psi\eta^y_R / \|\psi\eta^y_R\|_2. \tag{3.3.48}$$

By standard properties of IMS localization, for any $R \leq L/2$, we have

$$\int_{\mathbb{T}^3_L} T_L(\psi^y_R)\|\psi\eta^y_R\|_2^2 dy = \int_{\mathbb{T}^3_L} T_L(\psi\eta^y_R) dy = T_L(\psi) + \frac{\int |\nabla\eta|^2}{R^2}. \tag{3.3.49}$$

Moreover, by using that $|\psi|^2 = \int_{\mathbb{T}^3_L} |\psi\eta^y_R|^2 dy = \int_{\mathbb{T}^3_L} |\psi^y_R|^2 \|\psi\eta^y_R\|^2 dy$ and completing the square

$$W_L(\psi) = \int_{\mathbb{T}^3_L} \left[W_L(\psi^y_R) - \left\| |\psi^y_R|^2 - |\psi|^2 \right\|^2_{\mathring{H}^{-1}(\mathbb{T}^3_L)} \right] \|\psi\eta^y_R\|_2^2 dy. \tag{3.3.50}$$

Combining (3.3.49) and (3.3.50), we therefore obtain

$$\mathcal{E}_L(\psi) + \frac{C}{R^2} = \int_{\mathbb{T}^3_L} \left[\mathcal{E}_L(\psi^y_R) + \left\| |\psi^y_R|^2 - |\psi|^2 \right\|^2_{\mathring{H}^{-1}(\mathbb{T}^3_L)} \right] \|\psi\eta^y_R\|_2^2 dy. \tag{3.3.51}$$

Since the integrand on the r.h.s. is equal to the l.h.s. on average (indeed $\|\psi\eta^y_R\|_2^2 dy$ is a probability measure) there exists $\bar{y} \in \mathbb{T}^3_L$ such that

$$\mathcal{E}_L(\psi^{\bar{y}}_R) + \left\| |\psi^{\bar{y}}_R|^2 - |\psi|^2 \right\|^2_{\mathring{H}^{-1}(\mathbb{T}^3_L)} \leq \mathcal{E}_L(\psi) + \frac{C}{R^2}. \tag{3.3.52}$$

This fact has several consequences and it is particularly useful if we apply it to our sequence ψ_n with a radius $R = R_n \leq L_n/2$ (we take for simplicity $R = L_n/4$). Indeed, by the above discussion and (3.3.46), we obtain that there exists $\bar{y}_n \in \mathbb{T}^3_{L_n}$ such that the L^2-normalized functions

$$\bar{\psi}_n := \frac{\psi_n \eta^{\bar{y}_n}_{L_n/4}}{\|\psi_n \eta^{\bar{y}_n}_{L_n/4}\|_2} \tag{3.3.53}$$

are competitors both for the minimization of $\mathcal{E}_{L_n}$ and $\mathcal{E}$ (indeed, $\bar{\psi}_n$ can then be thought of as a function in $C^\infty_c(\mathbb{R}^3)$, supported on $B_{L_n/4}$) and satisfy

$$\begin{aligned} \mathcal{E}_{L_n}(\bar{\psi}_n) &\leq \mathcal{E}_{L_n}(\psi_n) + \frac{C}{L_n^2} \leq e_{L_n} + o_{L_n}(1), \\ \|\rho_{\bar{\psi}_n} - \rho_{\psi_n}\|^2_{\mathring{H}^{-1}(\mathbb{T}^3_{L_n})} &\leq \frac{C}{L_n^2}. \end{aligned} \tag{3.3.54}$$

In other words, we can localize any element of our sequence ψ_n to a ball of radius $R = L_n/4$ with an energy expense of order L_n^{-2}, and the localized function is close (in the sense of the second line of (3.3.54)) to ψ_n itself, up to an error again of order L_n^{-2}.

Moreover $T_{L_n}(\bar\psi_n) = T(\bar\psi_n)$ and, using Lemma 3.3.1 and the fact that $\mathrm{dist}_{\mathbb{T}^3_{L_n}}(x,y) = |x-y|$ for all $x, y \in B_{L_n/4}$, we have

$$|W_{L_n}(\bar\psi_n) - W(\bar\psi_n)| \lesssim \frac{1}{L_n}. \tag{3.3.55}$$

Therefore, using (3.3.54)

$$e_\infty \le \mathcal{E}(\bar\psi_n) \le \mathcal{E}_{L_n}(\bar\psi) + \frac{C}{L_n} \le e_{L_n} + o_{L_n}(1), \tag{3.3.56}$$

which shows the first claim in (3.3.47). By Theorem B and (3.3.56), it also follows that

$$\mathrm{dist}_{H^1}\left(\Theta(\Psi), \bar\psi_n\right) \xrightarrow{n\to\infty} 0. \tag{3.3.57}$$

Hence, up to an n-dependent translation and change of phase (which we can both assume to be zero without loss of generality by suitably redefining ψ_n), $\bar\psi_n \xrightarrow{H^1(\mathbb{R}^3)} \Psi$, and the convergence also holds in $L^p(\mathbb{R}^3)$ for any $2 \le p \le 6$. From this and the second line of (3.3.54), we would like to deduce that also ψ_n and Ψ_{L_n} are close. We first note that, by a simple application of Hölder's inequality, it follows that for any $f \in L^2(\mathbb{T}^3_L)$ with zero mean

$$\begin{aligned}\|f\|^2_{L^2(\mathbb{T}^3_L)} &\le \left(\sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3} |k|^{1/4}|f_k|^2\right)^{8/9}\left(\sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3} |k|^{-2}|f_k|^2\right)^{1/9}\\ &= \|f\|^{16/9}_{\mathring{H}^{1/8}(\mathbb{T}^3_L)}\|f\|^{2/9}_{\mathring{H}^{-1}(\mathbb{T}^3_L)}.\end{aligned} \tag{3.3.58}$$

We combine this with (3.3.54) and apply it to the zero mean function $(\rho_{\psi_n} - \rho_{\bar\psi_n})$, obtaining

$$\|\rho_{\bar\psi_n} - \rho_{\psi_n}\|^2_{L^2(\mathbb{T}^3_{L_n})} \lesssim \left(\frac{\|\rho_{\psi_n}\|^2_{\mathring{H}^{1/8}(\mathbb{T}^3_{L_n})} + \|\rho_{\bar\psi_n}\|^2_{\mathring{H}^{1/8}(\mathbb{T}^3_{L_n})}}{L_n^{1/4}}\right)^{8/9}. \tag{3.3.59}$$

Applying Lemma 3.3.4 to ψ_n and $\bar\psi_n$ (which are uniformly bounded in H^1 by Lemma 3.3.3) we conclude that $(\rho_{\psi_n} - \rho_{\bar\psi_n}) \xrightarrow{L^2} 0$.

As a consequence, since ψ_n and $\bar\psi_n$ have the same phase, ψ_n and $\bar\psi_n$ are arbitrarily close in L^4. Indeed,

$$\|\psi_n - \bar\psi_n\|^4_{L^4(\mathbb{T}^3_{L_n})} = \int_{\mathbb{T}^3_{L_n}} \left||\psi_n| - |\bar\psi_n|\right|^4 dx \le \int_{\mathbb{T}^3_{L_n}} (\rho_{\psi_n} - \rho_{\bar\psi_n})^2 dx \xrightarrow{n\to\infty} 0. \tag{3.3.60}$$

By the identification of $\mathbb{T}^3_{L_n}$ with $[-L_n/2, L_n/2]^3$, we finally get $\|\psi_n - \Psi\|_{L^4(\mathbb{R}^3)} \to 0$, if ψ_n is set to be 0 outside $[-L_n/2, L_n/2]^3$. Moreover, ψ_n converges to Ψ in $L^p(\mathbb{R}^3)$ for any $2 \le p < 6$, since $\|\psi_n\|_2 = 1$, $\psi_n \xrightarrow{L^4} \Psi$, $\|\Psi\|_2 = 1$ and $\|\psi_n\|_p$ is uniformly bounded for any $2 \le p \le 6$.

To show the second claim in (3.3.47), we need to show that the convergence actually holds in $H^1(\mathbb{T}^3_{L_n})$, i.e., that $\|\psi_n - \Psi_{L_n}\|_{H^1(\mathbb{T}^3_{L_n})} \to 0$. First, we show convergence in $H^1(B_R)$ for fixed R. Note that

$$\left(\|\psi_n\|_{H^1(\mathbb{T}^3_{L_n})} - \|\Psi\|_{H^1(\mathbb{R}^3)}\right) \to 0, \tag{3.3.61}$$

since

$$|T_{L_n}(\psi_n) - T_{L_n}(\bar{\psi_n})| = |\mathcal{E}_{L_n}(\psi_n) + W_{L_n}(\psi_n) - \mathcal{E}_{L_n}(\bar{\psi_n}) + W_{L_n}(\bar{\psi_n})| \\ \leq |\mathcal{E}_{L_n}(\psi_n) - \mathcal{E}_{L_n}(\bar{\psi_n})| + |W_{L_n}(\psi_n) - W_{L_n}(\bar{\psi_n})| \to 0, \quad (3.3.62)$$

and $T_{L_n}(\bar{\psi_n}) = T(\bar{\psi_n}) \to T(\Psi)$ by H^1 convergence. Moreover, given that ψ_n is uniformly bounded in $H^1(B_R)$ and $\psi_n \to \Psi$ in $L^2(B_R)$, we have $\psi_n \rightharpoonup \Psi$ in $H^1(B_R)$ for any R and this, together with (3.3.61) and weak lower semicontinuity of the norms, implies $\psi_n \to \Psi$ in $H^1(B_R)$ for any R. Finally, for any $\varepsilon > 0$ there exists $R = R(\varepsilon)$ such that $\|\Psi\|_{H^1(B_R^c)} \leq \varepsilon$ and, using strong H^1-convergence on balls and again (3.3.61), we obtain

$$\|\psi_n - \Psi_{L_n}\|_{H^1(\mathbb{T}^3_{L_n})} \leq \|\psi_n - \Psi\|_{H^1(B_R)} + \|\psi_n - \Psi\|_{H^1([-L_n/2,L_n/2]^3\setminus B_R)} \\ \leq \|\psi_n - \Psi\|_{H^1(B_R)} + \|\psi_n\|_{H^1([-L_n/2,L_n/2]^3\setminus B_R)} + \|\Psi\|_{H^1([-L_n/2,L_n/2]^3\setminus B_R)} \\ \leq \|\psi_n - \Psi\|_{H^1(B_R)} + 2\varepsilon + o_n(1) \to 2\varepsilon, \quad (3.3.63)$$

which concludes the proof of the second claim in (3.3.47).

Finally, we show the third claim in (3.3.47). This simply follows from the previous bounds, which guarantee that $\mathcal{E}_{L_n}(\psi_n) \to e_\infty$ and $T_{L_n}(\psi_n) \to T(\Psi)$ and hence

$$\mu^L_{\psi_n} = T_{L_n}(\psi_n) - 2W_{L_n}(\psi_n) = 2\mathcal{E}_{L_n}(\psi_n) - T_{L_n}(\psi_n) \to 2e_\infty - T(\Psi) = \mu_\Psi. \quad (3.3.64)$$

□

We conclude this section with a simple corollary of Proposition 3.3.1.

Corollary 3.3.1. *There exists L^* such that for $L > L^*$ and any $\psi \in \mathcal{M}^{\mathcal{E}}_L$ we have $\psi \neq \psi^y$ for $0 \neq y \in \mathbb{T}^3_L$.*

Proof. It is clearly sufficient to show the claim for $\psi \in \mathcal{M}^{\mathcal{E}}_L$ such that

$$\mathrm{dist}_{H^1}(\Theta_L(\psi), \Psi_L) = \|\psi - \Psi_L\|_{H^1(\mathbb{T}^3_L)} \quad (3.3.65)$$

and for $y \in \mathbb{T}^3_L$ such that $|y| \geq L/4$ (indeed, if the claim fails for some y' such that $|y'| < L/4$ it also fails for some y such that $|y| \geq L/4$). For any such ψ and y, Proposition 3.3.1 and the fact that $\Psi \neq \Psi^y$ for any $y \in \mathbb{R}^3$ guarantee the existence of L^* such that for any $L > L^*$ we have

$$\|\psi - \psi^y\|_{H^1(\mathbb{T}^3_L)} \geq \|\Psi^y_L - \Psi_L\|_{H^1(\mathbb{T}^3_L)} - 2\|\psi - \Psi_L\|_{H^1(\mathbb{T}^3_L)} \geq C > 0 \quad (3.3.66)$$

and this completes the proof. □

Study of the Hessian of $\mathcal{E}_L$

In this section we study the Hessian of $\mathcal{E}_L$ at its minimizers, showing that it is strictly positive, universally, for L big enough. Positivity is of course understood up to the trivial zero modes resulting from the symmetries of the problem (translations and changes of phase). This is obtained by comparing $\mathcal{E}_L$ with $\mathcal{E}$ and exploiting Theorem B.

For any minimizer $\psi \in \mathcal{M}^{\mathcal{E}}_L$, the Hessian of $\mathcal{E}_L$ at ψ is defined by

$$\lim_{\varepsilon\to 0} \frac{1}{\varepsilon^2}\left(\mathcal{E}_L\left(\frac{\psi + \varepsilon f}{\|\psi + \varepsilon f\|_2}\right) - e_L\right) = H^{\mathcal{E}_L}_\psi(f) \quad \forall f \in H^1(\mathbb{T}^3_L). \quad (3.3.67)$$

An explicit computation gives

$$H_\psi^{\mathcal{E}_L}(f) = \langle \mathrm{Im}\, f | L_\psi^L | \mathrm{Im}\, f\rangle + \langle \mathrm{Re}\, f | Q_\psi (L_\psi^L - 4X_\psi^{(l)}) Q_\psi | \mathrm{Re}\, f\rangle \,, \tag{3.3.68}$$

with $Q_\psi = \mathbb{1} - |\psi\rangle\langle\psi|$ and

$$L_\psi^L := -\Delta_L + V_{\sigma_\psi} - \mu_\psi^L \,, \quad X_\psi^{(l)}(x,y) := -\psi(x)\Delta_L^{-1}(x,y)\psi(y). \tag{3.3.69}$$

(We use the same notation for the operator $X_\psi^{(l)}$ and its integral kernel for simplicity.) We recall that $\mu_\psi^L = T_L(\psi) - 2W_L(\psi)$ and that $V_{\sigma_\psi} = 2\Delta_L^{-1}\rho_\psi$ and we note that $L_\psi^L \psi = 0$ is exactly the Euler–Lagrange equation derived in Lemma 3.3.3.

By minimality of ψ, we already know that $\inf \mathrm{spec}\, L_\psi^L = \inf \mathrm{spec}\, Q_\psi(L_\psi^L - 4X_\psi^{(l)})Q_\psi \geq 0$, and it is actually equal to 0 since ψ is in the kernel of both operators. Moreover, $\ker L_\psi^L = \mathrm{span}\{\psi\}$, since it is a Schrödinger operator of least (simple) eigenvalue 0. The situation is more complicated for $Q_\psi(L_\psi^L - 4X_\psi^{(l)})Q_\psi$, whose kernel contains at least ψ and $\partial_i\psi$ (by the translation invariance of the problem). Since both L_ψ^L and $Q_\psi(L_\psi^L - 4X_\psi^{(l)})Q_\psi$ have compact resolvents (they are given by bounded perturbations of $-\Delta_L$), they both have discrete spectrum. Our aim is two-fold: first we need to show that the kernel of $Q_\psi(L_\psi^L - 4X_\psi^{(l)})Q_\psi$ is exactly spanned by ψ and its partial derivatives, secondly we want to show that the spectral gap (above the trivial zero modes) of both operators is bounded by a universal positive constant.

Before stating the main result of this section, we introduce the relevant full-space objects: let again Ψ be the unique positive and radial full-space minimizer of the Pekar functional (3.3.3) and, analogously to (3.3.69), define

$$L_\Psi := -\Delta_{\mathbb{R}^3} + V_{\sigma_\Psi} - \mu_\Psi \,, \quad X_\Psi(x,y) := \Psi(x)(-\Delta_{\mathbb{R}^3})^{-1}(x,y)\Psi(y). \tag{3.3.70}$$

We introduce

$$h'_\infty := \inf_{\substack{f\in H^1_{\mathbb{R}}(\mathbb{R}^3),\|f\|_2=1\\ f\in(\mathrm{span}\{\Psi\})^\perp}} \langle f|L_\Psi|f\rangle \,,$$
$$h''_\infty := \inf_{\substack{f\in H^1_{\mathbb{R}}(\mathbb{R}^3),\|f\|_2=1\\ f\in(\mathrm{span}\{\Psi,\partial_1\Psi,\partial_2\Psi,\partial_3\Psi\})^\perp}} \langle f|L_\Psi - 4X_\Psi|f\rangle \,. \tag{3.3.71}$$

We emphasize that the results contained in [70] imply that $\min\{h'_\infty, h''_\infty\} > 0$. Moreover, it is easy to see, using that $V_{\sigma_\Psi}(x) \lesssim -|x|^{-1}$ for large x, that L_Ψ has infinitely many eigenvalues between 0, its least and simple eigenvalue with eigenfunction given by Ψ, and $-\mu_\Psi$, the bottom of its continuous spectrum. Since furthermore X_Ψ is positive, this implies, in particular, that

$$h''_\infty, h'_\infty < -\mu_\Psi, \tag{3.3.72}$$

which we shall use later.

Proposition 3.3.2. *For any $L>0$, we define*

$$h'_L := \inf_{\psi\in\mathcal{M}_L^{\mathcal{E}}} \inf_{\substack{f\in H^1_{\mathbb{R}}(\mathbb{T}^3_L),\|f\|_2=1\\ f\in(\mathrm{span}\{\psi\})^\perp}} \langle f|L_\psi^L|f\rangle \,, \tag{3.3.73}$$

$$h''_L := \inf_{\psi\in\mathcal{M}_L^{\mathcal{E}}} \inf_{\substack{f\in H^1_{\mathbb{R}}(\mathbb{T}^3_L),\|f\|_2=1\\ f\in(\mathrm{span}\{\psi,\partial_1\psi,\partial_2\psi,\partial_3\psi\})^\perp}} \langle f|L_\psi^L - 4X_\psi^{(l)}|f\rangle \,. \tag{3.3.74}$$

Then

$$\liminf_{L\to\infty} h'_L \geq h'_\infty, \quad \liminf_{L\to\infty} h''_L \geq h''_\infty. \tag{3.3.75}$$

It is not difficult to show that

$$\limsup_{L\to\infty} h'_L \leq h'_\infty, \quad \limsup_{L\to\infty} h''_L \leq h''_\infty, \tag{3.3.76}$$

simply by considering localizations of the full-space optimizers and using Proposition 3.3.1. Hence there is actually equality in (3.3.75).

To prove Proposition 3.3.2 we need the following two Lemmas.

Lemma 3.3.5. *For $\psi \in \mathcal{M}_L^{\mathcal{E}}$, the operator Y_ψ^L with integral kernel $Y_\psi^L(x,y) := \Delta_L^{-1}(x,y)\psi(y)$ is universally bounded from $L^2(\mathbb{T}_L^3)$ to $L^\infty(\mathbb{T}_L^3)$. This in particular implies that the operators $X_\psi^{(l)}$, defined in* (3.3.69)*, are universally bounded from $L^2(\mathbb{T}_L^3)$ to $L^2(\mathbb{T}_L^3)$.*

Proof. Using Lemma 3.3.1 and the normalization of ψ, we have

$$\begin{aligned} |Y_\psi^L(f)(x)| = \left| \int_{\mathbb{T}_L^3} \Delta_L^{-1}(x,y)\psi(y)f(y)dy \right| &\lesssim \|f\|_2 + \int_{\mathbb{T}_L^3} \frac{|\psi(y)f(y)|}{4\pi \operatorname{dist}_{\mathbb{T}_L^3}(x,y)} dy \\ &\lesssim \|f\|_2 + \int_{B_1(x)} \frac{|\psi(y)f(y)|}{\operatorname{dist}_{\mathbb{T}_L^3}(x,y)} dy \leq (1 + C\|\psi\|_\infty)\|f\|_2 \lesssim \|f\|_2. \end{aligned} \tag{3.3.77}$$

To conclude, we also made use of the fact that the minimizers are universally bounded in L^∞ by Lemma 3.3.3. □

Recall the definition of Ψ_L in (3.3.37).

Lemma 3.3.6. *For any $\varepsilon > 0$, there exists R'_ε and L'_ε (with $R'_\varepsilon \leq L'_\varepsilon/2$) such that for any $L > L'_\varepsilon$, any normalized f in $L^2(\mathbb{T}_L^3)$ supported on $B_{R'_\varepsilon}^c := [-L/2, L/2]^3 \setminus B_{R'_\varepsilon}$, and any $\psi \in \mathcal{M}_L^{\mathcal{E}}$ such that*

$$\|\psi - \Psi_L\|_{H^1(\mathbb{T}_L^3)} = \operatorname{dist}_{H^1}(\Theta_L(\psi), \Psi_L) \tag{3.3.78}$$

we have

$$\langle f | L_\psi^L - 4X_\psi^{(l)} | f \rangle \geq -\mu_\Psi - \varepsilon. \tag{3.3.79}$$

Proof. By definition of L_ψ^L and $X_\psi^{(l)}$, we have

$$\begin{aligned} \langle f | L_\psi^L - 4X_\psi^{(l)} | f \rangle &= T_L(f) - \mu_\psi^L + \langle f | V_{\sigma_\psi} | f \rangle - 4 \langle f | X_\psi^{(l)} | f \rangle \\ &\geq -\mu_\psi^L + \langle f | V_{\sigma_\psi} | f \rangle - 4 \langle f | X_\psi^{(l)} | f \rangle . \end{aligned} \tag{3.3.80}$$

By Proposition 3.3.1, taking L'_ε sufficiently large guarantees that

$$|\mu_\psi^L - \mu_\Psi| \leq \varepsilon/2. \tag{3.3.81}$$

Thus we only need to show that $\langle f | V_{\sigma_\psi} | f \rangle$ and $\langle f | X_\psi^{(l)} | f \rangle$ can be made arbitrary small by taking L'_ε and R'_ε sufficiently large. Since f is normalized and supported on $B_{R'_\varepsilon}^c$,

$$| \langle f | V_{\sigma_\psi} | f \rangle | \leq 2 \|V_{\sigma_\psi}\|_{L^\infty\left(B_{R'_\varepsilon}^c\right)}. \tag{3.3.82}$$

Moreover, using Lemma 3.3.1, splitting the integral over $B_t(x)$ and $B_t^c(x)$ (for some $t>0$), and assuming $x \in B^c_{R'_\varepsilon}$, we find

$$|V_{\sigma_\psi}(x)| \leq \frac{C}{L} + C\int_{\mathbb{T}^3_L} \frac{|\psi(y)|^2}{\mathrm{dist}_{\mathbb{T}^3_L}(x,y)}dy \leq \frac{C}{L} + Ct\|\psi\|^2_{L^6\left(B^c_{R'_\varepsilon - t}\right)} + 1/t. \tag{3.3.83}$$

On the other hand, by Lemma 3.3.5,

$$|\langle f|X^{(l)}_\psi|f\rangle| \leq C\|f\|_2 \int_{\mathbb{T}^3_L} \psi(y)|f(y)|dy \leq C\|\chi_{B^c_{R'_\varepsilon}}\psi\|_2. \tag{3.3.84}$$

Therefore, by applying Proposition 3.3.1, we can conclude that there exists L'_ε and R'_ε such that, for any $L > L'_\varepsilon$ and any L^2-normalized f supported on $B^c_{R'_\varepsilon}$, we have

$$\langle f|V_{\sigma_\psi}|f\rangle - 4\langle f|X^{(l)}_\psi|f\rangle \geq -\varepsilon/2, \tag{3.3.85}$$

which concludes our proof. □

Proof of Proposition 3.3.2. We only show the second inequality in (3.3.75), as its proof can easily be modified to also show the first. Moreover, we observe that the second inequality in (3.3.75) is equivalent to the statement that for any sequence $\psi_n \in \mathcal{M}_{L_n}$ with $L_n \to \infty$,

$$\liminf_n \inf_{\substack{f\in H^1(\mathbb{T}^3_{L_n}),\|f\|_2=1 \\ f\in \mathrm{span}\{\psi_n,\partial_1\psi_n,\partial_2\psi_n,\partial_3\psi_n\}^\perp}} \langle f|L^{L_n}_{\psi_n} - 4X^{L_n}_{\psi_n}|f\rangle \geq h''_\infty, \tag{3.3.86}$$

which we shall prove in the following.

We consider $\psi_n \in \mathcal{M}_{L_n}$, $L_n \to \infty$, and define

$$h_n := \inf_{\substack{f\in H^1(\mathbb{T}^3_{L_n}),\|f\|_2=1 \\ f\in \mathrm{span}\{\psi_n,\partial_1\psi_n,\partial_2\psi_n,\partial_3\psi_n\}^\perp}} \langle f|L^{L_n}_{\psi_n} - 4X^{L_n}_{\psi_n}|f\rangle. \tag{3.3.87}$$

By translation invariance of $\mathcal{E}_{L_n}$ and by Proposition 3.3.1, we can also restrict to sequences ψ_n converging to Ψ in $L^2(\mathbb{R}^3)$ and such that $\|\psi_n - \Psi_{L_n}\|_{H^1\left(\mathbb{T}^3_{L_n}\right)} \to 0$, where Ψ_{L_n} is defined in (3.3.37).

Let now g_n be a normalized function in $L^2(\mathbb{T}^3_{L_n})$, orthogonal to ψ_n and its partial derivatives, realizing h_n (which exists by compactness, and can be taken to be a real-valued function). We define the following partition of unity $0 \leq \eta^1_R, \eta^2_R \leq 1$, with $\eta^i_R \in C^\infty(\mathbb{R}^3)$, $\eta^i_R(x) = \eta_i(x/R)$ and

$$\eta_1(x) = \begin{cases} 1 & x \in B_1, \\ 0 & x \in B_2^c \end{cases} \qquad \eta_2 = \sqrt{1-|\eta_1|^2}. \tag{3.3.88}$$

We define $\eta^i_n := \eta^i_{L_n/8}$ and

$$g^i_n := \eta^i_n g_n / \|\eta^i_n g_n\|_2. \tag{3.3.89}$$

Standard properties of IMS localization imply that

$$\begin{aligned} h_n &= \langle g_n|L^{L_n}_{\psi_n} - 4X^{L_n}_{\psi_n}|g_n\rangle \\ &= \sum_{i=1,2} \|\eta^i_n g_n\|^2_2 \left\langle g^i_n \middle| L^{L_n}_{\psi_n} - 4X^{L_n}_{\psi_n} \middle| g^i_n \right\rangle \\ &\quad - \sum_{i=1,2} \Big(\langle g_n||\nabla\eta^i_n|^2|g_n\rangle + 2\langle g_n|[\eta^i_n,[\eta^i_n, X^{L_n}_{\psi_n}]]|g_n\rangle \Big). \end{aligned} \tag{3.3.90}$$

Clearly, the first summand in the second sum is of order $O(L_n^{-2})$, by the scaling of η_n^i. For the second summand, we observe that

$$[\eta_n^i, [\eta_n^i, X_{\psi_n}^{L_n}]](x,y) = \psi_n(x)(-\Delta_{L_n})^{-1}(x,y)\psi_n(y)\left(\eta_n^i(x) - \eta_n^i(y)\right)^2, \tag{3.3.91}$$

and proceed to bound the Hilbert-Schmidt norm of both operators ($i = 1, 2$), which will then bound the last line of (3.3.90). We make use of Lemma 3.3.1 to obtain

$$\begin{aligned}&\int_{\mathbb{T}^3_{L_n}\times\mathbb{T}^3_{L_n}} |\Delta_{L_n}^{-1}(x,y)|^2\psi_n(x)^2\psi_n(y)^2\left(\eta_i^R(x) - \eta_n^i(y)\right)^4 dxdy \\ &\lesssim \frac{1}{L_n^2} + \int_{\mathbb{T}^3_{L_n}\times\mathbb{T}^3_{L_n}} \frac{\left(\eta_n^i(x) - \eta_n^i(y)\right)^4}{d^2_{\mathbb{T}^3_{L_n}}(x,y)}\psi_n(x)^2\psi_n(y)^2 dxdy \leq \frac{1}{L_n^2} + \|\nabla\eta_n^i\|_\infty^2.\end{aligned} \tag{3.3.92}$$

Therefore, also the second summand in the error terms is order L_n^{-2}, which allows us to conclude that

$$\sum_{i=1,2} \|\eta_n^i g_n\|_2^2 \left\langle g_n^i \middle| L_{\psi_n}^{L_n} - 4X_{\psi_n}^{L_n} \middle| g_n^i\right\rangle = h_n + O(L_n^{-2}). \tag{3.3.93}$$

By Lemma 3.3.6 applied to g_n^2 (which is supported on $B^c_{L_n/4}$) and (3.3.72), we find

$$\left\langle g_n^2 \middle| L_{\psi_n}^{L_n} - 4X_{\psi_n}^{L_n} \middle| g_n^2\right\rangle \geq -\mu_\Psi + o_n(1) > h''_\infty + o_n(1). \tag{3.3.94}$$

Since the l.h.s. of (3.3.93) is a convex combination and $(L_{\psi_n}^{L_n} - 4X_{\psi_n}^{L_n})$ is uniformly bounded from below, (3.3.94) allows to restrict to sequences ψ_n such that

$$\|\eta_n^1 g_n\|_2 \geq C \tag{3.3.95}$$

uniformly in n and

$$\left\langle g_n^1 \middle| L_{\psi_n}^{L_n} - 4X_{\psi_n}^{L_n} \middle| g_n^1\right\rangle \leq h_n + o_n(1), \tag{3.3.96}$$

since our claim holds on any sequence for which (3.3.95) and (3.3.96) are not simultaneously satisfied. Using (3.3.95) it is easy to see that g_n^1 is almost orthogonal to ψ_n, in the sense that

$$|\left\langle g_n^1 \middle| \psi_n\right\rangle| = \frac{1}{\|g_n\eta_n^1\|_2}|\left\langle g_n(\eta_n^1 - 1) \middle| \psi_n\right\rangle| \leq \frac{1}{C}\|(1-\eta_n^1)\psi_n\|_2 \leq \frac{1}{C}\|\chi_{B^c_{L_n/8}}\psi_n\|_2 \xrightarrow{n\to\infty} 0. \tag{3.3.97}$$

Here we used the L^2-convergence of ψ_n to Ψ. Clearly, the same computation (together with the H^1-convergence of ψ_n to Ψ) shows that g_n^1 is also almost orthogonal to the partial derivatives of ψ_n.

To conclude, we wish to modify g_n^1 in order to obtain a function $\tilde{g}_n$ which satisfies the constraints (i.e., is a competitor) of the full-space variational problem introduced in (3.3.71). We also wish to have

$$\langle \tilde{g}_n | L_\Psi - 4X_\Psi | \tilde{g}_n\rangle = \left\langle g_n^1 \middle| L_{\psi_n}^{L_n} - 4X_{\psi_n}^{L_n} \middle| g_n^1\right\rangle + o_n(1). \tag{3.3.98}$$

Indeed, (3.3.98) together with (3.3.96) and the fact that $\tilde{g}_n$ is a competitor on $\mathbb{R}^3$, would imply that

$$h_n \geq \left\langle g_n^1 \middle| L_{\psi_n}^{L_n} - 4X_{\psi_n}^{L_n} \middle| g_n^1\right\rangle - o_n(1) = \langle \tilde{g}_n | L_\Psi - 4X_\Psi | \tilde{g}_n\rangle - o_n(1) \geq h''_\infty - o_n(1), \tag{3.3.99}$$

which finally yields the proof of the Proposition also for sequences ψ_n satisfying (3.3.95) and (3.3.96).

We have a natural candidate for $\tilde{g}_n$, which is simply

$$\tilde{g}_n := \frac{(\mathbb{1}-\mathcal{P})g_n^1}{\|(\mathbb{1}-\mathcal{P})g_n^1\|_2}, \tag{3.3.100}$$

with $\mathcal{P}(g_n^1) := \Psi\langle\Psi|g_n^1\rangle + \sum_{i=1,2,3}\frac{\partial_i\Psi}{\|\partial_i\Psi\|_2}\left\langle\frac{\partial_i\Psi}{\|\partial_i\Psi\|_2}\middle|g_n^1\right\rangle$. Clearly $\tilde{g}_n$ is a competitor for the full space minimization and we are only left with the task of proving that $\tilde{g}_n$ satisfies (3.3.98). We observe that, since g_n^1 is almost orthogonal to ψ_n and its partial derivatives, and using Proposition 3.3.1,

$$\begin{aligned}
&|\left\langle\Psi\middle|g_n^1\right\rangle| \leq \|\Psi-\psi_n\|_{L^2(B_{L_n/4})} + |\left\langle\psi_n\middle|g_n^1\right\rangle| = o_n(1),\\
&|\left\langle\partial_i\Psi\middle|g_n^1\right\rangle| \leq \|\Psi-\psi_L\|_{H^1(B_{L_n/4})} + |\left\langle\partial_i\psi_n\middle|g_n^1\right\rangle| = o_n(1).
\end{aligned} \tag{3.3.101}$$

Therefore

$$\|\mathcal{P}(g_n^1)\|_2 \to 0 \quad \text{and} \quad \|(\mathbb{1}-\mathcal{P})g_n^1\|_2 \to 1. \tag{3.3.102}$$

Hence, the normalization factor does not play any role in the proof of (3.3.98). Moreover

$$\begin{aligned}
&\left\langle(\mathbb{1}-\mathcal{P})g_n^1\middle|(L_\Psi-4X_\Psi)\middle|(\mathbb{1}-\mathcal{P})g_n^1\right\rangle\\
&= \left\langle g_n^1\middle|(L_\Psi-4X_\Psi)\middle|g_n^1\right\rangle + \left\langle\mathcal{P}(g_n^1)\middle|(L_\Psi-4X_\Psi)\middle|\mathcal{P}(g_n^1)\right\rangle - 2\left\langle g_n^1\middle|(L_\Psi-4X_\Psi)\middle|\mathcal{P}(g_n^1)\right\rangle,
\end{aligned} \tag{3.3.103}$$

and thus we can conclude that also $\mathcal{P}(g_n^1)$ does not play any role in the proof of (3.3.98), since $(L_\Psi-4X_\Psi)\mathcal{P}$ is a bounded operator ($\mathcal{P}$ has finite dimensional range contained in the domain of $(L_\Psi-4X_\Psi)$), $\mathcal{P}$ is a projection and $\|\mathcal{P}(g_n^1)\|_2\to 0$. With this discussion, we reduced our problem to showing that

$$\left\langle g_n^1\middle|(L_\Psi-4X_\Psi)\middle|g_n^1\right\rangle = \left\langle g_n^1\middle|(L_{\psi_n}^{L_n}-4X_{\psi_n}^{L_n})\middle|g_n^1\right\rangle + o_n(1). \tag{3.3.104}$$

Clearly the kinetic energy terms coincide for every n and $\mu_{\psi_n}^{L_n}\to\mu$, by Proposition 3.3.1. Therefore we only need to prove that

$$|\left\langle g_n^1\middle|V_{\sigma_{\psi_n}}-V_{\sigma_\Psi}\middle|g_n^1\right\rangle|, |\left\langle g_n^1\middle|X_{\psi_n}^{L_n}-X_\Psi\middle|g_n^1\right\rangle| \to 0. \tag{3.3.105}$$

For the first term, using that g_n^1 is supported on $B_{L_n/4}$, we have

$$|\left\langle g_n^1\middle|V_{\sigma_{\psi_n}}-V_{\sigma_\Psi}\middle|g_n^1\right\rangle| \leq \|V_{\sigma_\Psi}-V_{\sigma_{\psi_n}}\|_{L^\infty(B_{L_n/4})}. \tag{3.3.106}$$

If we define $\Psi_R := \chi_{B_R}\Psi$ and $(\psi_n)_R := \chi_{B_R}\psi_n$ we have $V_{\sigma_\Psi} = V_{\sigma_{\Psi_R}} + V_{\sigma_{[\Psi-\Psi_R]}}$ and $V_{\sigma_{\psi_n}} = V_{\sigma_{(\psi_n)_R}} + V_{\sigma_{[\psi_n-(\psi_n)_R]}}$. We consider $R=R(n)=L_n/8$ and observe that

$$|V_{\sigma_{[\Psi-\Psi_R]}}(x)| = 2\int_{\mathbb{R}^3}(-\Delta_{\mathbb{R}^3})^{-1}(x,y)(\Psi-\Psi_R)^2dy \lesssim \|\Psi-\Psi_R\|_6^2 + \|\Psi-\Psi_R\|_2^2 \to 0. \tag{3.3.107}$$

Similar computations, together with Lemma 3.3.1, yield similar estimates for $|V_{\sigma_{[\psi_n-(\psi_n)_R]}}(x)|$. Moreover, since $\operatorname{dist}_{\mathbb{T}^3_{L_n}}(x,y)=|x-y|$ for $x,y\in B_{L_n/8}$, we have, for any $x\in B_{L_n/8}$

$$\begin{aligned}|(V_{\sigma_{\Psi_R}}-V_{\sigma_{(\psi_n)_R}})(x)| &\lesssim \left|\int_{B_{L_n/4}}\frac{1}{|x-y|}(\Psi(y)-\psi_n(y))(\Psi(y)+\psi_n(y))dy\right|+\frac{1}{L_n}\\ &\lesssim \|\Psi+\psi_n\|_\infty\|\Psi-\psi_n\|_6+\|\Psi-\psi_n\|_2\|\Psi+\psi_n\|_2+\frac{1}{L_n}\to 0.\end{aligned} \tag{3.3.108}$$

Here we used again Lemma 3.3.1, the convergence of ψ_n to Ψ and the universal L^∞-boundedness of minimizers. Putting the pieces together we obtain

$$\begin{aligned}\|V_{\sigma_\Psi}-V_{\sigma_{\psi_n}}\|_{L^\infty(B_{L_n/4})} &\le \|V_{\sigma_{[\Psi-\Psi_R]}}\|_\infty+\|V_{\sigma_{[\psi_n-(\psi_n)_R]}}\|_\infty\\ &\quad+\|V_{\sigma_{\Psi_R}}-V_{\sigma_{(\psi_n)_R}}\|_{L^\infty(B_{R(n)})}\to 0,\end{aligned} \tag{3.3.109}$$

as desired. The study is similar for $\langle g_n^1|X^{L_n}_{\psi_n}-X_\Psi|g_n^1\rangle$, hence we shall not write it down explicitly.

We conclude that (3.3.104) holds and, by the discussion above, the proof is complete. □

Proof of Theorem 3.2.1

In this section we first prove universal local bounds for $\mathcal{E}_L$ around minimizers. These are a direct consequence of the results on the Hessian in the previous subsection, the proof follows along the lines of [43], [41, Appendix A] and [35, Appendix A]. Such universal local bounds yield universal local uniqueness of minimizers, i.e., the statement that minimizers that are not equivalent (i.e., not obtained one from the other by translations and changes of phase) must be universally apart (in $H^1(\mathbb{T}^3_L)$). Together with Proposition 3.3.1, this clearly implies uniqueness of minimizers for L big enough, which is the first part of Theorem 3.2.1. A little extra effort will then complete the proof of Theorem 3.2.1.

In this section, for any $\psi\in\mathcal{M}^{\mathcal{E}}_L$ and any $f\in L^2(\mathbb{T}^3_L)$, we write $e^{i\theta}\psi^y=P^{L^2}_{\Theta_L(\psi)}(f)$, respectively $e^{i\theta}\psi^y=P^{H^1}_{\Theta_L(\psi)}(f)$, to mean that $e^{i\theta}\psi^y$ realizes the L^2-distance, respectively the H^1-distance, between f and $\Theta_L(\psi)$. Note that by compactness these always exist, but they might not be unique. The possible lack of uniqueness is not a concern for our analysis, however.

Proposition 3.3.3 (Universal Local Bounds)**.** *There exist universal constants $K_1>0$ and $K_2>0$ and $L^{**}>0$ such that, for any $L>L^{**}$, any $\psi\in\mathcal{M}^{\mathcal{E}}_L$ and any L^2-normalized $f\in H^1(\mathbb{T}^3_L)$ with*

$$\operatorname{dist}_{H^1}(\Theta_L(\psi),f)\le K_1, \tag{3.3.110}$$

we have

$$\mathcal{E}_L(f)-e_L\ge K_2\|P^{L^2}_{\Theta_L(\psi)}(f)-f\|_{H^1(\mathbb{T}^3_L)}\ge K_2\operatorname{dist}^2_{H^1}(\Theta_L(\psi),f)\,. \tag{3.3.111}$$

Proof. We can restrict to *positive* $\psi\in\mathcal{M}^{\mathcal{E}}_L$ and normalized f such that

$$P^{L^2}_{\Theta_L(\psi)}(f)=\psi, \tag{3.3.112}$$

which clearly implies

$$\langle \psi | f \rangle \geq 0, \quad \langle \operatorname{Re} f | \partial_i \psi \rangle = 0. \tag{3.3.113}$$

Under this assumption, we prove that if (3.3.110) holds then

$$\mathcal{E}_L(\phi) - e_L \geq K_2 \|\psi - f\|^2_{H^1(\mathbb{T}^3_L)} \geq K_2 \operatorname{dist}^2_{H^1}(\Theta_L(\psi), f). \tag{3.3.114}$$

The general result follows immediately by invariance of $\mathcal{E}_L$ under translations and changes of phase.

We denote $\delta := f - \psi$ and proceed to expand $\mathcal{E}_L$ around ψ:

$$\mathcal{E}_L(f) = \mathcal{E}_L(\psi + \delta) = e_L + H^{\mathcal{E}_L}_\psi(\delta) + \operatorname{Err}_\psi(\delta). \tag{3.3.115}$$

We recall that $H^{\mathcal{E}_L}_\psi$ is simply the quadratic form associated to the Hessian of $\mathcal{E}_L$ at ψ and it is defined in (3.3.68). We denote $P_\psi := |\psi\rangle\langle\psi|$. The last term, which we see as an error contribution, is explicitly given by

$$\begin{aligned}\operatorname{Err}_\psi(\delta) = &- 8 \langle \operatorname{Re}\delta |\, X^{(l)}_\psi \,| P_\psi \operatorname{Re}\delta\rangle + 4 \langle P_\psi \operatorname{Re}\delta | X^{(l)}_\psi | P_\psi \operatorname{Re}\delta\rangle \\ &- 4 \left\langle |\delta|^2 \right| - \Delta_L^{-1} \left| \psi \operatorname{Re}\delta \right\rangle + W_L(\delta).\end{aligned} \tag{3.3.116}$$

Our first goal is to estimate $|\operatorname{Err}_\psi(\delta)|$. By (3.3.113) and the normalization of both ψ and f, we find

$$\|\delta\|_2^2 = 2 - 2\langle \psi | f \rangle. \tag{3.3.117}$$

Therefore, also using the positivity of ψ, we have

$$P_\psi \operatorname{Re}\delta = \psi(\langle \psi | f\rangle - 1) = -\frac{1}{2}\psi \|\delta\|_2^2. \tag{3.3.118}$$

We now apply Lemma 3.3.5 to obtain

$$\begin{aligned} &|\langle \operatorname{Re}\delta |\, X^{(l)}_\psi \,| P_\psi \operatorname{Re}\delta\rangle| \lesssim \|\operatorname{Re}\delta\|_2 \|P_\psi \operatorname{Re}\delta\|_2 \lesssim \|\delta\|_2^3, \\ &|\langle P_\psi \operatorname{Re}\delta | X^{(l)}_\psi | P_\psi \operatorname{Re}\delta\rangle| \lesssim \|P_\psi \operatorname{Re}\delta\|_2^2 \lesssim \|\delta\|_2^4, \\ &|\left\langle |\delta|^2 \right| - \Delta_L^{-1} \left| \psi \operatorname{Re}\delta\right\rangle| \lesssim \|\delta\|_2^2 \|\operatorname{Re}\delta\|_2 \leq \|\delta\|_2^3. \end{aligned} \tag{3.3.119}$$

Finally, by (3.3.22),

$$W_L(\delta) = \|\delta\|_2^4 W_L\left(\frac{\delta}{\|\delta\|_2}\right) \leq \|\delta\|_2^4 \left(\frac{1}{2} T_L\left(\frac{\delta}{\|\delta\|_2}\right) + C\right) \lesssim \|\delta\|_2^2 \|\delta\|^2_{H^1(\mathbb{T}^3_L)}. \tag{3.3.120}$$

Recalling (3.3.110), we can estimate

$$\|\delta\|_2 = \operatorname{dist}_{L^2}(f, \Theta_L(\psi)) \leq \operatorname{dist}_{H^1}(f, \Theta_L(\psi)) \leq K_1, \tag{3.3.121}$$

and this implies, combined with (3.3.119) and (3.3.120), that

$$|\operatorname{Err}_\psi(\delta)| \lesssim \|\delta\|^3_{H^1(\mathbb{T}^3_L)}. \tag{3.3.122}$$

We now want to bound $H_\psi^{\mathcal{E}_L}(\delta)$. We fix $0<\tau<\min\{h'_\infty,h''_\infty\}$, where h'_∞ and h''_∞ are defined in (3.3.71). Proposition 3.3.2 implies that there exists L^{**} such that for $L>L^{**}$ and $\psi\in\mathcal{M}_L^{\mathcal{E}}$, we have

$$L_\psi^L\geq\tau Q_\psi,\quad Q_\psi(L_\psi^L-4X_\psi^{(l)})Q_\psi\geq\tau Q'_\psi, \tag{3.3.123}$$

where we define $Q_\psi=\mathbb{1}-P_\psi$ and $Q'_\psi:=\mathbb{1}-P_\psi-\sum_{i=1,2,3}P_{\partial_i\psi/\|\partial_i\psi\|_2}$. We note that, by (3.3.113) and since ψ is orthogonal in L^2 to its partial derivatives, we have

$$Q_\psi(\operatorname{Re}f-\psi)=Q'_\psi(\operatorname{Re}f-\psi). \tag{3.3.124}$$

Therefore, recalling the definition of $H_\psi^{\mathcal{E}_L}$ given in (3.3.68),

$$\begin{aligned}H_\psi^{\mathcal{E}_L}(\delta)=&\ \langle\operatorname{Im}f|L_\psi^L|\operatorname{Im}f\rangle+\langle\operatorname{Re}f-\psi|Q_\psi(L_\psi^L-4X_\psi^{(l)})Q_\psi|\operatorname{Re}f-\psi\rangle\\ &\geq\tau(\|Q_\psi\operatorname{Im}f\|_2^2+\|Q'_\psi(\operatorname{Re}f-\psi)\|_2^2)=\tau\|Q_\psi\delta\|^2_{L^2(\mathbb{T}_L^3)}.\end{aligned} \tag{3.3.125}$$

Moreover, applying (3.3.117),

$$\|Q_\psi\delta\|^2_{L^2(\mathbb{T}_L^3)}=\|\delta\|_2^2-\langle\psi|\delta\rangle^2=\|\delta\|_2^2\left(1-\frac{1}{4}\|\delta\|_2^2\right)\geq\frac{1}{2}\|\delta\|_2^2, \tag{3.3.126}$$

and we can thus conclude that

$$H_\psi^{\mathcal{E}_L}(\delta)\geq\frac{\tau}{2}\|\delta\|_2^2. \tag{3.3.127}$$

On the other hand, by the universal boundedness of V_{σ_ψ} in $L^\infty(\mathbb{T}_L^3)$ and the universal boundedness of μ_ψ^L (see Proposition 3.3.1), we have, for some universal $C_1>0$,

$$L_\psi^L\geq-\Delta_L-C_1. \tag{3.3.128}$$

Similarly, also using Lemma 3.3.5, for some universal $C_2>0$,

$$Q(L_\psi^L-4X_\psi^{(l)})Q\geq-\Delta_L-C_2. \tag{3.3.129}$$

If we then define $C:=(\max\{C_1,C_2\}+1)$, we can conclude the validity of the universal bound

$$H_\psi^{\mathcal{E}_L}(\delta)\geq\|\delta\|^2_{H^1(\mathbb{T}_L^3)}-C\|\delta\|^2_{L^2(\mathbb{T}_L^3)}. \tag{3.3.130}$$

By interpolating between (3.3.127) and (3.3.130), we obtain

$$H_\psi^{\mathcal{E}_L}(\delta)\geq\frac{\tau}{\tau+2C}\|\delta\|^2_{H^1(\mathbb{T}_L^3)}. \tag{3.3.131}$$

Using (3.3.122) and (3.3.131) in (3.3.115), we can conclude that there exists a universal constant C such that for any $L>L^{**}$, any $0<\psi\in\mathcal{M}_L^{\mathcal{E}}$ and any normalized f satisfying (3.3.112),

$$\mathcal{E}_L(f)-e_L\geq\frac{1}{C}\|\delta\|^2_{H^1(\mathbb{T}_L^3)}-C\|\delta\|^3_{H^1(\mathbb{T}_L^3)}. \tag{3.3.132}$$

In particular, for K_2 sufficiently small, we can find a universal constant c such that (3.3.114) holds, *as long as*

$$\|\delta\|_{H^1(\mathbb{T}_L^3)}=\|P^{L^2}_{\Theta_L(\psi)}(f)-f\|_{H^1(\mathbb{T}_L^3)}\leq c. \tag{3.3.133}$$

To conclude the proof, it only remains to show that there exists a universal K_1 such that (3.3.133) holds as long as (3.3.110) holds. This can be achieved as follows. We have, using that both ψ and $P^{H^1}_{\Theta_L(\psi)}(f)$ are in $\mathcal{M}^{\mathcal{E}}_L$ and thus are universally bounded in $H^2(\mathbb{T}^3_L)$ (by Lemma 3.3.3) and recalling that $\psi = P^{L^2}_{\Theta_L(\psi)}(f)$,

$$\begin{aligned}
\|\psi - P^{H^1}_{\Theta_L(\psi)}(f)\|_{\mathring{H}^1(\mathbb{T}^3_L)} &\leq \|\psi - P^{H^1}_{\Theta_L(\psi)}(f)\|^{1/2}_{L^2(\mathbb{T}^3_L)} \| - \Delta_L(\psi - P^{H^1}_{\Theta_L(\psi)}(f))\|^{1/2}_{L^2(\mathbb{T}^3_L)} \\
&\lesssim \|\psi - P^{H^1}_{\Theta_L(\psi)}(f)\|^{1/2}_{L^2(\mathbb{T}^3_L)} \\
&\leq \left(\mathrm{dist}_{L^2}\left(\Theta_L(\psi), f\right) + \|f - P^{H^1}_{\Theta_L(\psi)}(f)\|_{L^2(\mathbb{T}^3_L)}\right)^{1/2} \\
&\lesssim \mathrm{dist}^{1/2}_{H^1}\left(\Theta_L(\psi), f\right). \qquad (3.3.134)
\end{aligned}$$

Therefore, for some universal C

$$\|f - \psi\|_{H^1(\mathbb{T}^3_L)} \leq \mathrm{dist}_{H^1}\left(\Theta_L(\psi), f\right) + C\,\mathrm{dist}^{1/2}_{H^1}\left(\Theta_L(\psi), f\right), \qquad (3.3.135)$$

and it suffices to take $K_1 \leq \left[(-C + \sqrt{C^2 + 4c})/2\right]^2$ to conclude our discussion. □

We are ready to prove Theorem 3.2.1.

Proof of Theorem 3.2.1. Fix K_1 as in Proposition 3.3.3. Using Proposition 3.3.1, we know that there exists $L_{K_1/2}$ such that, for any $L > L_{K_1/2}$ and any $\psi \in \mathcal{M}^{\mathcal{E}}_L$, we have

$$\mathrm{dist}_{H^1}\left(\Theta_L(\psi), \Psi_L\right) \leq K_1/2. \qquad (3.3.136)$$

We claim that (3.2.15) holds with $L_1 := \max\{L_{K_1/2}, L^*, L^{**}\}$, where L^* is the same as in Corollary 3.3.1 and L^{**} is the same as in Proposition 3.3.3.

Let $L > L_1$ and $\psi \in \mathcal{M}^{\mathcal{E}}_L$. Since $L > L_1 \geq L^*$, we have $\psi^y \neq \psi$ for any $0 \neq y \in \mathbb{T}^3_L$. Moreover, since $L > L_1 \geq L_{K_1/2}$ and using the triangle inequality, for any other $\psi_1 \in \mathcal{M}^{\mathcal{E}}_L$ we have

$$\mathrm{dist}_{H^1}\left(\Theta_L(\psi), \psi_1\right) \leq K_1. \qquad (3.3.137)$$

Since $L > L_1 \geq L^{**}$, we can apply Proposition 3.3.3, finding

$$K_2\,\mathrm{dist}^2_{H^1}(\Theta_L(\psi), \psi_1) \leq \mathcal{E}_L(\psi_1) - e_L = 0, \qquad (3.3.138)$$

i.e., $\psi_1 \in \Theta_L(\psi)$, and (3.2.15) holds for $L > L_1$.

For $\psi \in \mathcal{M}^{\mathcal{E}}_L = \Theta_L(\psi)$, and $L > L_1$, we now show the quadratic lower bound (3.2.16), independently of L. Lemma 3.3.3, which guarantees universal H^1-boundedness of minimizers, and estimate (3.3.22) ensure, by straightforward computations, that there exists $0 < \kappa^* < 1/2$ such that, if $f \in L^2(\mathbb{T}^3_L)$ is normalized and satisfies

$$\mathcal{E}_L(f) - e_L < \kappa^*\,\mathrm{dist}^2_{H^1}\left(\Theta_L(\psi), f\right), \qquad (3.3.139)$$

then f is universally bounded in $H^1(\mathbb{T}^3_L)$ and must satisfy

$$\mathcal{E}_L(f) - e_L < \delta_{K_1}, \qquad (3.3.140)$$

where δ_{K_1} is the δ_ε from Proposition 3.3.1 with $\varepsilon = K_1$. On the other hand, Proposition 3.3.1 and Proposition 3.3.3 combined with the fact that we have taken $L_1 \geq L_{K_1/2}$ (and that trivially $L_{K_1/2} \geq L_{K_1}$), guarantee that any L^2-normalized f satisfying (3.3.140) must satisfy

$$\mathcal{E}_L(f) - e_L \geq K_2 \operatorname{dist}^2_{H^1}(\Theta_L(\psi), f). \tag{3.3.141}$$

Therefore the bound (3.2.16) from Theorem 3.2.1 holds with the universal constant $\kappa_1 := \min\{\kappa^*, K_2\}$ and our proof is complete. □

This concludes our study of $\mathcal{E}_L$. We now move on to the study of the functional $\mathcal{F}_L$.

3.3.2 Study of $\mathcal{F}_L$

This section is structured as follows. In Section 3.3.2 we prove Corollary 3.2.1. In Section 3.3.2, we compute the Hessian of $\mathcal{F}_L$ at its minimizers, showing the validity of (3.2.22). This allows to obtain a more precise lower bound for $\mathcal{F}_L$ (compared to the bounds (3.2.19) and (3.2.20) from Corollary 3.2.1), which holds locally around the 3-dimensional surface of minimizers $\mathcal{M}^{\mathcal{F}}_L = \Omega_L(\varphi_L)$. Finally, in Section 3.3.2, we investigate closer the surface of minimizers $\Omega_L(\varphi_L)$ and the behavior of the functional $\mathcal{F}_L$ close to it. In particular, we show that the Hessian of $\mathcal{F}_L$ at its minimizers is strictly positive above its trivial zero modes and derive some key technical tools, which we exploit in Section 3.4.

Proof of Corollary 3.2.1

In this section, we show the validity of Corollary 3.2.1. We need the following Lemma. Recall that in our discussion constants are universal if they are independent of L for $L \geq L_0 > 0$.

Lemma 3.3.7. *For $\psi, \phi \in H^1(\mathbb{T}^3_L)$, $\|\psi\|_2 = \|\phi\|_2 = 1$,*

$$\langle \rho_\psi - \rho_\phi | (-\Delta_L)^{-1/2} | \rho_\psi - \rho_\phi \rangle \lesssim \| |\psi| - |\phi| \|^2_{H^1(\mathbb{T}^3_L)}. \tag{3.3.142}$$

Proof. We define $f(x) := |\psi(x)| + |\phi(x)|$ and $g(x) := |\psi(x)| - |\phi(x)|$. By the Hardy-Littlewood-Sobolev and the Sobolev inequality (see for example [10] for a comprehensive overview of such results on the torus), and using the normalization of ϕ and ψ we have

$$\begin{aligned}\langle \rho_\psi - \rho_\phi | (-\Delta_L)^{-1/2} | \rho_\psi - \rho_\phi \rangle &= \|(-\Delta_L)^{-1/4}(fg)\|_2^2 \leq C\|fg\|^2_{3/2} \leq C\|f\|_2^2\|g\|_6^2 \\ &\leq C'\|g\|^2_{H^1(\mathbb{T}^3_L)} = C'\| |\psi| - |\phi| \|^2_{H^1(\mathbb{T}^3_L)},\end{aligned} \tag{3.3.143}$$

which proves the Lemma. □

Proof of Corollary 3.2.1. With ψ_L as in Theorem 3.2.1, let $\varphi_L := \sigma_{\psi_L} \in C^\infty(\mathbb{T}^3_L)$. Observing that

$$\mathcal{G}_L(\psi, \varphi) = \mathcal{E}_L(\psi) + \|\sigma_\psi - \varphi\|_2^2, \tag{3.3.144}$$

and using Theorem 3.2.1 we can immediately conclude that in the regime $L > L_1$

$$\mathcal{M}^{\mathcal{F}}_L = \Omega_L(\varphi_L). \tag{3.3.145}$$

It is also immediate, recalling the definition of $\mathcal{G}_L$ in (3.2.7) and that $\psi_L > 0$, to conclude that ψ_L must be the unique positive ground state of h_{φ_L}.

To prove (3.2.19), we first of all observe that if $\varphi \in L^2(\mathbb{T}_L^3)$, we have

$$\mathcal{F}_L(\varphi) = |(\varphi)_0|^2 + \mathcal{F}_L(\hat{\varphi}). \tag{3.3.146}$$

Therefore, it is sufficient to restrict to φ with zero-average and show that in this case

$$\mathcal{F}_L(\varphi) - e_L \geq \min_{y \in \mathbb{T}_L^3} \langle \varphi - \varphi_L^y | \mathbb{1} - (\mathbb{1} + \kappa'(-\Delta_L)^{1/2})^{-1} | \varphi - \varphi_L^y \rangle . \tag{3.3.147}$$

Using Theorem 3.2.1, we obtain

$$\begin{aligned} \mathcal{G}_L(\psi, \varphi) - e_L &= \mathcal{E}_L(\psi) - e_L + \|\varphi - \sigma_\psi\|_2^2 \geq \mathcal{E}_L(|\psi|) - e_L + \|\varphi - \sigma_\psi\|_2^2 \\ &\geq \kappa_1 \operatorname{dist}_{H^1}^2(|\psi|, \Theta(\psi_L)) + \|\varphi - \sigma_\psi\|_2^2 \\ &= \kappa_1 \||\psi| - \psi_L^y\|_{H^1(\mathbb{T}_L^3)}^2 + \|\varphi - \sigma_\psi\|_2^2, \end{aligned} \tag{3.3.148}$$

for some $y \in \mathbb{T}_L^3$. We now apply Lemma 3.3.7 and recall that $\varphi_L^y = \sigma_{\psi_L^y}$, obtaining with a simple completion of the square

$$\begin{aligned} \mathcal{G}_L(\psi, \varphi) - e_L &\geq \kappa' \left\langle \rho_\psi - \rho_{\psi_L^y} \middle| (-\Delta_L)^{-1/2} \middle| \rho_\psi - \rho_{\psi_L^y} \right\rangle + \|\varphi - \sigma_\psi\|_2^2 \\ &= \|F^{1/2}(\sigma_\psi - \varphi_L^y) + F^{-1/2}(\varphi_L^y - \varphi)\|_2^2 \\ &\quad + \langle \varphi - \varphi_L^y | \mathbb{1} - F^{-1} | \varphi - \varphi_L^y \rangle , \end{aligned} \tag{3.3.149}$$

where $F = \mathbb{1} + \kappa'(-\Delta_L)^{1/2}$. Dropping the first term and minimizing over ψ yields our claim. Finally, (3.2.20) immediately follows from (3.2.19) and the spectral gap of the Laplacian, using the fact that φ_L and all its translates have zero average since $\varphi_L = \sigma_{\psi_L}$. □

The Hessian of $\mathcal{F}_L$

For any $\varphi \in L^2_{\mathbb{R}}(\mathbb{T}_L^3)$, we introduce the notation

$$e(\varphi) := \inf \operatorname{spec} h_\varphi, \tag{3.3.150}$$

and observe that $\mathcal{F}_L$, defined in (3.2.10), can equivalently be written as

$$\mathcal{F}_L(\varphi) = \|\varphi\|_2^2 + e(\varphi), \quad \varphi \in L^2_{\mathbb{R}}(\mathbb{T}_L^3). \tag{3.3.151}$$

We compute the Hessian of $\mathcal{F}_L$ at its minimizers using standard arguments in perturbation theory, showing the validity of expression (3.2.22). We need the following two Lemmas.

Lemma 3.3.8. *For $L \geq L_0 > 0$, any $\varphi \in L^2(\mathbb{T}_L^3)$ and any $T > 0$*

$$\|(-\Delta_L + T)^{-1}\varphi\| = \|\varphi(-\Delta_L + T)^{-1}\| \leq C_T \|\varphi\|_{L^2(\mathbb{T}_L^3) + L^\infty(\mathbb{T}_L^3)} \tag{3.3.152}$$

for some constant $C_T > 0$ with $\lim_{T\to\infty} C_T = 0$. Here φ is understood as a multiplication operator, $\|\cdot\|$ denotes the operator norm on $L^2(\mathbb{T}_L^3)$, and

$$\|\varphi\|_{L^2(\mathbb{T}_L^3)+L^\infty(\mathbb{T}_L^3)} := \inf_{\substack{\varphi_1 + \varphi_2 = \varphi \\ \varphi_1 \in L^2(\mathbb{T}_L^3),\, \varphi_2 \in L^\infty(\mathbb{T}_L^3)}} \left(\|\varphi_1\|_{L^2(\mathbb{T}_L^3)} + \|\varphi_2\|_{L^\infty(\mathbb{T}_L^3)} \right). \tag{3.3.153}$$

Note that

$$\|\varphi\|_{L^2(\mathbb{T}_L^3)} \le L^{3/2}\|\varphi\|_{L^2(\mathbb{T}_L^3)+L^\infty(\mathbb{T}_L^3)} \le L^{3/2}\|\varphi\|_{L^2(\mathbb{T}_L^3)}, \tag{3.3.154}$$

which clearly makes the two norms equivalent. Nevertheless, we find it more natural to work with a bound of the form (3.3.152), where C_T is independent of L.

Lemma 3.3.8 implies that, for any $\varphi \in L^2(\mathbb{T}_L^3)+L^\infty(\mathbb{T}_L^3)$, the multiplication operator associated with φ is infinitesimally relatively bounded with respect to $-\Delta_L$. More precisely, for any $\delta > 0$, there exists $C\left(\delta, \|\varphi\|_{L^2(\mathbb{T}_L^3)+L^\infty(\mathbb{T}_L^3)}\right)$ depending on φ only through $\|\varphi\|_{L^2(\mathbb{T}_L^3)+L^\infty(\mathbb{T}_L^3)}$, such that for any $f \in \mathrm{Dom}(-\Delta_L)$

$$\|\varphi f\| \le \delta\|\Delta_L f\| + C\left(\delta, \|\varphi\|_{L^2(\mathbb{T}_L^3)+L^\infty(\mathbb{T}_L^3)}\right)\|f\|. \tag{3.3.155}$$

Whenever infinitesimal relative boundedness holds with a constant $C(\delta)$ uniform over a class of operators, we will say that the class is uniformly infinitesimally relatively bounded. In this case, Lemma 3.3.8 ensures that multiplication operators associated to functions in $(L^2 + L^\infty)$-balls are uniformly infinitesimally relatively bounded with respect to $-\Delta_L$.

Proof. We first observe that, by self-adjointness of $(-\Delta_L + T)^{-1}$, it is sufficient to show that the claimed bound holds for $\|\varphi(-\Delta_L+T)^{-1}\|$. For any $f, \varphi \in L^2(\mathbb{T}_L^3)$ and any decomposition of the form $\varphi = \varphi_1 + \varphi_2$ with $\varphi_1 \in L^2(\mathbb{T}_L^3)$ and $\varphi_2 \in L^\infty(\mathbb{T}_L^3)$ we have

$$\begin{aligned}\|\varphi(-\Delta_L + T)^{-1} f\|_2 &\le \|\varphi_1\|_2\|(-\Delta_L + T)^{-1} f\|_\infty + \|\varphi_2\|_\infty\|(-\Delta_L + T)^{-1} f\|_2 \\ &\le \|\varphi_1\|_2\|(-\Delta_L + T)^{-1} f\|_\infty + T^{-1}\|\varphi_2\|_\infty\|f\|_2. \end{aligned} \tag{3.3.156}$$

Moreover,

$$\begin{aligned}\|(-\Delta_L + T)^{-1} f\|_\infty &\le \sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{L^{3/2}(|k|^2+T)}|f_k| \le \left(\frac{1}{L^3}\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3}\frac{1}{(|k|^2+T)^2}\right)^{1/2}\|f\|_2 \\ &\le C\left(\int_{\mathbb{R}^3}\frac{1}{(|x|^2+T)^2}\right)^{1/2}\|f\|_2 = CT^{-1/2}\|f\|_2. \end{aligned} \tag{3.3.157}$$

Therefore, picking $C_T := \max\left\{T^{-1}, CT^{-1/2}\right\}$ yields

$$\|\varphi(-\Delta_L + T)^{-1} f\|_2 \le C_T\left(\|\varphi_1\|_2 + \|\varphi_2\|_\infty\right)\|f\|_2, \tag{3.3.158}$$

optimizing over φ_1 and φ_2 completes the proof. □

Lemma 3.3.9. *For* $\varphi \in L^2(\mathbb{T}_L^3)$

$$\|(-\Delta_L)^{-1/2}\varphi\|_{L^\infty(\mathbb{T}_L^3)+L^2(\mathbb{T}_L^3)} \lesssim \|(-\Delta_L+1)^{-1/2}\varphi\|_{L^2(\mathbb{T}_L^3)}. \tag{3.3.159}$$

Proof. We write $f_1 = \chi_{[0,1)}$ and $f_2 = \chi_{[1,+\infty)}$ and

$$\varphi_1 = f_1\left[(-\Delta_L)^{-1/2}\right]\varphi, \quad \varphi_2 = f_2\left[(-\Delta_L)^{-1/2}\right]\varphi. \tag{3.3.160}$$

Clearly $(-\Delta_L)^{-1/2}\varphi = \varphi_1 + \varphi_2$. Moreover

$$\begin{aligned}
\|(-\Delta_L)^{-1/2}\varphi\|_{L^\infty+L^2} &\leq \|\varphi_1\|_\infty + \|\varphi_2\|_2 \\
&\leq \left(\sum_{\substack{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3\\|k|<1}} \frac{1}{L^3|k|^2}\right)^{1/2} \left(\sum_{\substack{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3\\|k|<1}} |\varphi_k|^2\right)^{1/2} + \left(\sum_{\substack{k\in\frac{2\pi}{L}\mathbb{Z}^3\\|k|\geq 1}} \frac{|\varphi_k|^2}{|k|^2}\right)^{1/2} \\
&\lesssim \left(\sum_{\substack{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3\\|k|<1}} |\varphi_k|^2\right)^{1/2} + \left(\sum_{\substack{k\in\frac{2\pi}{L}\mathbb{Z}^3\\|k|\geq 1}} \frac{|\varphi_k|^2}{|k|^2}\right)^{1/2} \\
&\lesssim \left(\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{|k|^2+1}|\varphi_k|^2\right)^{1/2} = C\|(-\Delta_L+1)^{-1/2}\varphi\|_{L^2(\mathbb{T}_L^3)}.
\end{aligned} \tag{3.3.161}$$

This concludes the proof. □

Lemmas 3.3.8 and 3.3.9 together yield the following Corollary, whose proof is omitted as it is now straightforward.

Corollary 3.3.2. *For any φ such that $\|(-\Delta_L+1)^{-1/2}\varphi\|_2$ is finite, the multiplication operator V_φ (defined in* (3.2.8)*) is infinitesimally relatively bounded with respect to $(-\Delta_L)$. Moreover, for $T>0$ there exists C_T such that*

$$\|(-\Delta_L+T)^{-1}V_\varphi\| \leq C_T\|(-\Delta_L+1)^{-1/2}\varphi\|_2, \quad \textit{and} \quad C_T \searrow 0 \ \textit{as}\ T\to\infty. \tag{3.3.162}$$

In particular, Corollary 3.3.2 implies that the family of multiplication operators associated to $\{V_\varphi \,|\, \|(-\Delta_L+1)^{-1/2}\varphi\|_2 \leq M\}$ is uniformly infinitesimally relatively bounded with respect to $-\Delta_L$ for any M.

With these tools at hand we now investigate $\mathcal{F}_L$ close to its minimum and, in particular, compute the Hessian of $\mathcal{F}_L$ at its minimizers. We follow very closely the analogous analysis carried out in [41]. By translation invariance of the problem, it is clearly sufficient to perform the computation with respect to φ_L, where φ_L is the same as in Corollary 3.2.1.

Proposition 3.3.4. *For $L>L_1$ let $\varphi\in L^2_{\mathbb{R}}(\mathbb{T}^3_L)$ be such that*

$$\|(-\Delta_L+1)^{-1/2}(\varphi-\varphi_L)\|_{L^2(\mathbb{T}^3_L)} \leq \varepsilon_L \tag{3.3.163}$$

for some $\varepsilon_L>0$ small enough. Then

$$\begin{aligned}
&|\mathcal{F}_L(\varphi) - e_L - \langle\varphi-\varphi_L|\mathbb{1}-K_L|\varphi-\varphi_L\rangle| \\
&\lesssim_L \|(-\Delta_L+1)^{-1/2}(\varphi-\varphi_L)\|_2 \langle\varphi-\varphi_L|J_L|\varphi-\varphi_L\rangle,
\end{aligned} \tag{3.3.164}$$

where

$$\begin{aligned}
K_L &:= 4(-\Delta_L)^{-1/2}\psi_L\frac{Q_{\psi_L}}{h_{\varphi_L}-e(\varphi_L)}\psi_L(-\Delta_L)^{-1/2}, \\
J_L &= 4(-\Delta_L)^{-1/2}\psi_L(-\Delta_L+1)^{-1}\psi_L(-\Delta_L)^{-1/2},
\end{aligned} \tag{3.3.165}$$

and ψ_L, which we recall is the (positive) ground state of h_{φ_L}, is understood, in the expressions for K_L and J_L, as a multiplication operator.

Note that this implies that $H^{\mathcal{F}_L}_{\varphi_L} = \mathbb{1} - K_L$, as claimed in (3.2.22). In particular, $K_L \leq \mathbb{1}$ by minimality of φ_L. It is also clear, by definition, that $K_L \geq 0$. We emphasize that J_L is trace class, being the square of $(-\Delta_L + 1)^{-1/2}\psi_L(-\Delta_L)^{-1/2}$, which is Hilbert-Schmidt since ψ_L is in L^2, as a function of x, and $f(k) := (|k|^2 + 1)^{-1/2}|k|^{-1}$ is in L^2, as a function of k. From the trace class property of J_L, together with the boundedness of $(-\Delta_L+1)^{1/2}\frac{Q_{\psi_L}}{h_{\varphi_L}-e(\varphi_L)}(-\Delta_L+1)^{1/2}$ (which follows from Corollary 3.3.2), we immediately infer the trace class property of K_L. We even show in Lemma 3.3.10 that $J_L, K_L \lesssim_L (-\Delta_L+1)^{-2}$.

We shall in the following denote by K^y_L, respectively J^y_L, the unitary equivalent operators obtained from K_L and J_L by a translation by y. Note that K^y_L and J^y_L appear if one expands $\mathcal{F}_L$ with respect to φ^y_L instead of φ_L. Moreover, the invariance under translations of $\mathcal{F}_L$ implies that

$$\operatorname{span}\{\nabla\varphi_L\} \subset \ker(\mathbb{1} - K_L). \tag{3.3.166}$$

We show in Section 3.3.2 that these two sets coincide. Finally, even though both ε_L and the estimate (3.3.164) in Proposition 3.3.4 depend on L, with a little extra work one can show that the bound is actually uniform in L (for large L). For simplicity we opt for the current version of Proposition 3.3.4, as it is sufficient for the purpose of our investigation, which is set on a torus of fixed linear size $L > L_1$.

Proof. We shall denote $h_0 := h_{\varphi_L}$. By assumption (3.3.163) and since $\varphi_L \in L^2(\mathbb{T}^3_L)$, we can apply Corollary 3.3.2 to φ_L and to $(\varphi - \varphi_L)$. This way we see that $V_{\varphi-\varphi_L}$ is uniformly infinitesimally relatively bounded with respect to h_0 for any φ satisfying (3.3.163).

It is clear that h_0 admits a simple and isolated least eigenvalue $e(\varphi_L)$. Standard results in perturbation theory then imply that there exist $\varepsilon_L > 0$ and a contour γ around $e(\varphi_L)$ such that for any φ satisfying (3.3.163) $e(\varphi)$ is the only eigenvalue of $h_\varphi = h_0 + V_{\varphi-\varphi_L}$ inside γ. (For fixed φ, the statement above is a standard result in perturbation theory, see [101, Theorem XII.8]; moreover it is also possible to get a φ-independent γ encircling $e(\varphi)$, see [101, Theorem XII.11] and recall that $V_{\varphi-\varphi_L}$ are *uniformly* infinitesimally relatively bounded with respect to h_0.) We can then write

$$e(\varphi) = \operatorname{Tr}\int_\gamma \frac{z}{z-(h_0+V_{\varphi-\varphi_L})}\frac{dz}{2\pi i}. \tag{3.3.167}$$

Moreover, by the uniform infinitesimal relative boundedness of $V_{\varphi-\varphi_L}$ with respect to h_0, we have

$$\sup_{z\in\gamma}\|V_{\varphi-\varphi_L}(z-h_0)^{-1}\| < 1, \tag{3.3.168}$$

for ε_L sufficiently small. For any $z \in \gamma$, we can thus use the resolvent identity in the form

$$\begin{aligned}\frac{1}{z-h_0-V_{\varphi-\varphi_L}} &= \left(\mathbb{1} - \frac{Q_{\psi_L}}{z-h_0}V_{\varphi-\varphi_L}\right)^{-1}\frac{Q_{\psi_L}}{z-h_0} \\ &\quad \left(\mathbb{1} - \frac{Q_{\psi_L}}{z-h_0}V_{\varphi-\varphi_L}\right)^{-1}\frac{P_{\psi_L}}{z-h_0}\left(\mathbb{1} - V_{\varphi-\varphi_L}\frac{1}{z-h_0}\right)^{-1}.\end{aligned} \tag{3.3.169}$$

The first term is analytic inside the contour γ and hence it gives zero after integration when inserted in (3.3.167). Inserting the second term of (3.3.169), which is rank one, in (3.3.167) and using Fubini's Theorem to interchange the trace and the integral, we obtain

$$e(\varphi) = \int_\gamma \frac{z}{z - e(\varphi_L)} \left\langle \psi_L \middle| \left(\mathbb{1} - V_{\varphi-\varphi_L} \frac{1}{z - h_0}\right)^{-1} \left(\mathbb{1} - \frac{Q_{\psi_L}}{z - h_0} V_{\varphi-\varphi_L}\right)^{-1} \middle| \psi_L \right\rangle \frac{dz}{2\pi i}. \tag{3.3.170}$$

For simplicity, we introduce the notation

$$A = V_{\varphi-\varphi_L} \frac{1}{z - h_0}, \quad B = \frac{Q_{\psi_L}}{z - h_0} V_{\varphi-\varphi_L}. \tag{3.3.171}$$

Because of (3.3.168), both A and B are smaller than 1 in norm, uniformly in $z \in \gamma$. We shall use the identity

$$\begin{aligned} \frac{1}{\mathbb{1} - A} \frac{1}{\mathbb{1} - B} =& \mathbb{1} + A + A(A + B) + \frac{B}{\mathbb{1} - B} \\ &+ \frac{A^3}{\mathbb{1} - A} + \frac{A^2}{\mathbb{1} - A} B + \frac{A}{\mathbb{1} - A} \frac{B^2}{\mathbb{1} - B}. \end{aligned} \tag{3.3.172}$$

We insert the various terms in (3.3.170) and do the contour integration. The term $\mathbb{1}$ gives $e(\varphi_L)$. The term A, recalling that $(-\Delta_L)^{-1/2} \rho_{\psi_L} = \varphi_L$, yields

$$\langle \psi_L | V_{\varphi-\varphi_L} | \psi_L \rangle = 2 \langle \varphi - \varphi_L | \varphi_L \rangle. \tag{3.3.173}$$

A standard calculation shows that the term $A(A + B)$ gives

$$\left\langle \psi_L \middle| V_{\varphi-\varphi_L} \frac{Q_{\psi_L}}{e(\varphi_L) - h_0} V_{\varphi-\varphi_L} \middle| \psi_L \right\rangle = - \langle \varphi - \varphi_L | K_L | \varphi - \varphi_L \rangle. \tag{3.3.174}$$

Furthermore, since $Q_{\psi_L} \psi_L = 0$, the term $B(\mathbb{1} - B)^{-1}$ yields zero. Recalling that $\mathcal{F}_L(\varphi) = \|\varphi\|^2 + e(\varphi)$ we obtain from (3.3.170)

$$\begin{aligned} &\mathcal{F}_L(\varphi) - \mathcal{F}_L(\varphi_L) - \langle \varphi - \varphi_L | \mathbb{1} - K_L | \varphi - \varphi_L \rangle \\ &= \int_\gamma \frac{z}{z - e(\varphi_L)} \left\langle \psi_L \middle| \frac{A^3}{\mathbb{1} - A} + A \left(\frac{A}{\mathbb{1} - A} + \frac{1}{\mathbb{1} - A} \frac{B}{\mathbb{1} - B} \right) B \middle| \psi_L \right\rangle \frac{dz}{2\pi i}. \end{aligned} \tag{3.3.175}$$

We observe that, since γ is uniformly bounded and uniformly bounded away from $e(\varphi_L)$, we can get rid of the integration, i.e., it suffices to bound

$$\begin{aligned} (I) &:= \sup_{z \in \gamma} \left| \left\langle \psi_L \middle| \frac{A^3}{\mathbb{1} - A} \middle| \psi_L \right\rangle \right|, \\ (II) &:= \sup_{z \in \gamma} \left| \left\langle \psi_L \middle| A \left(\frac{A}{\mathbb{1} - A} + \frac{1}{\mathbb{1} - A} \frac{B}{\mathbb{1} - B} \right) B \middle| \psi_L \right\rangle \right|, \end{aligned} \tag{3.3.176}$$

with the r.h.s. of (3.3.164) to conclude the proof. We note that

$$\langle \varphi - \varphi_L | J_L | \varphi - \varphi_L \rangle = \left\| (-\Delta_L + 1)^{1/2} V_{\varphi-\varphi_L} \psi_L \right\|_2^2, \tag{3.3.177}$$

and that, by infinitesimal relative boundedness of V_{φ_L} with respect to $(-\Delta_L)$ and since γ is uniformly bounded away from $e(\varphi_L)$, there exists some constant $C_L > 0$ such that

$$\sup_{z \in \gamma} \left\| (-\Delta_L + 1)^{1/2} (z - h_0)^{-k} (-\Delta_L + 1)^{1/2} \right\| \leq C_L \quad \text{for } k = 1, 2. \tag{3.3.178}$$

Therefore,

$$\begin{aligned}
(I) &= \sup_{z\in\gamma} \left|(z-e(\varphi_L))^{-1} \langle V_{\varphi-\varphi_L}\psi_L|(z-h_0)^{-1}A(\mathbb{1}-A)^{-1}|V_{\varphi-\varphi_L}\psi_L\rangle\right| \\
&\lesssim_L \sup_{z\in\gamma} \left\|(-\Delta_L+1)^{1/2}(z-h_0)^{-1}\frac{A}{\mathbb{1}-A}(-\Delta_L+1)^{1/2}\right\| \langle \varphi-\varphi_L|J_L|\varphi-\varphi_L\rangle\,, \\
&\lesssim_L \sup_{z\in\gamma} \left\|(-\Delta_L+1)^{-1/2}\frac{A}{\mathbb{1}-A}(-\Delta_L+1)^{1/2}\right\| \langle \varphi-\varphi_L|J_L|\varphi-\varphi_L\rangle\,, \qquad (3.3.179)\\
(II) &\leq \sup_{z\in\gamma} \left\|\frac{A}{\mathbb{1}-A}+\frac{1}{\mathbb{1}-A}\frac{B}{\mathbb{1}-B}\right\| \langle\psi_L|AA^\dagger|\psi_L\rangle^{1/2} \langle\psi_L|BB^\dagger|\psi_L\rangle^{1/2} \\
&\lesssim_L \sup_{z\in\gamma} \left\|\frac{A}{\mathbb{1}-A}+\frac{1}{\mathbb{1}-A}\frac{B}{\mathbb{1}-B}\right\| \langle \varphi-\varphi_L|J_L|\varphi-\varphi_L\rangle\,. \qquad (3.3.180)
\end{aligned}$$

Since

$$A(\mathbb{1}-A)^{-1} = V_{\varphi-\varphi_L}(z-h_\varphi)^{-1}, \qquad (3.3.181)$$

it follows that

$$\begin{aligned}
&\left\|(-\Delta_L+1)^{-1/2}\frac{A}{\mathbb{1}-A}(-\Delta_L+1)^{1/2}\right\| \\
&\leq \|(-\Delta_L+1)^{-1/2}V_{\varphi-\varphi_L}(-\Delta_L)^{-1/2}\|\|(-\Delta_L)^{1/2}(z-h_\varphi)^{-1}(-\Delta_L)^{1/2}\| \\
&\lesssim_L \|(-\Delta_L+1)^{-1}(\varphi-\varphi_L)\|, \qquad (3.3.182)
\end{aligned}$$

where we used the relative boundedness of h_φ w.r.t to $-\Delta_L$ and Corollary 3.3.2. This yields the right bound for (I). Similar estimates yield the right bounds for $\|A(\mathbb{1}-A)^{-1}\|$ and $\|(\mathbb{1}-A)^{-1}B(\mathbb{1}-B)^{-1}\| \lesssim_L \|B\|$, concluding the proof. □

As a final result of this subsection, we prove the following Lemma about the operators K_L and J_L.

Lemma 3.3.10. *Let K_L and J_L be the operators defined in* (3.3.165)*. We have*

$$K_L, J_L \lesssim_L (-\Delta_L+1)^{-2}. \qquad (3.3.183)$$

Proof. We prove the result for J_L. By the relative boundedness of h_{φ_L} with respect to $-\Delta_L$ the same proof applies to K_L. We shall show that $(-\Delta_L+1)(-\Delta_L)^{-1/2}\psi_L(-\Delta_L+1)^{-1/2}$ is bounded as an operator on $L^2(\mathbb{T}^3_L)$. In fact, for $f\in L^2(\mathbb{T}^3_L)$,

$$\begin{aligned}
&\|(-\Delta_L+1)(-\Delta_L)^{-1/2}\psi_L(-\Delta_L+1)^{-1/2}f\|_2^2 \\
&= \sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3}\left(\frac{|k|^2+1}{|k|}\right)^2\left|\sum_{\xi\in\frac{2\pi}{L}\mathbb{Z}^3}(\psi_L)_{k-\xi}\frac{f_\xi}{(|\xi|^2+1)^{1/2}}\right|^2 \\
&\leq \|(-\Delta_L+1)^{3/2}\psi_L\|_2^2\sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3}\left(\frac{|k|^2+1}{|k|}\right)^2\sum_{\xi\in\frac{2\pi}{L}\mathbb{Z}^3}\frac{|f_\xi|^2}{(|k-\xi|^2+1)^3(|\xi|^2+1)} \\
&\lesssim_L \sum_{\xi\in\frac{2\pi}{L}\mathbb{Z}^3}\frac{|f_\xi|^2}{|\xi|^2+1}\sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3}\frac{(|k|^2+1)^2}{|k|^2(|k-\xi|^2+1)^3} \lesssim_L \|f\|_2^2, \qquad (3.3.184)
\end{aligned}$$

where we used that $\psi_L\in C^\infty(\mathbb{T}^3_L)$ and that $\sum_{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3}\frac{(|k|^2+1)^2}{|k|^2(|k-\xi|^2+1)^3}\lesssim|\xi|^2+1$. Therefore

$$J_L \leq \|(-\Delta_L+1)(-\Delta_L)^{-1/2}\psi_L(-\Delta_L+1)^{-1/2}\|^2(-\Delta_L+1)^{-2} \lesssim_L (-\Delta_L+1)^{-2}, \qquad (3.3.185)$$

as claimed. □

Local Properties of $\mathcal{M}_L^{\mathcal{F}}$ and $\mathcal{F}_L$

For $L > L_1$ we introduce the notation

$$\Pi_\nabla^L := L^2\text{-projection onto } \operatorname{span}\{\nabla\varphi_L\}, \tag{3.3.186}$$

which is going to be used throughout this section and Section 3.4. According to Theorem 3.2.1, the condition $L > L_1$ guarantees that $\psi_L^y \neq \psi_L$ for any $\psi_L \in \mathcal{M}_L^{\mathcal{E}}$ and any $y \neq 0$, which implies that $\operatorname{ran}\Pi_\nabla^L$ is three dimensional (i.e that the partial derivatives of φ_L are linearly independent); if not, there would exist $\nu \in \mathbb{S}^2$ such that $\partial_\nu\psi_L = 0$ and this would imply $\psi_L = \psi_L^y$ for any y parallel to ν.

For technical reasons, we also introduce a family of weighted norms which will be needed in Section 3.4. For $T \geq 0$, we define

$$\|\varphi\|_{W_T} := \langle\varphi|W_T|\varphi\rangle^{1/2}, \tag{3.3.187}$$

where W_T acts in k-space as multiplication by

$$W_T(k) = \begin{cases} 1 & |k| \leq T \\ (|k|^2+1)^{-1} & |k| > T. \end{cases} \tag{3.3.188}$$

Note that $\|\varphi\|_{W_0}^2 = \langle\varphi|(-\Delta_L+1)^{-1}|\varphi\rangle$ and $\|\varphi\|_{W_\infty} = \|\varphi\|_2$.

For the purpose of this section we could formulate the following Lemma only with respect to $\|\cdot\|_2 = \|\cdot\|_{W_\infty}$, but we opt for this more general version since we shall need it in Section 3.4.

Lemma 3.3.11. *For any $L > L_1$, there exists ε'_L (independent of T) such that for any $\varphi \in L^2_{\mathbb{R}}(\mathbb{T}^3_L)$ with $\operatorname{dist}_{W_T}(\varphi, \Omega_L(\varphi_L)) \leq \varepsilon'_L$ there exist a* unique *couple (y_φ, v_φ), depending on T, with $y_\varphi \in \mathbb{T}^3_L$ and $v_\varphi \in (\operatorname{span}_{i=1,2,3}\{W_T\partial_i\varphi_L\})^\perp$, such that*

$$\varphi = \varphi_L^{y_\varphi} + (v_\varphi)^{y_\varphi} \quad \textit{and} \quad \|v_\varphi\|_{W_T} \leq \varepsilon'_L. \tag{3.3.189}$$

As Proposition 3.3.4 above, we opt for an L-dependent version of Lemma 3.3.11 for simplicity, as it is sufficient for our purposes. We nevertheless believe it is possible to prove a corresponding statement that is uniform in L. Note that Lemma 3.3.11 is equivalent to the statement that there exists a T-independent ε'_L such that the W_T-projection onto $\Omega_L(\varphi_L)$ is uniquely defined in an ε'_L-neighborhood of $\Omega_L(\varphi_L)$ with respect to the W_T-norm, and that, for any φ therein, $\varphi_L^{y_\varphi}$ characterizes the W_T-projection of φ onto $\Omega_L(\varphi_L)$, so that

$$\operatorname{dist}_{W_T}(\varphi, \Omega_L(\varphi_L)) = \|\varphi - \varphi_L^{y_\varphi}\|_{W_T} = \|v_\varphi\|_{W_T}. \tag{3.3.190}$$

Proof. We begin by observing that the Lemma is equivalent to showing that for any $\|\cdot\|_{W_T}$-normalized $v \in (\operatorname{span}_{i=1,2,3}\{W_T\partial_i\varphi_L\})^\perp$, any $\varepsilon \leq \varepsilon'_L$ and any $0 \neq y \in \mathbb{T}^3_L$ we have

$$\varepsilon < \|\varphi_L + \varepsilon v - \varphi_L^y\|_{W_T}. \tag{3.3.191}$$

Indeed, if the Lemma holds then $\varphi = \varphi_L + \varepsilon v$ does not admit other decompositions of the form (3.3.189), which implies that, for any $y \neq 0$, (3.3.191) holds (otherwise there would exist $y \neq 0$ minimizing the W_T-distance of φ from $\Omega_L(\varphi_L)$ and such y would necessarily yield a second decomposition of the form (3.3.189)). On the other hand, if the statement (3.3.191) holds and the Lemma does not, then there exists φ such that $\operatorname{dist}_{W_T}(\varphi, \Omega_L(\varphi_L)) \leq \varepsilon'_L$ and also such that (y_1, v_1) and (y_2, v_2) yield two different decompositions of the form (3.3.189) for φ (note that at least one decomposition of the form (3.3.189) always exist, as there exist at least one element of $\Omega_L(\varphi_L)$ realizing the W_T-distance of φ from $\Omega_L(\varphi_L)$). By considering φ^{-y_1} (respectively φ^{-y_2}) we find $\|v_1\|_{W_T} > \|v_2\|_{W_T}$ (respectively $\|v_2\|_{W_T} > \|v_1\|_{W_T}$), which is clearly a contradiction. We shall hence proceed to prove the statement (3.3.191).

Taylor's formula and the regularity of φ_L imply the existence of T-independent constant C_L^1 such that

$$\varphi_L^y = \varphi_L + y \cdot (\nabla \varphi_L) + g_y, \quad \text{with} \quad \|g_y\|_{W_T} \leq \|g_y\|_2 \leq C_L^1 |y|^2. \tag{3.3.192}$$

As remarked after (3.3.186), the kernel of Π_∇^L is three-dimensional, hence there exists a constant C_L^2 independent of T such that

$$\min_{\nu \in \mathbb{S}^2} \|\nu \cdot \nabla \varphi_L\|_{W_T} \geq \min_{\nu \in \mathbb{S}^2} \|\nu \cdot \nabla \varphi_L\|_{W_0} \geq C_L^2. \tag{3.3.193}$$

Therefore, using that $v \perp_{W_T} \nabla \varphi_L$ in combination with (3.3.192) and (3.3.193), we find, for

$$|y| < (C_L^2 - 2\varepsilon C_L^1)^{1/2} (C_L^1)^{-1}, \tag{3.3.194}$$

that

$$\|\varphi_L + \varepsilon v - \varphi_L^y\|_{W_T} = \|\varepsilon v - y \cdot (\nabla \varphi_L) - g_y\|_{W_T} \geq \left(\varepsilon^2 + |y|^2 C_L^2\right)^{1/2} - C_L^1 |y|^2 > \varepsilon, \tag{3.3.195}$$

i.e., that (3.3.191) holds for y satisfying (3.3.194). Furthermore, we have

$$\|\varphi_L + \varepsilon v - \varphi_L^y\|_{W_T}^2 \geq \varepsilon^2 + \|\varphi_L - \varphi_L^y\|_{W_T} \left(\|\varphi_L - \varphi_L^y\|_{W_T} - 2\varepsilon\right), \tag{3.3.196}$$

and this implies that (3.3.191) holds for any y such that

$$\|\varphi_L - \varphi_L^y\|_{W_T} > 2\varepsilon. \tag{3.3.197}$$

Using again (3.3.193) and (3.3.192), there exist $C_L^3, c_L^1, c_L^4 > 0$ independent of T such that

$$\begin{aligned} \|\varphi_L - \varphi_L^y\|_{W_T} = \|y \cdot (\nabla \varphi_L) + g_y\|_{W_T} \geq C_L^2 |y| - C_L^1 |y|^2 \geq C_L^3 |y|, \quad \text{for} \quad |y| \leq c_L^1, \\ \|\varphi_L - \varphi_L^y\|_{W_T} > c_L^4 \quad \text{for} \quad |y| > c_L^1, \end{aligned} \tag{3.3.198}$$

where the second line simply follows from $\|\cdot\|_{W_T} \geq \|\cdot\|_{W_0}$, the fact that $\varphi_L \neq \varphi_L^y$ for any $0 \neq y \in [-L/2, L/2]^3$ and the continuity of φ_L. Combining (3.3.197) and (3.3.198), we conclude that (3.3.191) holds if either $|y| > c_L^1$ or

$$|y| > 2\varepsilon (C_L^3)^{-1}. \tag{3.3.199}$$

Picking ε'_L sufficiently small, the fact that (3.3.191) holds both under the conditions (3.3.194) and (3.3.199) shows that it holds for any $y \in \mathbb{T}_L^3$, and this completes the proof. □

We conclude our study of the Pekar functional $\mathcal{F}_L$ by showing that $\ker(\mathbb{1} - K_L) = \operatorname{span}\{\nabla \varphi_L\} = \operatorname{ran} \Pi_\nabla^L$. Since clearly $\operatorname{ran} \Pi_\nabla^L \subset \ker(\mathbb{1} - K_L)$, this is a consequence of the following Proposition.

Proposition 3.3.5. *Recalling the definition of τ_L from Corollary 3.2.1, we have*

$$\mathbb{1} - K_L \geq \tau_L (\mathbb{1} - \Pi_\nabla^L). \tag{3.3.200}$$

Proof. We need to show that for all normalized $v \in \operatorname{ran}(\mathbb{1} - \Pi^L_\nabla)$ the bound

$$\langle v|\mathbb{1} - K_L|v\rangle \geq \tau_L \tag{3.3.201}$$

holds. Using Lemma 3.3.11 in the case $T = \infty$, for any such v and ε small enough, denoting $\varphi = \varphi_L + \varepsilon v$, we obtain

$$\operatorname{dist}^2_{L^2}(\varphi, \Omega_L(\varphi_L)) = \varepsilon^2. \tag{3.3.202}$$

Moreover, since $\|(-\Delta_L + 1)^{-1}(\varphi - \varphi_L)\| \leq \varepsilon\|v\|_2 = \varepsilon$, for ε small enough we can expand $\mathcal{F}_L(\varphi)$ with respect to φ_L using Proposition 3.3.4. Combining this with (3.2.20), we arrive at

$$\tau_L \varepsilon^2 \leq \mathcal{F}_L(\varphi_L + \varepsilon v) - e_L \leq \varepsilon^2 \langle v|\mathbb{1} - K_L|v\rangle + \varepsilon^3 \langle v|J_L|v\rangle . \tag{3.3.203}$$

Since ε can be taken arbitrarily small, the proof is complete. □

3.4 Proof of Main Results

In this Section we give the proof of Theorem 3.2.2. In Section 3.4.1 we prove the upper bound in (3.2.24). In Section 3.4.2 we estimate the cost of substituting the full Hamiltonian $\mathbb{H}_L$ with a cut-off Hamiltonian depending only on finitely many phonon modes, a key step in providing a lower bound for $\inf \operatorname{spec} \mathbb{H}_L$. Finally, in Section 3.4.3, we show the validity of the lower bound in (3.2.24).

The approach used in Sections 3.4.1 and 3.4.2 follows closely the one used in [41], even if, in our setting, minor complications arise in the proof of the upper bound due the presence of the zero modes of the Hessian. For the lower bound in Section 3.4.3, however, a substantial amount of additional work is needed to deal with the translation invariance, which complicates the proof significantly.

3.4.1 Upper Bound

In this section we construct a trial state, which will be used to obtain an upper bound on the ground state energy of $\mathbb{H}_L$ for fixed $L > L_1$. This is carried out using the Q-space representation of the bosonic Fock space $\mathcal{F}(L^2(\mathbb{T}^3_L))$ (see [100]). Even though the estimates contained in this section are L-dependent, we believe it is possible, with little modifications to the proof, to obtain the same upper bound with the same error estimates uniformly in L.

Our trial state depends non-trivially only on finitely many phonon variables, and we proceed to describe it more in detail. If one picks Π to be a *real* finite rank projection on $L^2(\mathbb{T}^3_L)$, then

$$\mathcal{F}(L^2(\mathbb{T}^3_L)) \cong \mathcal{F}(\Pi L^2(\mathbb{T}^3_L)) \otimes \mathcal{F}((\mathbb{1} - \Pi)L^2(\mathbb{T}^3_L)). \tag{3.4.1}$$

The first factor $\mathcal{F}(\Pi L^2(\mathbb{T}^3_L))$ can isomorphically be identified with $L^2(\mathbb{R}^N)$, where N is the complex dimension of $\operatorname{ran}\Pi$. In particular, there is a one-to-one correspondence between any real $\varphi \in \operatorname{ran}\Pi$ and $\lambda = (\lambda_1, \ldots, \lambda_N) \in \mathbb{R}^N$, explicitly given by

$$\varphi = \sum_{i=1}^N \lambda_i \varphi_i \cong (\lambda_1, \ldots, \lambda_N) = \lambda, \tag{3.4.2}$$

where $\{\varphi_i\}_{i=1}^N$ denotes an orthonormal basis of $\operatorname{ran}\Pi$ consisting of real-valued functions. The trial state we use corresponds to the vacuum in the second factor $\mathcal{F}((\mathbb{1} - \Pi)L^2(\mathbb{T}^3_L))$ and shall hence be written only as a function of x (the electron variable) and λ (the finitely many phonon variables selected by Π). We begin by specifying some properties we wish Π to satisfy. Consider φ_L from Corollary 3.2.1 and define Π to be a projection of the form $\Pi = \Pi' + \Pi_\nabla^L$, where Π_∇^L is defined in (3.3.186) and Π' is an $(N-3)$-dimensional projection on $\operatorname{span}\{\nabla\varphi_L\}^\perp = \operatorname{ran}(\mathbb{1} - \Pi_\nabla^L)$ that will be further specified later but will always be taken so that $\varphi_L \in \operatorname{ran}\Pi$. Our trial state is of the form

$$\Psi(x,\varphi) = G(\varphi)\eta(\varphi)\psi_\varphi(x), \tag{3.4.3}$$

where

- $x \in \mathbb{T}_L^3$ and φ is a real element of $\operatorname{ran}\Pi$ (identified with $\lambda \in \mathbb{R}^N$ as in (3.4.2)),
- $G(\varphi)$ is a Gaussian factor explicitly given by

$$G(\varphi) = \exp\Big(-\alpha^2 \left\langle \varphi - \varphi_L \middle| [\Pi(\mathbb{1} - K_L)\Pi]^{1/2} \middle| \varphi - \varphi_L \right\rangle\Big), \tag{3.4.4}$$

- η is a 'localization factor' given by

$$\eta(\varphi) = \chi\left(\varepsilon^{-1}\|(-\Delta_L + 1)^{-1/2}(\varphi - \varphi_L)\|_{L^2(\mathbb{T}_L^3)}\right), \tag{3.4.5}$$

  for some $0 < \varepsilon < \varepsilon_L$ (with ε_L as in Proposition 3.3.4), where $0 \le \chi \le 1$ is a smooth cut-off function such that $\chi(t) = 1$ for $t \le 1/2$ and $\chi(t) = 0$ for $t \ge 1$,
- ψ_φ is the unique positive ground state of $h_\varphi = -\Delta_L + V_\varphi$.

We note that our state actually depends on two parameters (N and ε) and, of course, on the specific choice of Π'. We choose $\{\varphi_i\}_{i=1,\dots,N}$ to be a real orthonormal basis of eigenfunctions of $[\Pi(\mathbb{1} - K_L)\Pi]$ corresponding to eigenvalues $\mu_i = 0$ for $i = 1,2,3$ and $\mu_i \ge \tau_L > 0$ for $i = 4,\dots,N$. Recalling Proposition 3.3.5, this amounts to choosing $\{\varphi_i\}_{i=1,2,3}$ to be a real orthonormal basis of $\operatorname{ran}\Pi_\nabla^L$ and $\{\varphi_i\}_{i=4,\dots,N}$ to be a real orthonormal basis of eigenfunctions of $[\Pi'(\mathbb{1} - K_L)\Pi']$. With this choice, we have (with a slight abuse of notation)

$$G(\varphi) = G(\lambda_4,\dots,\lambda_N) = \exp\left(-\alpha^2 \sum_{i=4}^N \mu_i^{1/2}(\lambda_i - \lambda_i^L)^2\right), \tag{3.4.6}$$

where $\varphi_L \cong \lambda_L = (0,0,0,\lambda_4^L,\dots,\lambda_N^L)$, since $\varphi_L \in \operatorname{ran}\Pi$ by construction, and the first three coordinates are 0 since $\varphi_L \in \left(\operatorname{ran}\Pi_\nabla^L\right)^\perp$.

We first show that even if G does not have finite $L^2(\mathbb{R}^N)$-norm, Ψ does due to the presence of η. We define

$$T_\varepsilon := \{\|(-\Delta_L + 1)^{-1/2}(\varphi - \varphi_L)\| \le \varepsilon\} \subset \mathbb{R}^N \tag{3.4.7}$$

and

$$\gamma_L := \inf_{\substack{\varphi \in \operatorname{ran}\Pi_\nabla^L \\ \|\varphi\|_2 = 1}} \langle \varphi | (-\Delta_L + 1)^{-1} | \varphi \rangle > 0. \tag{3.4.8}$$

Then, on T_ε, recalling that $\Pi_\nabla^L \varphi_L = 0$, we have

$$\gamma_L^{1/2}\sqrt{\lambda_1^2+\lambda_2^2+\lambda_3^2} = \gamma_L^{1/2}\|\Pi_\nabla^L\varphi\| \leq \|(-\Delta_L+1)^{-1/2}\Pi_\nabla^L(\varphi-\varphi_L)\|_2$$
$$\leq \|(-\Delta_L+1)^{-1/2}\Pi'(\varphi-\varphi_L)\|_2+\varepsilon \leq \|\Pi'(\varphi-\varphi_L)\|+\varepsilon = \left(\sum_{i=4}^N(\lambda_i-\lambda_i^L)^2\right)^{1/2}+\varepsilon \tag{3.4.9}$$

and this implies, using the normalization of ψ_φ, that

$$\|\Psi\|^2 = \int_{\mathbb{R}^N} G(\lambda_4,\ldots,\lambda_N)^2\eta(\lambda)^2 d\lambda_1\ldots d\lambda_N \leq \int_{\mathbb{R}^N} G(\lambda_4,\ldots,\lambda_N)^2 \mathbb{1}_{T_\varepsilon}(\lambda)d\lambda_1\cdots d\lambda_N$$
$$\leq \frac{4\pi}{3}\int_{\mathbb{R}^{N-3}} G(\lambda_4,\ldots,\lambda_N)^2\gamma_L^{-3/2}\left[\left(\sum_{i=4}^N(\lambda_i-\lambda_i^L)^2\right)^{1/2}+\varepsilon\right]^3 d\lambda_4\cdots d\lambda_N < \infty. \tag{3.4.10}$$

We spend a few words to motivate our choice of Ψ. The absolute value squared of Ψ has to be interpreted as a probability density over the couples (φ, x), with φ being a classical state for the phonon field and x the position of the electron. In the electron coordinate, our Ψ corresponds to the ground state of h_φ for any value of φ. This implies, by straightforward computations, that the expectation value of the Fröhlich Hamiltonian in Ψ equals the one of $e(\varphi)+\mathbb{N}$, $e(\varphi)$ being the ground state energy of h_φ and $\mathbb{N}$ the number operator. Moreover, because of the factor η, we are localizing our state to the regime where the Hessian expansion of $e(\varphi)$ from Proposition 3.3.4 holds. To leading order, this effectively makes our system formally correspond to a system of infinitely many harmonic oscillators with frequencies given by the eigenvalues of $(\mathbb{1}-K_L)^{1/2}$, with a Gaussian ground state. To carry out this analysis out rigorously, we need to choose a suitable finite rank projection Π, as detailed in the remained of this section.

We are now ready to delve into the details of the proof. It is easy to see that the interaction term appearing in the Fröhlich Hamiltonian acts in the Q-space representation as the multiplication by $V_\varphi(x)$. Therefore, since Ψ corresponds to the vacuum on $(\mathbb{1}-\Pi)L^2(\mathbb{T}_L^3)$ and only depends on x through the factor $\psi_\varphi(x)$, the g.s. of h_φ, it follows that

$$\langle\Psi|\mathbb{H}_L|\Psi\rangle = \langle\Psi|e(\varphi)+\mathbb{N}|\Psi\rangle \tag{3.4.11}$$

where $\varphi = \Pi\varphi \cong \lambda \in \mathbb{R}^N$ and the inner product on the r.h.s. is naturally interpreted as the one on $L^2(\mathbb{T}_L^3)\otimes L^2(\mathbb{R}^N)$. In the Q-space representation, the number operator takes the form

$$\mathbb{N} = \sum_{n=1}^N\left(-\frac{1}{4\alpha^4}\partial_{\lambda_n}^2+\lambda_n^2-\frac{1}{2\alpha^2}\right) = \frac{1}{4\alpha^4}(-\Delta_\lambda)+|\lambda|^2-\frac{N}{2\alpha^2}. \tag{3.4.12}$$

Using the fact that η is supported on the set T_ε defined in (3.4.7), we can use the Hessian expansion from Proposition 3.3.4 to obtain bounds on $e(\lambda)$. Consequently, for a suitable positive constant C_L,

$$\langle\Psi|\mathbb{H}_L|\Psi\rangle \leq \langle\Psi|e_L+\langle\varphi-\varphi_L|\mathbb{1}-K_L+\varepsilon C_L J_L|\varphi-\varphi_L\rangle|\Psi\rangle$$
$$+\left\langle\Psi\middle|\frac{1}{4\alpha^4}(-\Delta_\lambda)-\frac{N}{2\alpha^2}\middle|\Psi\right\rangle$$
$$= \left(e_L-\frac{1}{2\alpha^2}\operatorname{Tr}(\Pi)\right)\|\Psi\|^2+A+B, \tag{3.4.13}$$

with

$$A = \left\langle \Psi \middle| \frac{1}{4\alpha^4}(-\Delta_\lambda) + \sum_{i=4}^{N} \mu_i(\lambda_i - \lambda_i^L)^2 \middle| \Psi \right\rangle, \tag{3.4.14}$$

$$B = \varepsilon C_L \langle \Psi | \langle \varphi - \varphi_L | J_L | \varphi - \varphi_L \rangle | \Psi \rangle . \tag{3.4.15}$$

We shall now proceed to bound A and B. First, we recall that by Lemma 3.3.10

$$J_L \lesssim_L (-\Delta_L + 1)^{-2}. \tag{3.4.16}$$

Therefore, since η is supported on T_ε, we have

$$B \lesssim_L \varepsilon^3 \|\Psi\|^2. \tag{3.4.17}$$

To bound A a bit more work is required. A direct calculation shows that

$$\left[\frac{1}{4\alpha^4}(-\Delta_\lambda) + \sum_{i=4}^{N} \mu_i(\lambda_i - \lambda_i^L)^2\right] G = \frac{1}{2\alpha^2} \operatorname{Tr}\Big([\Pi(\mathbb{1} - K_L)\Pi]^{1/2}\Big) G. \tag{3.4.18}$$

The previous identity, together with straightforward manipulations involving integration by parts, shows that

$$\begin{aligned} A &= \frac{1}{4\alpha^4}\left(\langle \psi_\varphi G \eta | \psi_\varphi(-\Delta_\lambda G)\eta\rangle + \int_{\mathbb{T}_L^3 \times \mathbb{R}^N} G^2 |\nabla_\lambda(\eta\psi_\varphi)|^2\right) + \left\langle \Psi \middle| \sum_{i=4}^{N} \mu_i(\lambda - \lambda_i^L)^2 \middle| \Psi \right\rangle \\ &\leq \frac{1}{2\alpha^2} \operatorname{Tr}\Big([\Pi(\mathbb{1} - K_L)\Pi]^{1/2}\Big)\|\Psi\|^2 \\ &\quad + \frac{1}{2\alpha^4}\left[\int_{\mathbb{T}_L^3 \times \mathbb{R}^N} G^2\eta^2|\nabla_\lambda\psi_\varphi|^2 + \int_{\mathbb{T}_L^3 \times \mathbb{R}^N} G^2 |\nabla_\lambda \eta|^2 |\psi_\varphi|^2\right] \\ &=: \frac{1}{2\alpha^2} \operatorname{Tr}\Big([\Pi(\mathbb{1} - K_L)\Pi]^{1/2}\Big)\|\Psi\|^2 + A_1 + A_2. \end{aligned} \tag{3.4.19}$$

We proceed to bound A_1. By standard first order perturbation theory (using that the phase of ψ_φ is chosen so that it is the unique positive minimizer of h_φ) we have

$$\partial_{\lambda_n}\psi_\varphi = -\frac{Q_{\psi_\varphi}}{h_\varphi - e(\varphi)} V_{\varphi_n}\psi_\varphi, \tag{3.4.20}$$

where we recall that $Q_{\psi_\varphi} = \mathbb{1} - |\psi_\varphi\rangle\langle\psi_\varphi|$. This implies that, for fixed φ,

$$\begin{aligned} \int_{\mathbb{T}_L^3} |\nabla_\lambda \psi_\varphi(x)|^2 dx &= \sum_{n=1}^{N} \left\| \frac{Q_{\psi_\varphi}}{h_\varphi - e(\varphi)} V_{\varphi_n}\psi_\varphi \right\|^2_{L^2(\mathbb{T}_L^3)} \\ &= \sum_{n=1}^{N} \langle \varphi_n | (-\Delta_L)^{-1/2} \psi_\varphi \left(\frac{Q_{\psi_\varphi}}{h_\varphi - e(\varphi)}\right)^2 \psi_\varphi (-\Delta_L)^{-1/2} | \varphi_n \rangle \\ &= \operatorname{Tr}\left(\Pi(-\Delta_L)^{-1/2}\psi_\varphi \left(\frac{Q_{\psi_\varphi}}{h_\varphi - e(\varphi)}\right)^2 \psi_\varphi(-\Delta_L)^{-1/2}\Pi\right), \end{aligned} \tag{3.4.21}$$

where ψ_φ is interpreted as a multiplication operator in the last two expressions. Since $(-\Delta_L+1)^{1/2}\left(\frac{Q_{\psi_\varphi}}{h_\varphi - e(\varphi)}\right)^2(-\Delta_L+1)^{1/2}$ is uniformly bounded over the support of η (the potential

V_φ being uniformly infinitesimally relatively bounded with respect to $-\Delta_L$ by Corollary 3.3.2) and recalling the normalization of ψ_φ, we get

$$\begin{aligned}&\mathrm{Tr}\left(\Pi(-\Delta_L)^{-1/2}\psi_\varphi\left(\frac{Q_{\psi_\varphi}}{h_\varphi - e(\varphi)}\right)^2\psi_\varphi(-\Delta_L)^{-1/2}\Pi\right)\\&\lesssim_L \mathrm{Tr}\Big(\Pi(-\Delta_L)^{-1/2}\psi_\varphi(-\Delta_L+1)^{-1}\psi_\varphi(-\Delta_L)^{-1/2}\Pi\Big) \lesssim_L 1.\end{aligned} \tag{3.4.22}$$

In summary, we conclude that

$$A_1 \lesssim_L \frac{1}{\alpha^4}\|\Psi\|^2. \tag{3.4.23}$$

Finally, we proceed to bound A_2. Recalling the definition of η and T_ε, we see that

$$\begin{aligned}|\nabla_\lambda \eta|^2 &= \left|\nabla_\lambda\left[\chi\left(\varepsilon^{-1}\|(-\Delta_L+1)^{-1/2}(\varphi-\varphi_L)\|_{L^2(\mathbb{T}_L^3)}\right)\right]\right|^2\\&\lesssim \varepsilon^{-2}\mathbb{1}_{T_\varepsilon}(\varphi)\left|\nabla_\lambda\|(-\Delta_L+1)^{-1/2}(\varphi-\varphi_L)\|_{L^2(\mathbb{T}_L^3)}\right|^2\\&\lesssim \varepsilon^{-2}\mathbb{1}_{T_\varepsilon}(\varphi)\frac{\|(-\Delta_L+1)^{-1}(\varphi-\varphi_L)\|^2}{\|(-\Delta_L+1)^{-1/2}(\varphi-\varphi_L)\|^2} \leq \mathbb{1}_{T_\varepsilon}(\varphi)\varepsilon^{-2},\end{aligned} \tag{3.4.24}$$

where we used that η is supported on T_ε and that χ is smooth and compactly supported. Therefore, using also the normalization of ψ_φ, we obtain

$$A_2 \lesssim \frac{1}{\alpha^4\varepsilon^2}\|\mathbb{1}_{T_\varepsilon}G\|^2_{L^2(\mathbb{R}^N)}. \tag{3.4.25}$$

We now need to bound $\|\mathbb{1}_{T_\varepsilon}G\|_{L^2(\mathbb{R}^N)}$ in terms of $\|\Psi\| = \|\eta G\|_{L^2(\mathbb{R}^N)}$. We define

$$S_\nu := \{\varphi \in \operatorname{ran}\Pi \mid \|\Pi'(\varphi-\varphi_L)\|_2 \leq \nu\} \tag{3.4.26}$$

and observe that on $S_\nu \cap T_\varepsilon$ we have, by the triangle inequality,

$$\|(-\Delta_L+1)^{-1/2}\Pi^L_\nabla\varphi\|_2 \leq \varepsilon+\nu, \tag{3.4.27}$$

and that on S_ν^c

$$G(\lambda) \leq \exp\Big(-\alpha^2\tau_L^{1/2}\nu^2\Big), \tag{3.4.28}$$

where we used that $[\Pi(\mathbb{1}-K_L)\Pi]^{1/2} \geq \tau_L^{1/2}\Pi'$ (with τ_L being the constant appearing in Proposition 3.3.5). We then have, using (3.4.27), that

$$\begin{aligned}\|\mathbb{1}_{T_\varepsilon}G\|_2^2 &= \|\mathbb{1}_{T_\varepsilon\cap S_\nu}G\|_2^2 + \|\mathbb{1}_{T_\varepsilon\cap S_\nu^c}G\|_2^2\\&\leq \int_{\{\|(-\Delta_L+1)^{-1/2}\Pi^L_\nabla\varphi\|_2\leq\varepsilon+\nu\}\cap S_\nu} G^2 d\lambda_1\dots d\lambda_N + \int_{T_\varepsilon\cap S_\nu^c} G^2 d\lambda_1\dots d\lambda_N.\end{aligned} \tag{3.4.29}$$

We now perform the change of variables $(\lambda_1,\lambda_2,\lambda_3) = 3(\lambda_1',\lambda_2',\lambda_3')$ in the first integral and the change of variables $\lambda-\lambda_L = 2(\lambda'-\lambda_L)$ in the second integral and fix $\nu = \varepsilon/8$, obtaining

$$\begin{aligned}\|\mathbb{1}_{T_\varepsilon}G\|_2^2 &\leq 27\int_{\{\|(-\Delta_L+1)^{-1/2}\Pi^L_\nabla\varphi\|_2\leq(\varepsilon+\nu)/3\}\cap S_\nu} G^2 d\lambda + 2^N\int_{T_{\varepsilon/2}\cap S^c_{\nu/2}} G(\lambda')^8 d\lambda'\\&\leq \Big(27+2^N\exp\Big(-6\alpha^2\tau_L^{1/2}\nu^2/4\Big)\Big)\int_{T_{\varepsilon/2}} G^2 d\lambda\\&\leq \Big(27+2^N\exp\Big(-6\alpha^2\tau_L^{1/2}\nu^2/4\Big)\Big)\|\Psi\|^2,\end{aligned} \tag{3.4.30}$$

where in the second step we used that $\{\|(-\Delta_L+1)^{-1/2}\Pi^L_\nabla\varphi\|_2 \leq (\varepsilon+\nu)/3\} \cap S_\nu \subset T_{\varepsilon/2}$ by the triangle inequality if $\nu=\varepsilon/8$, and (3.4.28) to estimate the Gaussian factor on $S^c_{\nu/2}$. Therefore, as long as $\sqrt{N} \leq C^1_L \alpha\varepsilon$ for a sufficiently small C^1_L, we conclude that

$$A_2 \lesssim \frac{1}{\alpha^4\varepsilon^2}\|\Psi\|^2. \tag{3.4.31}$$

Plugging estimates (3.4.17), (3.4.19), (3.4.23), and (3.4.31) into (3.4.13), we infer, for $\sqrt{N} \leq C^1_L\alpha\varepsilon$, that for a sufficiently large C^2_L

$$\frac{\langle\Psi|\mathbb{H}_L|\Psi\rangle}{\langle\Psi|\Psi\rangle} \leq e_L - \frac{1}{2\alpha^2}\operatorname{Tr}\Big(\Pi - [\Pi(\mathbb{1}-K_L)\Pi]^{1/2}\Big) + C^2_L(\varepsilon^3+\alpha^{-4}\varepsilon^{-2}). \tag{3.4.32}$$

We now proceed to choose a real orthonormal basis for $\operatorname{ran}\Pi$ which is convenient to bound the r.h.s. of (3.4.32). Let $\{g_j\}_{j\in\mathbb{N}}$ be an orthonormal basis of eigenfunctions of K_L with corresponding eigenvalue k_j, ordered such that $k_{j+1} \geq k_j$. By Proposition 3.3.5 we have $k_j = 1$ for $j=1,2,3$ and $k_j<1$ for $j>3$. Moreover, Π^L_∇ coincides with the projection onto $\operatorname{span}\{g_1,g_2,g_3\}$. We pick Π' to be the projection onto $\operatorname{span}\{g_4,\dots,g_N\}$ if φ_L is spanned by $\{g_1,\dots,g_N\}$ and onto $\operatorname{span}\{g_4,\dots,g_{N-1},\varphi_L\}$ otherwise. With this choice the eigenvalues μ_i of $\Pi(\mathbb{1}-K_L)\Pi$ appearing in the Gaussian factor G are equal to

$$\mu_j = 1-k_j, \quad j=1,\dots,N-1, \quad \mu_N = \begin{cases} 1-k_N & \text{if } \varphi_L \in \operatorname{span}\{g_1,\dots,g_N\}, \\ \langle\tilde\varphi_L|\mathbb{1}-K_L|\tilde\varphi_L\rangle & \text{otherwise,}\end{cases} \tag{3.4.33}$$

with $\tilde\varphi_L := \frac{\varphi_L - \sum_{j=4}^{N-1} g_j\langle g_j|\varphi_L\rangle}{\|\varphi_L - \sum_{j=4}^{N-1} g_j\langle g_j|\varphi_L\rangle\|_2}$. In any case

$$\begin{aligned}&\operatorname{Tr}\Big(\Pi - [\Pi(\mathbb{1}-K_L)\Pi]^{1/2}\Big)\\ &\geq \sum_{j=1}^{N-1}(1-(1-k_j)^{1/2}) = \operatorname{Tr}\Big(\mathbb{1}-(\mathbb{1}-K_L)^{1/2}\Big) - \sum_{j=N}^{\infty}(1-(1-k_j)^{1/2}).\end{aligned} \tag{3.4.34}$$

In order to estimate $\sum_{j=N}^\infty(1-(1-k_j)^{1/2})$, we note that Lemma 3.3.10 implies that $k_j \lesssim_L (l_j+1)^{-2}$, where l_j denotes the ordered eigenvalues of $-\Delta_L$. Since $l_j \sim j^{2/3}$ for $j \gg 1$, we have

$$\sum_{j=N}^{\infty}(1-(1-k_j)^{1/2}) \lesssim_L N^{-1/3}. \tag{3.4.35}$$

This allows us to conclude that

$$\frac{\langle\Psi|\mathbb{H}_L|\Psi\rangle}{\langle\Psi|\Psi\rangle} \leq e_L - \frac{1}{2\alpha^2}\operatorname{Tr}\Big(\mathbb{1}-(\mathbb{1}-K_L)^{1/2}\Big) + C^3_L(\varepsilon^3+\alpha^{-4}\varepsilon^{-2}+\alpha^{-2}N^{-1/3}), \tag{3.4.36}$$

as long as $\sqrt{N} \leq C^1_L\alpha\varepsilon$. The error term is minimized, under this constraint, for $\varepsilon \sim \alpha^{-8/11}$ and $N \sim \alpha^2\varepsilon^2 \sim \alpha^{6/11}$, which yields

$$\frac{\langle\Psi|\mathbb{H}_L|\Psi\rangle}{\langle\Psi|\Psi\rangle} \leq e_L - \frac{1}{2\alpha^2}\operatorname{Tr}\Big(\mathbb{1}-(\mathbb{1}-K_L)^{1/2}\Big) + C_L\alpha^{-24/11}, \tag{3.4.37}$$

as claimed in (3.2.24).

3.4.2 The Cutoff Hamiltonian

As a first step to derive the lower bound in (3.2.24), we show that it is possible to apply an ultraviolet cutoff of size Λ to $\mathbb{H}_L$ at an expense of order $\Lambda^{-5/2}$ (this is proven in Proposition 3.4.3 in Section 3.4.2). Our approach follows closely the one in [41]. It relies on an application of a triple Lieb–Yamazaki bound (extending the method of [83]) which we carry out in Section 3.4.2), and on a consequent use (in Section 3.4.2) of a Gross transformation [58, 94].

We shall in the following, for any *real-valued* $f \in L^2(\mathbb{T}_L^3)$, denote

$$\Phi(f) := a^\dagger(f) + a(f), \tag{3.4.38}$$
$$\Pi(f) := \Phi(if) = i(a^\dagger(f) - a(f)). \tag{3.4.39}$$

We recall that the interaction term in the Fröhlich Hamiltonian is given by

$$-a^\dagger(v_L^x) - a(v_L^x) = -\Phi(v_L^x), \tag{3.4.40}$$

where v_L was defined in (3.2.3) and a and $a^\dagger$ satisfy the rescaled commutation relations (3.2.5). We shall apply an ultraviolet cutoff of size Λ in k-space, which amounts to substituting the interaction term with

$$-a^\dagger(v_{L,\Lambda}^x) - a(v_{L,\Lambda}^x) = -\Phi(v_{L,\Lambda}^x), \tag{3.4.41}$$

where

$$v_{L,\Lambda}(y) := \sum_{\substack{0\neq k \in \frac{2\pi}{L}\mathbb{Z}^3 \\ |k|<\Lambda}} \frac{1}{|k|} \frac{e^{-ik\cdot y}}{L^3}. \tag{3.4.42}$$

To quantify the expense of such a cutoff we clearly need to bound

$$-a^\dagger(w_{L,\Lambda}^x) - a(w_{L,\Lambda}^x) = -\Phi(w_{L,\Lambda}^x), \tag{3.4.43}$$

where

$$w_{L,\Lambda}(y) = v_L(y) - v_{L,\Lambda}(y) = \sum_{\substack{k \in \frac{2\pi}{L}\mathbb{Z}^3 \\ |k|\geq\Lambda}} \frac{1}{|k|} \frac{e^{-ik\cdot y}}{L^3}. \tag{3.4.44}$$

Triple Lieb–Yamazaki Bounds

Let us introduce the notation $p = (p_1, p_2, p_3) = -i\nabla_x$ for the electron momentum operator. Note that on any function of the form $f(x, y) = f(y - x)$, such as $w_{L,\Lambda}^x$ for example, the operator p simply acts as multiplication by k in k-space and agrees, up to a sign, with $-i\nabla_y$.

The purpose of this section is to prove the following Proposition.

Proposition 3.4.1. *Let* $w_{L,\Lambda}$ *be defined as in* (3.4.44) *and* $\Lambda > 1$. *Then*

$$a^\dagger(w_{L,\Lambda}^x) + a(w_{L,\Lambda}^x) = \Phi(w_{L,\Lambda}^x) \lesssim (|p|^2 + \mathbb{N} + 1)^2(\Lambda^{-5/2} + \alpha^{-1}\Lambda^{-3/2}), \tag{3.4.45}$$

as quadratic forms on $L^2(\mathbb{T}_L^3) \otimes \mathcal{F}(L^2(\mathbb{T}_L^3))$.

We first need the following Lemma.

Lemma 3.4.1. *Let $w_{L,\Lambda}$ be defined as in* (3.4.44) *and $\Lambda > 1$. Then for any $j,l,m \in \{1,2,3\}$*

$$a^\dagger\left[(\partial_j\partial_l\partial_m(-\Delta_L)^{-3}w_{L,\Lambda})^x\right] a\left[(\partial_j\partial_l\partial_m(-\Delta_L)^{-3}w_{L,\Lambda})^x\right] \lesssim \Lambda^{-5}\mathbb{N}, \tag{3.4.46}$$

$$\|\partial_j\partial_l(-\Delta_L)^{-2}w_{L,\Lambda}\|^2_{L^2(\mathbb{T}^3_L)} \lesssim \Lambda^{-3}, \tag{3.4.47}$$

$$a^\dagger\left[(\partial_j\partial_l(-\Delta_L)^{-2}w_{L,\Lambda})^x\right] a\left[(\partial_j\partial_l(-\Delta_L)^{-2}w_{L,\Lambda})^x\right] \lesssim \Lambda^{-5}(|p|^2 + L^{-3}\Lambda^{-1})\mathbb{N}, \tag{3.4.48}$$

as quadratic forms on $L^2(\mathbb{T}^3_L) \otimes \mathcal{F}(L^2(\mathbb{T}^3_L))$.

Proof. For any $j,l,m \in \{1,2,3\}$, (3.4.46) follows from $a^\dagger(g)a(g) \le \|g\|_2^2\mathbb{N}$ for $g \in L^2(\mathbb{T}^3_L)$, and then proceeding along the same lines of the proof of (3.4.47). To prove (3.4.47) we estimate

$$\|\partial_j\partial_l(-\Delta_L)^{-2}w_{L,\Lambda}\|^2_{L^2(\mathbb{T}^3_L)} = \frac{1}{L^3}\sum_{\substack{|k|\ge\Lambda \\ k\in\frac{2\pi}{L}\mathbb{Z}^3}} \frac{k_j^2k_l^2}{|k|^{10}} \lesssim \int_{B^c_\Lambda}\frac{1}{|t|^6}dt = \frac{4\pi}{3}\Lambda^{-3}. \tag{3.4.49}$$

If we denote $f^x_{j,l} := (-\partial_j\partial_l(-\Delta_L)^{-2}w_{L,\Lambda})^x$, in order to show (3.4.48) it suffices to prove that

$$\left|f^x_{j,l}\right\rangle\left\langle f^x_{j,l}\right| \lesssim \Lambda^{-5}\left(|p|^2 + \Lambda^{-1}\right) \quad \text{on} \quad L^2(\mathbb{T}^3_L)\otimes L^2(\mathbb{T}^3_L), \tag{3.4.50}$$

where the bracket notation refers to the second factor in the tensor product, i.e., the left side is a rank-one projection on the second factor parametrized by x, which acts via multiplication on the first factor. For any $\Psi \in L^2(\mathbb{T}^3_L)\otimes L^2(\mathbb{T}^3_L)$ with Fourier coefficients $\Psi_{q,k}$, we have

$$\begin{aligned}
&\left\langle\Psi\middle|\left|f^x_{j,l}\right\rangle\left\langle f^x_{j,l}\right|\middle|\Psi\right\rangle = \int dx\left|\int dy\overline{f^x_{j,l}(y)}\Psi(x,y)\right|^2 = \sum_{q\in\frac{2\pi}{L}\mathbb{Z}^3}\left|\sum_{\substack{k\in\frac{2\pi}{L}\mathbb{Z}^3\\|k|\ge\Lambda}}\frac{k_jk_l}{L^{3/2}|k|^5}\Psi_{q-k,k}\right|^2 \\
&\le \left[\sum_{q\in\frac{2\pi}{L}\mathbb{Z}^3}\left(\sum_{\substack{k\in\frac{2\pi}{L}\mathbb{Z}^3\\|k|\ge\Lambda,\ k\ne q}}\frac{1}{L^3|k|^6|q-k|^2}\right)\left(\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3}|q-k|^2|\Psi_{q-k,k}|^2\right) + \sum_{\substack{q\in\frac{2\pi}{L}\mathbb{Z}^3\\|q|\ge\Lambda}}\frac{|\Psi_{0,q}|^2}{L^3|q|^6}\right] \\
&\le \sup_{q\in\frac{2\pi}{L}\mathbb{Z}^3}\left(\sum_{\substack{k\in\frac{2\pi}{L}\mathbb{Z}^3\\|k|\ge\Lambda,\ k\ne q}}\frac{L^{-3}}{|k|^6|q-k|^2}\right)\langle\Psi||p|^2|\Psi\rangle + L^{-3}\Lambda^{-6}\|\Psi\|^2 \\
&\lesssim \langle\Psi|\Lambda^{-5}(|p|^2 + L^{-3}\Lambda^{-1})|\Psi\rangle,
\end{aligned} \tag{3.4.51}$$

which shows our claim. We only need to justify the last step, i.e., that the supremum appearing in (3.4.51) is bounded by $C\Lambda^{-5}$. We have

$$\begin{aligned}
\sum_{\substack{0\ne k\in\frac{2\pi}{L}\mathbb{Z}^3\\|k|\ge\Lambda,\ k\ne q}}\frac{L^{-3}}{|k|^6|q-k|^2} &\lesssim \int_{B^c_\Lambda}\frac{1}{|x|^6|q-x|^2}dx = \Lambda^{-5}\int_{B^c_1}\frac{1}{|x|^6|\Lambda^{-1}q-x|^2} \\
&\le \Lambda^{-5}\left(\int_{B_1(\Lambda^{-1}q)}\frac{1}{|\Lambda^{-1}q-x|^2} + \int_{B^c_1}|x|^{-6}\right) \le \frac{16\pi}{3}\Lambda^{-5}.
\end{aligned} \tag{3.4.52}$$

This concludes the proof. □

We are now able to prove Proposition 3.4.1.

Proof of Proposition 3.4.1. Following the approach by Lieb and Yamazaki in [83], we have

$$\sum_{j=1}^{3}[p_j, a(p_j|p|^{-2}w^x_{L,\Lambda})] = -a(w^x_{L,\Lambda}). \tag{3.4.53}$$

Applying this three times, we obtain

$$\sum_{j,k,l=1}^{3} [p_j, [p_k, [p_l, a(p_jp_kp_l|p|^{-6}w^x_{L,\Lambda})]]] = -a(w^x_{L,\Lambda}). \tag{3.4.54}$$

Similarly,

$$\sum_{j,k,l=1}^{3} [p_j, [p_k, [p_l, a^\dagger(p_jp_kp_l|p|^{-6}w^x_{L,\Lambda})]]] = a^\dagger(w^x_{L,\Lambda}). \tag{3.4.55}$$

Therefore, if we define

$$\begin{aligned} B_{jkl} &:= a^\dagger(p_jp_kp_l|p|^{-6}w^x_{L,\Lambda}) - a(p_jp_kp_l|p|^{-6}w^x_{L,\Lambda}) \\ &= a^\dagger\left[(\partial_j\partial_l\partial_m(-\Delta_L)^{-3}w_{L,\Lambda})^x\right] - a\left[(\partial_j\partial_l\partial_m(-\Delta_L)^{-3}w_{L,\Lambda})^x\right], \end{aligned} \tag{3.4.56}$$

we have

$$a^\dagger(w^x_{L,\Lambda}) + a(w^x_{L,\Lambda}) = \Phi(w^x_{L,\Lambda}) = \sum_{j,k,l=1}^{3} [p_j, [p_k, [p_l, B_{jkl}]]]. \tag{3.4.57}$$

Using that $B^\dagger_{jkl} = -B_{jkl}$ and that B_{jkl} is invariant under exchange of indices, we arrive at

$$\Phi(w^x_{L,\Lambda}) = \sum_{j,k,l=1}^{3} \left(p_jp_k[p_l, B_{jkl}] + [B^\dagger_{jkl}, p_l]p_jp_k\right) - 2\sum_{j,k,l=1}^{3} \left(p_jp_kB_{jkl}p_l + p_lB^\dagger_{jkl}p_jp_k\right). \tag{3.4.58}$$

By the Cauchy–Schwarz inequality, we have for any $\lambda > 0$

$$-p_jp_kB_{jkl}p_l - p_lB^\dagger_{jkl}p_jp_k \le \lambda p_j^2p_k^2 + \lambda^{-1}p_lB^\dagger_{jkl}B_{jkl}p_l. \tag{3.4.59}$$

Moreover, using (3.4.46) and the rescaled commutation relations (3.2.5) satisfied by a and $a^\dagger$, we have

$$B^\dagger_{jkl}B_{jkl} \le C\left(4\mathbb{N} + 2\alpha^{-2}\right)\Lambda^{-5}. \tag{3.4.60}$$

Using (3.4.59) and (3.4.60) and picking $\lambda = C^{1/2}\Lambda^{-5/2}$ we conclude that

$$-2\sum_{j,k,l=1}^{3} \left(p_jp_kB_{jkl}p_l + p_lB^\dagger_{jkl}p_jp_k\right) \lesssim \Lambda^{-5/2}\left(|p|^4 + 3|p|^2(4\mathbb{N} + 2\alpha^{-1})\right). \tag{3.4.61}$$

We now define

$$\begin{aligned} C_{jk} &:= \sum_{l=1}^{3}[p_l, B_{jkl}] = a^\dagger(p_jp_k|p|^{-4}w^x_{L,\Lambda}) + a(p_jp_k|p|^{-4}w^x_{L,\Lambda}) \\ &= a^\dagger\left[(\partial_j\partial_k(-\Delta_L)^{-2}w_{L,\Lambda})^x\right] + a\left[(\partial_j\partial_k(-\Delta_L)^{-2}w_{L,\Lambda})^x\right] = C^\dagger_{jk}. \end{aligned} \tag{3.4.62}$$

Using (3.4.47), (3.4.48) and the Cauchy-Schwarz inequality, we have for any $\lambda > 0$

$$p_j p_k C_{jk} + C_{jk} p_j p_k \leq \lambda p_j^2 p_k^2 + \lambda^{-1} C_{jk}^2. \tag{3.4.63}$$

Moreover,

$$\begin{aligned} C_{jk}^2 &\leq 4a^\dagger(p_j p_k |p|^{-4} w_{L,\Lambda}^x) a(p_j p_k |p|^{-4} w_{L,\Lambda}^x) + 2\alpha^{-2} \| p_j p_k |p|^{-4} w_{L,\Lambda}^x \|_2^2 \\ &\lesssim \Lambda^{-5}(|p|^2 + \Lambda^{-1})\mathbb{N} + \alpha^{-2}\Lambda^{-3}. \end{aligned} \tag{3.4.64}$$

Picking $\lambda = \Lambda^{-5/2} + \alpha^{-1}\Lambda^{-3/2}$, we therefore conclude that

$$\begin{aligned} &\sum_{j,k,l=1}^{3} \Big(p_j p_k [p_l, B_{jkl}] + [B_{jkl}^\dagger, p_l] p_j p_k \Big) \\ &\lesssim (\Lambda^{-5/2} + \alpha^{-1}\Lambda^{-3/2})[|p|^4 + \mathbb{N}(|p|^2 + L^{-3}\Lambda^{-1}) + 1]. \end{aligned} \tag{3.4.65}$$

Applying (3.4.61) and (3.4.65) in (3.4.58), we finally obtain

$$\begin{aligned} \Phi(w_{L,\Lambda}^x) &\lesssim (\Lambda^{-5/2} + \alpha^{-1}\Lambda^{-3/2}) \Big[|p|^4 + \mathbb{N}(|p|^2 + L^{-3}\Lambda^{-1}) + 1 \Big] \\ &\quad + \Lambda^{-5/2} \Big(|p|^4 + 3|p|^2(4\mathbb{N} + 2\alpha^{-1}) \Big) \\ &\lesssim (|p|^2 + \mathbb{N} + 1)^2 (\Lambda^{-5/2} + \alpha^{-1}\Lambda^{-3/2}), \end{aligned} \tag{3.4.66}$$

as claimed. □

Gross Transformation

The bound (3.4.45), derived in Proposition 3.4.1, is not immediately useful as it stands. In order to relate the r.h.s. of (3.4.45) to the square of the Fröhlich Hamiltonian $\mathbb{H}_L$ in (3.2.4), we shall apply a Gross transformation [58], [94].

For a real-valued $f \in H^1(\mathbb{T}_L^3)$, recalling that $f^x(\,\cdot\,) = f(\,\cdot - x)$, we consider the following unitary transformation on $L^2(\mathbb{T}_L^3) \otimes \mathcal{F}$

$$U = e^{a(\alpha^2 f^x) - a^\dagger(\alpha^2 f^x)} = e^{i\Pi(\alpha^2 f^x)}, \tag{3.4.67}$$

where U is understood to act as a 'multiplication' with respect to the x variable. For any $g \in L^2(\mathbb{T}_L^3)$, we have

$$U a(g) U^\dagger = a(g) + \langle g | f^x \rangle \quad \text{and} \quad U a^\dagger(g) U^\dagger = a^\dagger(g) + \langle f^x | g \rangle\,, \tag{3.4.68}$$

and therefore

$$U \mathbb{N} U^\dagger = \mathbb{N} + \Phi(f^x) + \|f\|_2^2. \tag{3.4.69}$$

Moreover,

$$U p U^\dagger = p + \alpha^2 \Phi(p f^x) = p + \alpha^2 \Phi[(i\nabla f)^x]. \tag{3.4.70}$$

This implies that

$$U p^2 U^\dagger = p^2 + \alpha^4 (\Phi[(i\nabla f)^x])^2 + 2\alpha^2 p \cdot a[(i\nabla f)^x] + 2\alpha^2 a^\dagger[(i\nabla f)^x] \cdot p + \alpha^2 \Phi[(-\Delta_L f)^x]. \tag{3.4.71}$$

Therefore, we also have

$$U\mathbb{H}_L U^\dagger = |p|^2 + \alpha^4(\Phi[(i\nabla f)^x])^2 + 2\alpha^2 p\cdot a[(i\nabla f)^x] + 2\alpha^2 a^\dagger[(i\nabla f)^x]\cdot p \\ + \Phi[(-\alpha^2\Delta_L f + f - v_L)^x] + \mathbb{N} + \|f\|_2^2 - 2\langle v_L|f\rangle . \tag{3.4.72}$$

We denote

$$g = -\alpha^2\Delta_L f + f - v_L, \tag{3.4.73}$$

and we shall pick

$$f(y) = \left[(-\alpha^2\Delta_L+1)^{-1}(-\Delta_L)^{-1/2}\chi_{B^c_{K^2}}(-\Delta_L)\right](0,y) \\ = \sum_{\substack{|k|\geq K\\ k\in\frac{2\pi}{L}\mathbb{Z}^3}} \frac{1}{(\alpha^2|k|^2+1)|k|}\frac{e^{-ik\cdot y}}{L^3} \tag{3.4.74}$$

for some $K>0$. Recalling (3.4.42), this implies that

$$g(y) = -v_{L,K}(y) = -\sum_{\substack{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3\\ |k|<K}} \frac{1}{|k|}\frac{e^{-ik\cdot y}}{L^3}. \tag{3.4.75}$$

For simplicity we suppress the dependence on K in the notation for f and g, but we will keep track of the parameter K by denoting the operator U related to this choice of f (depending on α and K) via (3.4.67) by U_α^K. We shall need the following estimates for norms involving f and g. We have

$$\|g\|_2^2 = \sum_{\substack{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3\\ |k|<K}} \frac{1}{L^3|k|^2} \lesssim K, \tag{3.4.76}$$

$$\|f\|_2^2 = \sum_{\substack{0\neq k\in\frac{2\pi}{L}\mathbb{Z}^3\\ |k|\geq K}} \frac{1}{L^3|k|^2(\alpha^2|k|^2+1)^2} \lesssim \alpha^{-4}\int_{B_K^c}\frac{1}{|t|^6}dt \lesssim \alpha^{-4}K^{-3}, \tag{3.4.77}$$

$$\langle v_L|f\rangle = \sum_{\substack{k\in\frac{2\pi}{L}\mathbb{Z}^3\\ |k|\geq K}} \frac{1}{L^3|k|^2(\alpha^2|k|^2+1)} \lesssim \alpha^{-2}\int_{B_K^c}\frac{1}{|t|^4}dt \lesssim \alpha^{-2}K^{-1}, \tag{3.4.78}$$

$$\|\nabla f\|_2^2 = \sum_{\substack{k\in\frac{2\pi}{L}\mathbb{Z}^3\\ |k|\geq K}} \frac{1}{L^3(\alpha^2|k|^2+1)^2} \lesssim \alpha^{-4}\int_{B_K^c}\frac{1}{|t|^4}dt \lesssim \alpha^{-4}K^{-1}. \tag{3.4.79}$$

We now state and prove the main result of this subsection, the proof of which follows the approach used in [57] for the analogous statement on $\mathbb{R}^3$, and in [41] for the analogous statement on a domain with Dirichlet boundary conditions.

Proposition 3.4.2. *For any $\varepsilon>0$ there exist $K_\varepsilon>0$ and $C_\varepsilon>0$ such that, for all $\alpha\gtrsim 1$ and any $\Psi\in L^2(\mathbb{T}_L^3)\otimes\mathcal{F}$ in the domain of $|p|^2+\mathbb{N}$*

$$(1-\varepsilon)\|(|p|^2+\mathbb{N})\Psi\| - C_\varepsilon\|\Psi\| \leq \|U_\alpha^{K_\varepsilon}\mathbb{H}_L(U_\alpha^{K_\varepsilon})^\dagger\Psi\| \leq (1+\varepsilon)\|(|p|^2+\mathbb{N})\Psi\| + C_\varepsilon\|\Psi\|. \tag{3.4.80}$$

Proof. We shall use the following standard (given the rescaled commutation relations satisfied by a and $a^\dagger$) properties, which hold for any $\Psi \in \mathcal{F}$, any $f \in L^2(\mathbb{T}^3_L)$ and any function $h : [0,\infty) \to \mathbb{R}$

$$\|a(f)\Psi\| \le \|f\|_2 \|\sqrt{\mathbb{N}}\Psi\|, \quad \|a^\dagger(f)\Psi\| \le \|f\|_2 \|\sqrt{\mathbb{N}+\alpha^{-2}}\Psi\|, \tag{3.4.81}$$
$$h(\mathbb{N}+\alpha^{-2})a = a h(\mathbb{N}), \quad h(\mathbb{N})a^\dagger = a^\dagger h(\mathbb{N}+\alpha^{-2}). \tag{3.4.82}$$

It is then straightforward, with the aid of the estimates (3.4.76), (3.4.77), (3.4.78) and (3.4.79), to show, for any $\Psi \in L^2(\mathbb{T}^3_L)\otimes \mathcal{F}$, any $\delta > 0$ and any $K > 0$, that

$$\alpha^4 \|(\Phi[(i\nabla f)^x])^2\Psi\| \lesssim \alpha^4 \|\nabla f\|^2 \|(\mathbb{N}+\alpha^{-2})\Psi\| \lesssim K^{-1}\|(\mathbb{N}+\alpha^{-2})\Psi\|, \tag{3.4.83}$$
$$\|\Phi(g^x)\Psi\| \lesssim K^{1/2}\|\sqrt{\mathbb{N}+\alpha^{-2}}\Psi\| \lesssim \delta\|(\mathbb{N}+\alpha^{-2})\Psi\| + \delta^{-1}K\|\Psi\|, \tag{3.4.84}$$
$$\alpha^2\|a^\dagger[(i\nabla f)^x]\cdot p\Psi\| \lesssim K^{-1/2}\|\sqrt{\mathbb{N}+\alpha^{-2}}\sqrt{|p|^2}\Psi\| \lesssim K^{-1/2}\|(|p|^2+\mathbb{N}+\alpha^2)\Psi\|. \tag{3.4.85}$$

It remains to bound the term

$$\|\alpha^2 p\cdot a[(i\nabla f)^x]\Psi\| \le \|\alpha^2 a[(i\nabla f)^x]\cdot p\Psi\| + \|a[(-\alpha^2\Delta_L f)^x]\Psi\| =: (\mathrm{I}) + (\mathrm{II}). \tag{3.4.86}$$

As in (3.4.85), we can easily bound

$$(\mathrm{I}) \lesssim K^{-1/2}\|(|p|^2+\mathbb{N}+\alpha^{-2})\Psi\|. \tag{3.4.87}$$

By (3.4.73) and (3.4.75) and recalling (3.4.42) and (3.4.44), we have

$$a[(-\alpha^2\Delta_L f)^x] = a[(g-f+v_L)^x] = -a(f^x) + a(w^x_{L,K}). \tag{3.4.88}$$

With the same arguments used in the proof of Lemma 3.4.1 we obtain

$$\|a(w^x_{L,K})\Psi\| \lesssim K^{-1/2}\|\sqrt{\mathbb{N}(|p|^2+K^{-1})}\Psi\|, \tag{3.4.89}$$

and therefore, using (3.4.77) to bound $\|a(f^x)\Psi\|$, we arrive at

$$\begin{aligned}(II) &\lesssim \alpha^{-2}K^{-3/2}\|\sqrt{\mathbb{N}}\Psi\| + K^{-1/2}\|\sqrt{\mathbb{N}(|p|^2+K^{-1})}\Psi\| \\ &\lesssim \alpha^{-2}K^{-3/2}(\|(\mathbb{N}+\alpha^{-2})\Psi\| + \|\Psi\|) + K^{-1/2}\|(|p|^2+\mathbb{N}+K^{-1})\Psi\|.\end{aligned} \tag{3.4.90}$$

Combining (3.4.83), (3.4.84), (3.4.85), (3.4.87), (3.4.90), (3.4.77) and (3.4.78) with (3.4.72), we obtain, for any $K \ge 1$

$$\|U^K_\alpha \mathbb{H}_L (U^k_\alpha)^\dagger\Psi\| \le [1 + C(K^{-1/2}+\delta)]\|(|p|^2+\mathbb{N})\Psi\| + C(\delta^{-1}K + 3\alpha^{-2}K^{-1})\|\Psi\|, \tag{3.4.91}$$
$$\|U^K_\alpha \mathbb{H}_L (U^K_\alpha)^\dagger\Psi\| \ge [1 - C(K^{-1/2}+\delta)]\|(|p|^2+\mathbb{N})\Psi\| - C(\delta^{-1}K + 3\alpha^{-2}K^{-1})\|\Psi\|, \tag{3.4.92}$$

which allows to conclude the proof by picking $K_\varepsilon \sim \varepsilon^{-2}$, $\delta \sim \varepsilon$ and $C_\varepsilon \sim \varepsilon^{-3}$. □

Remark 3.4.1. *Proposition 3.4.2 has as an important consequence the fact that the ground state energy of $\mathbb{H}_L$ is uniformly bounded for $\alpha \gtrsim 1$.*

Final Estimates for Cut-off Hamiltonian

With Propositions 3.4.1 and 3.4.2 at hand, we are finally ready to prove the main result of this section. Note that all the estimates performed in this section are actually independent of L.

Proposition 3.4.3. *Let*

$$\mathbb{H}_L^\Lambda = -\Delta_L - \Phi(v_{L,\Lambda}^x) + \mathbb{N}, \tag{3.4.93}$$

where $v_{L,\Lambda}$ is defined in (3.4.42)*. Then, for any $\Lambda \gtrsim 1$ and $\alpha \gtrsim 1$,*

$$\inf \operatorname{spec} \mathbb{H}_L - \inf \operatorname{spec} \mathbb{H}_L^\Lambda \gtrsim -(\Lambda^{-5/2} + \alpha^{-1}\Lambda^{-3/2} + \alpha^{-2}\Lambda^{-1}). \tag{3.4.94}$$

Note that for the error term introduced in (3.4.94) to be negligible compared to α^{-2} it suffices to pick $\Lambda \gg \alpha^{4/5}$.

Proof. We begin by recalling that Proposition 3.4.1 implies that

$$a(w_{L,\Lambda}^x) + a^\dagger(w_{L,\Lambda}^x) = \Phi(w_{L,\Lambda}^x) \lesssim (\Lambda^{-5/2} + \alpha^{-1}\Lambda^{-3/2})(|p|^2 + \mathbb{N} + 1)^2. \tag{3.4.95}$$

Applying the unitary Gross transformation U_α^K introduced in the previous subsection (with f defined in (3.4.74) and K large enough for Proposition 3.4.2 to hold for some $0 < \varepsilon < 1$) to both sides of the previous inequality and recalling (3.4.68), we obtain

$$\begin{aligned}(U_\alpha^K)^\dagger \Phi(w_{L,\Lambda}^x) U_\alpha^K &= \Phi(w_{L,\Lambda}^x) + 2\langle f | w_{L,\Lambda}\rangle \\ &\lesssim (\Lambda^{-5/2} + \alpha^{-1}\Lambda^{-3/2})(U_\alpha^K)^\dagger (|p|^2 + \mathbb{N} + 1)^2 U_\alpha^K.\end{aligned} \tag{3.4.96}$$

Proposition 3.4.2 implies that

$$(U_\alpha^K)^\dagger (|p|^2 + \mathbb{N} + 1)^2 U_\alpha^K \lesssim (\mathbb{H}_L + C)^2, \tag{3.4.97}$$

where C is a positive constant (independent of α for $\alpha \gtrsim 1$). Recalling the definitions of f and $w_{L,\Lambda}$ we also have

$$|\langle f | w_{L,\Lambda}\rangle| \le \sum_{\substack{0 \neq k \in \frac{2\pi}{L}\mathbb{Z}^3 \\ |k| > \Lambda}} \frac{1}{L^3(\alpha^2|k|^2 + 1)|k|^2} \lesssim \alpha^{-2}\Lambda^{-1}, \tag{3.4.98}$$

and this allows us to conclude, in combination with (3.4.96) and (3.4.97), that

$$\Phi(w_{L,\Lambda}^x) \lesssim (\Lambda^{-5/2} + \alpha^{-1}\Lambda^{-3/2} + \alpha^{-2}\Lambda^{-1})(\mathbb{H}_L + C)^2. \tag{3.4.99}$$

Hence

$$\langle \Psi | \mathbb{H}_L | \Psi \rangle \ge \langle \Psi | \mathbb{H}_L^\Lambda | \Psi \rangle - (\Lambda^{-5/2} + \alpha^{-1}\Lambda^{-3/2} + \alpha^{-2}\Lambda^{-1}) \langle \Psi | (\mathbb{H}_L + C)^2 | \Psi \rangle. \tag{3.4.100}$$

By Remark 3.4.1, to compute the ground state energy of $\mathbb{H}_L$ it is clearly sufficient to restrict to the spectral subspace relative to $|\mathbb{H}_L| \le C$ for some suitable C, which then yields (3.4.94). This concludes the proof and the section. □

3.4.3 Final Lower Bound

In this section we show the validity of the lower bound in (3.2.24), thus completing the proof of Theorem 3.2.2. With Proposition 3.4.3 at hand, we have good estimates on the cost of substituting $\mathbb{H}_L$ with $\mathbb{H}_L^\Lambda$ and, in particular, we know that the difference between the ground state energies of the two is negligible for $\Lambda \gg \alpha^{4/5}$. We are thus left with the task of giving a lower bound on $\inf \operatorname{spec} \mathbb{H}_L^\Lambda$.

While the previous steps in the lower bound follow closely the analogous strategy in [41], the translation invariance of our model leads to substantial complications in the subsequent steps, and the analysis given in this subsection is the main novel part of our proof. In contrast to the case considered in [41], the set of minimizers $\mathcal{M}_L^{\mathcal{F}} = \Omega_L(\varphi_L)$ is a three-dimensional manifold, and in order to decouple the resulting zero-modes of the Hessian of the Pekar functional we find it necessary introduce a suitable diffeomorphism that 'flattens' the manifold of minimizers and the region close to it. Special attention also has to be paid on the metric in which this closeness is measured, necessitating the introduction of the family of norms in (3.3.188).

We emphasize that the non-uniformity in L also results from the subsequent analysis, where the compactness of resolvent of $-\Delta_L$ enters in an essential way.

Let Π denote the projection

$$\operatorname{ran}\Pi = \operatorname{span}\left\{L^{-3/2}e^{ik\cdot x},\ k \in \frac{2\pi}{L}\mathbb{Z}^3,\ |k| \le \Lambda\right\}, \quad N = \dim_{\mathbb{C}} \operatorname{ran}\Pi. \tag{3.4.101}$$

For later use we note that

$$N \sim \left(\frac{L}{2\pi}\right)^3 \Lambda^3 \quad \text{as } \Lambda \to \infty. \tag{3.4.102}$$

The Fock space $\mathcal{F}(L^2(\mathbb{T}_L^3))$ naturally factorizes into the tensor product $\mathcal{F}(\Pi L^2(\mathbb{T}_L^3)) \otimes \mathcal{F}((\mathbb{1} - \Pi)L^2(\mathbb{T}_L^3))$ and $\mathbb{H}_L^\Lambda$ is of the form $\mathbb{A} \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{N}^>$, with $\mathbb{A}$ acting on $L^2(\mathbb{T}_L^3) \otimes \mathcal{F}(\Pi L^2(\mathbb{T}_L^3))$ and $\mathbb{N}^>$ being the number operator on $\mathcal{F}((\mathbb{1} - \Pi)L^2(\mathbb{T}_L^3))$. In particular, $\inf \operatorname{spec} \mathbb{H}_L^\Lambda = \inf \operatorname{spec} \mathbb{A}$.

As in Section 3.4.1, we can, for any L^2-orthonormal basis of real-valued functions $\{f_n\}$ of $\operatorname{ran}\Pi$, identify $\mathcal{F}(\Pi L^2(\mathbb{T}_L^3))$ with $L^2(\mathbb{R}^N)$ through the Q-space representation (see [100]). In particular, any real-valued $\varphi \in \operatorname{ran}\Pi$ corresponds to a point $\lambda \in \mathbb{R}^N$ via

$$\varphi = \Pi\varphi = \sum_{n=1}^N \lambda_n f_n \cong (\lambda_1, \dots, \lambda_N) = \lambda. \tag{3.4.103}$$

Note that, compared to Section 3.4.1, we are using a different choice of Π here for the decomposition $L^2(\mathbb{T}_L^3) = \operatorname{ran}\Pi \oplus (\operatorname{ran}\Pi)^\perp$.

In the representation given by (3.4.103), the operator $\mathbb{A}$ is given by

$$\mathbb{A} = -\Delta_L + V_\varphi(x) + \sum_{n=1}^N \left(-\frac{1}{4\alpha^4}\partial_{\lambda_n}^2 + \lambda_n^2 - \frac{1}{2\alpha^2}\right) \tag{3.4.104}$$

on $L^2(\mathbb{T}_L^3) \otimes L^2(\mathbb{R}^N)$. For a lower bound, we can replace $h_\varphi = -\Delta_L + V_\varphi$ with the infimum of its spectrum $e(\varphi)$, obtaining

$$\inf \operatorname{spec} \mathbb{H}_L^\Lambda \ge \inf \operatorname{spec} \mathbb{K}, \tag{3.4.105}$$

where $\mathbb{K}$ is the operator on $L^2(\mathbb{R}^N)$ defined as

$$\mathbb{K} = -\frac{1}{4\alpha^4}\sum_{n=1}^{N}\partial_{\lambda_n}^2 - \frac{N}{2\alpha^2} + \mathcal{F}_L(\varphi) = \frac{1}{4\alpha^4}(-\Delta_\lambda) - \frac{N}{2\alpha^2} + \mathcal{F}_L(\lambda), \tag{3.4.106}$$

where $\mathcal{F}_L$, which is understood as a multiplication operator in (3.4.106), can be seen as a function of $\varphi \in \mathrm{span}_{\mathbb{R}}\{f_j\}_{j=1}^N$ or $\lambda \in \mathbb{R}^N$ through the identification (3.4.103).

Using IMS localization we shall split $\mathbb{R}^N$ into two regions, one localized around the surface of minimizers of $\mathcal{F}_L$, i.e., $\mathcal{M}_L^{\mathcal{F}} = \Omega_L(\varphi_L)$, and the other localized away from it. On each of these regions we can bound $\mathcal{F}_L$ from below with the estimates contained in Proposition 3.3.4 and in Corollary 3.2.1, respectively. Because of the prefactor α^{-4} in front of $-\Delta_\lambda$ the outer region turns out to be negligible compared to the inner one (at least if we define the inner and outer region with respect to an appropriate norm). At the same time, employing an appropriate diffeomorphism, the inner region can be treated as if $\Omega_L(\varphi_L)$ was a a flat torus, leading to a system of harmonic oscillators whose ground state energy can be calculated explicitly.

The start be specifying the norm with respect to which we measure closeness to $\Omega_L(\varphi_L)$. Recall the definition of the W_T-norms given in (3.3.188). Note that for $T \geq \Lambda$ the L^2-norm coincides with the W_T-norm on $\operatorname{ran}\Pi$, which makes $0 < T < \Lambda$ the relevant regime for our discussion. In fact, we shall pick

$$1 \ll T \ll \Lambda^{2/3}, \quad \alpha^{4/5} \ll \Lambda, \tag{3.4.107}$$

where $T \gg 1$ is needed for the inner region to yield the right contribution, and $T \ll \Lambda^{2/3}$ ensures that the outer region contribution is negligible.

We proceed by introducing an IMS type localization with respect to $\|\cdot\|_{W_T}$. Let $\chi : \mathbb{R}_+ \to [0,1]$ be a smooth function such that $\chi(t) = 1$ for $t \leq 1/2$ and $\chi(t) = 0$ for $t \geq 1$. Let $\varepsilon > 0$ and let j_1 and j_2 denote the multiplication operators on $L^2(\mathbb{R}^N)$

$$j_1 = \chi\left(\varepsilon^{-1}\mathsf{dist}_{W_T}(\varphi, \Omega_L(\varphi_L))\right), \quad j_2 = \sqrt{1 - j_1^2}. \tag{3.4.108}$$

Then

$$\mathbb{K} = j_1\mathbb{K}j_1 + j_2\mathbb{K}j_2 - \mathbb{E}, \tag{3.4.109}$$

where $\mathbb{E}$ is the IMS localization error given by

$$\mathbb{E} = \frac{1}{4\alpha^4}\sum_{n=1}^{N}\left(|\partial_{\lambda_n}j_1|^2 + |\partial_{\lambda_n}j_2|^2\right). \tag{3.4.110}$$

To bound $\mathbb{E}$ we apply Lemma 3.3.11, which states that for ε sufficiently small, for any $\varphi \in \mathsf{supp}j_1$, there exists a *unique* $y_\varphi \in \mathbb{T}_L^3$ such that

$$\mathrm{dist}_{W_T}^2(\varphi, \Omega_L(\varphi_L)) = \left\langle \varphi - \varphi_L^{y_\varphi} \middle| W_T \middle| \varphi - \varphi_L^{y_\varphi} \right\rangle. \tag{3.4.111}$$

Likewise, for any $n \in \{1, \dots, N\}$ and any h sufficiently small there exists a unique $y_{n,h} \in \mathbb{T}_L^3$ such that

$$\mathrm{dist}_{W_T}^2(\varphi + hf_n, \Omega_L(\varphi_L)) = \left\langle \varphi + hf_n - \varphi_L^{y_{n,h}} \middle| W_T \middle| \varphi + hf_n - \varphi_L^{y_{n,h}} \right\rangle. \tag{3.4.112}$$

It is easy to see, using again Lemma 3.3.11, that $\lim_{h\to 0} y^{h,n} = y^{\varphi}$ for any n. Therefore, using that $\mathrm{dist}_{W_T}(\varphi + hf_n, \Omega_L(\varphi_L)) \leq \|\varphi - \varphi_L^{y_\varphi}\|_{W_T}$ and $\mathrm{dist}_{W_T}(\varphi, \Omega_L(\varphi_L)) \leq \|\varphi - \varphi_L^{y_{h,n}}\|_{W_T}$, we arrive at

$$\begin{aligned}
&2 \langle f_n | W_T \left|\varphi - \varphi_L^{y_\varphi}\right\rangle = \lim_{h\to 0} 2 \langle f_n | W_T \left|\varphi - \varphi_L^{y_{h,n}}\right\rangle \\
&\leq \lim_{h\to 0} h^{-1} \left(\mathrm{dist}^2_{W_T}(\varphi + hf_n, \Omega_L(\varphi_L)) - \mathrm{dist}^2_{W_T}(\varphi, \Omega_L(\varphi_L))\right) \\
&\leq 2 \langle f_n | W_T \left|\varphi - \varphi_L^{y_\varphi}\right\rangle,
\end{aligned} \tag{3.4.113}$$

which shows that

$$\partial_{\lambda_n} \mathrm{dist}^2_{W_T}(\varphi, \Omega_L(\varphi_L)) = 2 \langle f_n | W_T(\varphi - \varphi_L^{y_\varphi})\rangle. \tag{3.4.114}$$

Using that $|\chi'|, \left|\left[(1-\chi^2)^{1/2}\right]'\right| \lesssim \mathbb{1}_{[1/2,1]}$, for $k = 1, 2$ we obtain

$$\begin{aligned}
|[\partial_{\lambda_n} j_k](\varphi)|^2 &\lesssim \varepsilon^{-4} \left|\partial_{\lambda_n} \mathrm{dist}^2_{W_T}(\varphi, \Omega_L(\varphi_L))\right|^2 \mathbb{1}_{\left\{\mathrm{dist}_{W_T}(\varphi, \Omega_L(\varphi_L)) \leq \varepsilon\right\}} \\
&\lesssim \varepsilon^{-4} |\langle f_n | W_T(\varphi - \varphi_L^{y_\varphi})\rangle|^2 \mathbb{1}_{\left\{\mathrm{dist}_{W_T}(\varphi, \Omega_L(\varphi_L)) \leq \varepsilon\right\}}.
\end{aligned} \tag{3.4.115}$$

Summing over n, using that $\|W_T\| \leq 1$ and that $\{f_n\}$ is an orthonormal system, we arrive at

$$\mathbb{E} \lesssim \alpha^{-4}\varepsilon^{-2}, \tag{3.4.116}$$

and thus the localization error is negligible as long as $\varepsilon \gg \alpha^{-1}$. Hence, we are left with the task of providing lower bounds for $j_1 \mathbb{K} j_1$ and $j_2 \mathbb{K} j_2$ under the constraint $\varepsilon \gg \alpha^{-1}$. We carry out these estimates in the next two subsections, 3.4.3 and 3.4.3. Finally, in Section 3.4.3, we combine these bounds to prove the lower bound in (3.2.24).

Bounds on $j_1 \mathbb{K} j_1$

Let us look closer at the intersection of the ε-neighborhood of $\Omega_L(\varphi_L)$ with respect to the W_T-norm with $\mathrm{ran}\,\Pi$, i.e., the set

$$[\Pi\Omega_L(\varphi_L)]_{\varepsilon,T} := \{\varphi \in \mathrm{ran}\,\Pi \,|\, \bar{\varphi} = \varphi,\ \mathsf{dist}_{W_T}(\varphi, \Omega_L(\varphi_L)) \leq \varepsilon\} = \mathsf{supp} j_1 \cap \mathrm{ran}\,\Pi. \tag{3.4.117}$$

In the following we shall show that this set is, for ε small enough, a tubular neighborhood of $\Pi\Omega_L(\varphi_L)$, which can be mapped via a suitable diffeomorphism (given in Definition 3.4.1) to a tubular neighborhood of a flat torus.

Since $\varphi \in \mathrm{ran}\,\Pi$ and Π commutes both with W_T and with the transformation $g \mapsto g^y$ for any $y \in \mathbb{T}^3_L$, we have

$$\mathrm{dist}^2_{W_T}(\varphi, \Omega_L(\varphi_L)) = \|(\mathbb{1} - \Pi)\varphi_L\|^2_{W_T} + \mathrm{dist}^2_{W_T}(\varphi, \Omega_L(\Pi\varphi_L)). \tag{3.4.118}$$

This implies that $[\Pi\Omega_L(\varphi_L)]_{\varepsilon,T}$ is non-empty if and only if

$$r_{T,\varepsilon} := \sqrt{\varepsilon^2 - \|(\mathbb{1} - \Pi)\varphi_L\|^2_{W_T}} > 0. \tag{3.4.119}$$

Since $\varphi_L \in C^\infty(\mathbb{T}^3_L)$, $r_{T,\varepsilon} > 0$ as long as

$$\varepsilon \gtrsim_L \Lambda^{-h} \tag{3.4.120}$$

for some $h > 0$ and Λ sufficiently large. In particular, (3.4.120) is satisfied with $h = 5/4$ for α large enough since, as discussed above, we need to pick $\varepsilon \gg \alpha^{-1}$ and $\Lambda \gg \alpha^{4/5}$ for the IMS and the cutoff errors to be negligible.

Lemma 3.3.11 implies that any $\varphi \in [\Pi\Omega_L(\varphi_L)]_{\varepsilon,T}$, for $\varepsilon \leq \varepsilon'_L$ (independently of T and N), admits a unique W_T-projection $\varphi_L^{y_\varphi}$ onto $\Omega_L(\varphi_L)$ and

$$\varphi = \varphi_L^{y_\varphi} + (v_\varphi)^{y_\varphi}, \quad \text{with} \quad v_\varphi \in (\operatorname{span}\{W_T \nabla \varphi_L\})^{\perp_{L^2}}. \tag{3.4.121}$$

Since W_T and Π commute, $\Omega_L(\varphi_L)$ is 'parallel' to $\operatorname{ran}\Pi$ with respect to $\|\cdot\|_{W_T}$, i.e., $\operatorname{dist}_{W_T}(\operatorname{ran}\Pi, \varphi_L^y)$ is independent of y and the W_T-projection of φ_L^y onto Π is simply $\Pi(\varphi_L^y) = (\Pi\varphi_L)^y$. Therefore, for $\varepsilon \leq \varepsilon'_L$, any $\varphi \in [\Pi\Omega_L(\varphi_L)]_{\varepsilon,T}$ admits a *unique* W_T-projection $(\Pi\varphi_L)^{y_\varphi}$ onto $\Omega_L(\Pi\varphi_L)$ and (3.4.121) induces a unique decomposition of the form

$$\varphi = (\Pi\varphi_L)^{y_\varphi} + (\eta_\varphi)^{y_\varphi}, \quad \text{with} \quad \eta_\varphi \in (\operatorname{span}\{\Pi W_T \nabla \varphi_L\})^{\perp_{L^2}}, \ \|\eta_\varphi\|_{W_T} \leq r_{T,\varepsilon}, \tag{3.4.122}$$

where $\eta_\varphi = \Pi v_\varphi$ (note that $(\mathbb{1} - \Pi)v_\varphi = -(\mathbb{1} - \Pi)\varphi_L$). This allows to introduce the following diffeomorphism, which is a central object in our discussion. It maps $[\Pi\Omega_L(\varphi_L)]_{\varepsilon,T}$ onto a tubular neighborhood of a flat torus. We shall call this diffeomorphism *Gross coordinates*, as it is inspired by an approach introduced in [59].

Definition 3.4.1 (Gross coordinates)**.** *For*

$$B_\varepsilon^{T,\Lambda} := \left\{\eta \in \operatorname{span}_{\mathbb{R}}\{\Pi W_T \nabla \varphi_L\}^{\perp_{L^2}} \cap \operatorname{ran}\Pi \mid \|\eta\|_{W_T} \leq r_{T,\varepsilon}\right\} \subset \operatorname{ran}\Pi, \tag{3.4.123}$$

we define the Gross coordinates map u as

$$\begin{aligned} u : [\Pi\Omega_L(\varphi_L)]_{\varepsilon,T} &\to \mathbb{T}_L^3 \times B_\varepsilon^{T,\Lambda}, \\ \varphi &\mapsto (y_\varphi, \eta_\varphi), \end{aligned} \tag{3.4.124}$$

where y_φ and η_φ are defined through the decomposition (3.4.122)*.*

By the discussion above it is clear that u is well-defined and invertible, for $\varepsilon \leq \varepsilon'_L$ (defined in Lemma 3.3.11), with inverse u^{-1} given by

$$\begin{aligned} u^{-1} : \mathbb{T}_L^3 \times B_\varepsilon^{T,\Lambda} &\to [\Pi\Omega_L(\varphi_L)]_{\varepsilon,T} \\ (y, \eta) &\mapsto (\Pi\varphi_L)^y + \eta^y. \end{aligned} \tag{3.4.125}$$

We emphasize that the whole aim of the discussion above is to show that u is well-defined, since once that has been shown the invertibility of u and the form of u^{-1} are obvious. In other words, the map u^{-1} as defined in (3.4.125) is trivially-well defined, but it is injective and surjective with inverse u only thanks to the existence and uniqueness of the decomposition (3.4.122).

To show that u is a smooth diffeomorphism, we prefer to work with its inverse u^{-1}, which we proceed to write down more explicitly. For this purpose, we pick a real L^2-orthonormal basis $\{f_k\}_{k=1}^N$ of $\operatorname{ran}\Pi$, such that f_1, f_2 and f_3 are an orthonormal basis of $\operatorname{span}\{\Pi W_T \nabla \varphi_L\}$ and $f_4 = \frac{\Pi\varphi_L}{\|\Pi\varphi_L\|_2}$. Note that $\operatorname{span}\{\Pi W_T \nabla \varphi_L\}$ is three dimensional, as remarked after (3.3.186), at least for N and T large enough, and that f_4 is indeed orthogonal to f_1, f_2 and f_3 since in k-space W_T and Π are even multiplication operators while the partial derivatives are odd multiplication operators. We denote the projection onto $\operatorname{span}_{k=1,2,3}\{\Pi W_T \partial_k \varphi_L\}$ by

$$\Pi_{\nabla,T}^L := \sum_{k=1}^3 |f_k\rangle \langle f_k|. \tag{3.4.126}$$

Having fixed a real orthonormal L^2-basis, we can identify any real-valued function in $\operatorname{ran}\Pi$ (and hence also any function in $[\Pi\Omega_L(\varphi_L)]_{\varepsilon,T}$) with a point $(\lambda_1,\dots,\lambda_N)$ via (3.4.103). In these coordinates, the orthogonal transformation that acts on functions in $\operatorname{ran}\Pi$ as the translation by y, i.e., $\varphi \mapsto \varphi^y$, reads

$$R(y) := \sum_{k=1}^{N} |f_k^y\rangle \langle f_k| , \tag{3.4.127}$$

and we can write $B_\varepsilon^{T,\Lambda}$ in (3.4.123) as

$$B_\varepsilon^{T,\Lambda} := \left\{ \eta = (\eta_4,\dots,\eta_N) \in \operatorname{span}_{\mathbb{R}}\{f_4,\dots,f_N\} \,\middle|\, \left\| \sum_{k=4}^{N} \eta_k f_k \right\|_{W_T} \leq r_{T,\varepsilon} \right\}. \tag{3.4.128}$$

In this basis, we can write u^{-1} explicitly as

$$u^{-1}(y,\eta) = (\Pi\varphi_L)^y + \eta^y = R(y)(0,0,0,\|\Pi\varphi_L\|_2 + \eta_4, \eta_5, \dots, \eta_N). \tag{3.4.129}$$

The following Lemma uses this explicit expression for u^{-1} and shows that it is a smooth diffeomorphism (therefore showing that the Gross coordinates map u is as well).

Lemma 3.4.2. *Let u^{-1} be the map defined in (3.4.129). There exists $\varepsilon_L^1 \leq \varepsilon_L'$ (independent of T and N) and $N_L > 0$ such that for any $\varepsilon \leq \varepsilon_L^1$, any $T > 0$ and any $N > N_L$ the map u^{-1} is a C^∞-diffeomorphism from $\mathbb{T}_L^3 \times B_\varepsilon^{T,\Lambda}$ onto $[\Pi\Omega_L(\varphi_L)]_{\varepsilon,T}$. Moreover, for $\varepsilon \leq \varepsilon_L^1$, $|\det Du^{-1}|$ and all its derivatives are uniformly bounded independently of T and N.*

Proof. We introduce the notation $J(y,\eta) = Du^{-1}(y,\eta)$ and $d(y,\eta) := |\det J(y,\eta)|$. Note that $R(y)$ in (3.4.127) satisfies $R(-y) = R(y)^{-1} = R(y)^t$ since $\{f_j^y\}_{j=1}^N$ is an orthonormal basis of $\operatorname{ran}\Pi$ for any y. Hence, for $j = 1,\dots,N$ we have

$$(u^{-1})_j(y,\eta) = \left\langle f_j \middle| u^{-1}(y,\eta) \right\rangle = \left\langle R(-y) f_j \middle| \Pi\varphi_L + \sum_{l=4}^{N} \eta_l f_l \right\rangle. \tag{3.4.130}$$

This yields the smoothness of u^{-1} in η and in y (noting that $\{f_j\}_{j=1}^N \subset \operatorname{ran}\Pi$ is a set of smooth functions for any N). We proceed to compute J. We have, for $4 \leq k \leq N$,

$$\partial_{\eta_k}(u^{-1})_j(y,\eta) = \langle R(-y) f_j | f_k \rangle = \langle f_j | R(y) f_k \rangle , \tag{3.4.131}$$

and

$$\begin{aligned} \partial_{y_k}(u^{-1})_j(y,\eta) &= \left\langle f_j \middle| \partial_{y_k} R(y) \left(\Pi\varphi_L + \sum_{l=4}^{N} \eta_l f_l \right) \right\rangle \\ &= -\left\langle f_j \middle| R(y)\partial_k \left(\Pi\varphi_L + \sum_{l=4}^{N} \eta_l f_l \right) \right\rangle \end{aligned} \tag{3.4.132}$$

for $1 \leq k \leq 3$. Therefore

$$\begin{aligned} J(y,\eta) &= R(y) \left[\sum_{k=1}^{3} |v_k\rangle \langle f_k| + \sum_{k\geq 4} |f_k\rangle \langle f_k| \right] \\ &= R(y) \left(\mathbb{1} - \Pi_{\nabla,T}^L + \sum_{k=1}^{3} |v_k\rangle \langle f_k| \right) =: R(y) J_0(\eta), \end{aligned} \tag{3.4.133}$$

where $v_k(\eta) := -\partial_k u^{-1}(0,\eta) = -\partial_k \left(\Pi\varphi_L + \sum_{l=4}^N \eta_l f_l\right)$. Since $R(y)$ is orthogonal, we see that $d = |\det J_0|$ (implying, in particular, that d is independent of y).

Observe that

$$J_0 = \begin{pmatrix} A_0 & 0 \\ A_1 & \mathbb{1} \end{pmatrix}, \tag{3.4.134}$$

where A_0 is the 3×3 matrix given by

$$(A_0)_{jk} = \langle f_j|v_k\rangle = \left\langle f_j \middle| -\partial_k \left(\Pi\varphi_L + \sum_{l=4}^N \eta_l f_l\right)\right\rangle, \quad j,k\in\{1,2,3\}, \tag{3.4.135}$$

and A_1 is the $(N-3)\times 3$ matrix defined by

$$(A_1)_{jk} = \left\langle f_{j+3} \middle| -\partial_k \left(\Pi\varphi_L + \sum_{l=4}^N \eta_l f_l\right)\right\rangle \quad j\in\{1,\dots,N-3\},\;\; k\in\{1,2,3\}. \tag{3.4.136}$$

Since J_0 is the identity in the bottom-right $(N-3)\times(N-3)$ corner and 0 in the top-right $3\times(N-3)$ corner, $d = |\det A_0|$. On $\operatorname{ran}\Pi^L_{\nabla,T}$ the operators ∂_k with $k=1,2,3$ and W_T^{-1} are uniformly bounded in N and T. Recall also that $\|\eta\|_{W_T} \le \varepsilon_L^1$. Hence, for some constant C_L independent of N and T, and for any $j,k\in\{1,2,3\}$, we have

$$|(A_0)_{jk}| \le \|\partial_k f_j\|_2 \|\Pi\varphi_L\|_2 + \|W_T^{-1}\partial_k f_j\|_{W_T}\|\eta\|_{W_T} \le C_L. \tag{3.4.137}$$

Moreover, for any $j,k\in\{1,2,3\}$ and any $l,l_1,l_2\in\{4,\dots,N\}$, we also have

$$\partial_{\eta_l}(A_0)_{jk} = \langle \partial_k f_j | f_l\rangle, \quad \partial_{\eta_{l_1}}\partial_{\eta_{l_2}}(A_0)_{jk} = 0. \tag{3.4.138}$$

Clearly, (3.4.137) and (3.4.138) together with the fact that $d = |\det A_0|$ show that d and all its derivatives are uniformly bounded in N and T. To show that there exists ε_L^1 and N_L such that $d \ge C_L > 0$ for all $\varepsilon \le \varepsilon_L^1$, $T>0$ and $N > N_L$, we show that the image of the 3-dimensional unit sphere under A_0 is uniformly bounded away from 0, which clearly yields our claim. For this purpose, we observe that the k-th column of A_0 is given by $\Pi^L_{\nabla,T}\left[-\partial_k\left(\Pi\varphi_L + \sum_{l=4}^N \eta_l f_l\right)\right]$ and therefore, for any unit vector $a = (a_1,a_2,a_3)\in\mathbb{R}^3$,

$$A_0 a = \sum_{k=1}^3 a_k \Pi^L_{\nabla,T}\left[-\partial_k\left(\Pi\varphi_L + \sum_{l=4}^N \eta_l f_l\right)\right] = -\Pi^L_{\nabla,T}\partial_a u^{-1}(0,\eta), \tag{3.4.139}$$

where we denote $\sum_{k=1}^3 a_k\partial_k = \partial_a$. To bound the norm of $A_0 a$ from below, it is then sufficient to test $\partial_a u^{-1}(0,\eta)$ against one normalized element of $\operatorname{ran}\Pi^L_{\nabla,T}$, say $\frac{\Pi W_T \partial_a\varphi_L}{\|\Pi W_T\partial_a\varphi_L\|_2}$. We obtain

$$\begin{aligned}
\|A_0 a\|_2^2 = \|\Pi^L_{\nabla,T}\partial_a u^{-1}(0,\eta)\|_2^2 &\ge \left|\left\langle \frac{\Pi W_T\partial_a\varphi_L}{\|\Pi W_T\partial_a\varphi_L\|_2}\middle| \partial_a\left(\Pi\varphi_L + \sum_{l=4}^N \eta_l f_l\right)\right\rangle\right|^2 \\
&= \|\Pi W_T\partial_a\varphi_L\|_2^{-2}\left|\|\Pi W_T^{1/2}\partial_a\varphi_L\|_2^2 - \left\langle \Pi\partial_a^2\varphi_L\middle|\eta\right\rangle_{W_T}\right|^2 \\
&\ge \|\partial_a\varphi_L\|_2^{-2}\left(\|\Pi W_0^{1/2}\partial_a\varphi_L\|_2^2 - \|\Pi\partial_a^2\varphi_L\|_{W_T}\|\eta\|_{W_T}\right)_+^2 \\
&\ge \|\partial_a\varphi_L\|_2^{-2}\left(\|\Pi W_0^{1/2}\partial_a\varphi_L\|_2^2 - \varepsilon\|\partial_a^2\varphi_L\|_2\right)_+^2,
\end{aligned} \tag{3.4.140}$$

where we used that $\|\eta\|_{W_T} \le \varepsilon$, $0 \le W_T \le \mathbb{1}$ and $\Pi \le \mathbb{1}$, and $(\,\cdot\,)_+$ denotes the positive part. As remarked after (3.3.186), $\partial_a \varphi_L = (-\Delta_L)^{-1/2}\partial_a|\psi_L|^2 \neq 0$ and since $\varphi_L \in C^\infty$, $\partial_a\varphi_L$ and $\partial_a^2\varphi_L$ are uniformly bounded in a. We can thus find $N_L > 0$ and ε_L^1 such that the r.h.s. of (3.4.140) is bounded from below by some constant $C_L > 0$ uniformly for $T > 0$, $N > N_L$ and $\varepsilon \le \varepsilon_L^1$. This shows that A_0 (and hence J) is invertible at every point and that $d \ge C_L > 0$ uniformly in $T > 0$, $N > N_L$ and $\varepsilon \le \varepsilon_L^1$, as claimed. This concludes the proof. □

Since u is a diffeomorphism, we can introduce a unitary operator that lifts u^{-1} to L^2, defined by

$$\begin{aligned} U &: L^2(\mathbb{T}_L^3 \times B_\varepsilon^{T,\Lambda}) \longrightarrow L^2([\Pi\Omega_L(\varphi_L)]_{\varepsilon,T}) \\ U(\psi) &:= |\det(Du)|^{1/2}\psi\circ u. \end{aligned} \tag{3.4.141}$$

Recall that j_1 is supported in $[\Pi\Omega_L(\varphi_L)]_{\varepsilon,T}$, hence we can apply U to $j_1\mathbb{K}j_1$, obtaining an operator that acts on functions on $\mathbb{T}_L^3 \times \mathbb{R}^{N-3}$ that are supported in $\mathbb{T}_L^3 \times B_\varepsilon^{T,\Lambda}$. In particular,

$$j_1\mathbb{K}j_1 \ge j_1^2 \inf\operatorname{spec}_{H_0^1(\mathbb{T}_L^3\times B_\varepsilon^{T,\Lambda})}[U^*\mathbb{K}U], \tag{3.4.142}$$

where the subscript indicates that the operator has to be understood as the corresponding quadratic form with form domain $H_0^1(\mathbb{T}_L^3 \times B_\varepsilon^{T,\Lambda})$ (i.e., with Dirichlet boundary conditions on the boundary of $B_\varepsilon^{T,\Lambda}$). We are hence left with the task of giving a lower bound on $\inf\operatorname{spec}_{H_0^1(\mathbb{T}_L^3\times B_\varepsilon^{T,\Lambda})}[U^*\mathbb{K}U]$, which will be done in the remainder of this subsection.

Recalling the definition of $\mathbb{K}$ given in (3.4.106), we proceed to find a convenient lower bound for $U^*\mathcal{F}_LU$. Any $(\Pi\varphi_L)^{y_\varphi} + (w_\varphi)^{y_\varphi} = \varphi \in [\Pi\Omega_L(\varphi_L)]_{\varepsilon,T}$ satisfies (3.3.163) with $\varphi_L^{y_\varphi}$ in place of φ_L, and we can therefore expand $\mathcal{F}_L(\varphi)$ using Proposition 3.3.4, obtaining

$$\begin{aligned} \mathcal{F}_L(\varphi) - e_L &\ge \langle (w_\varphi)^{y_\varphi} - ((\mathbb{1}-\Pi)\varphi_L)^{y_\varphi} | \mathbb{1} - K_L^{y_\varphi} - \varepsilon C_L J_L^{y_\varphi} | (w_\varphi)^{y_\varphi} - ((\mathbb{1}-\Pi)\varphi_L)^{y_\varphi}\rangle \\ &= \langle \varphi_L | (\mathbb{1}-\Pi)(\mathbb{1} - K_L - \varepsilon C_L J_L)(\mathbb{1}-\Pi)|\varphi_L\rangle \\ &\quad - 2\,\langle (\mathbb{1}-\Pi)\varphi_L |\, \mathbb{1} - K_L - \varepsilon C_L J_L\, | w_\varphi\rangle + \langle w_\varphi | \mathbb{1} - K_L - \varepsilon C_L J_L | w_\varphi\rangle\,. \end{aligned} \tag{3.4.143}$$

Since K_L and J_L are trace class operators,

$$(\mathbb{1}-\Pi)(\mathbb{1} - K_L - \varepsilon C_L J_L)(\mathbb{1}-\Pi) > 0 \tag{3.4.144}$$

holds for Λ sufficiently large and ε sufficiently small. Moreover, since $\varphi_L \in C^\infty(\mathbb{T}_L^3)$

$$\begin{aligned} &|\,\langle (\mathbb{1}-\Pi)\varphi_L |\, \mathbb{1} - K_L - \varepsilon C_L J_L\, | w_\varphi\rangle\,| \\ &\quad \le \|W_T^{-1/2}(\mathbb{1} - K_L - \varepsilon C_L J_L)(\mathbb{1}-\Pi)\varphi_L\|_2 \|w_\varphi\|_{W_T} = O(\varepsilon\Lambda^{-h}) \end{aligned} \tag{3.4.145}$$

for arbitrary $h > 0$ and uniformly in T. This implies that, for any $\varphi = (\Pi\varphi_L)^{y_\varphi} + (w_\varphi)^{y_\varphi} \in [\Pi\Omega_L(\varphi_L)]_{\varepsilon,T}$, any Λ sufficiently large, any ε sufficiently small and an arbitrary h

$$\mathcal{F}_L(\varphi) = \mathcal{F}_L((\Pi\varphi_L)^{y_\varphi} + (w_\varphi)^{y_\varphi}) \ge e_L - O(\varepsilon\Lambda^{-h}) + \langle w_\varphi | \mathbb{1} - K_L - \varepsilon C_L J_L | w_\varphi\rangle\,. \tag{3.4.146}$$

Therefore, if we define the $[(N-3)\times(N-3)]$-matrix M with coefficients

$$M_{k,j} := \langle f_{k+3} |\, \mathbb{1} - K_L - \varepsilon C_L J_L\, | f_{j+3}\rangle\,, \tag{3.4.147}$$

then, by (3.4.146), the multiplication operator $U^*\mathcal{F}_L U$ satisfies

$$(U^*\mathcal{F}_L U)(y,\eta) \geq e_L + \langle \eta | M | \eta \rangle - O(\varepsilon \Lambda^{-h}). \tag{3.4.148}$$

It is easy to see that M is a positive matrix, at least for ε sufficiently small and T and Λ sufficiently large. Indeed, the positivity of M is equivalent to the positivity of $(\mathbb{1} - K_L - \varepsilon C_L J_L)$ on $\operatorname{ran}(\Pi - \Pi^L_{\nabla,T})$ and, by Proposition 3.3.5, $(\mathbb{1} - K_L - \varepsilon C_L J_L)$ is positive on any vector space with trivial intersection with $\operatorname{ran}\Pi^L_\nabla$. Clearly, since $\Pi^L_{\nabla,T} \to \Pi^L_\nabla$ as $T \to \infty$, the bound

$$M \geq c_L > 0 \tag{3.4.149}$$

holds, uniformly in T, Λ and for ε sufficiently small.

We now proceed to bound $-U^*\Delta_\lambda U$ from below.

Lemma 3.4.3. *Let U be the unitary transformation defined in* (3.4.141). *There exists $C_L > 0$, independent of N, T and ε, such that, for $\varepsilon \leq \varepsilon_L^1$, $T > 0$ and $N > N_L$*

$$U^*\left(-\Delta_\lambda\right) U \geq -\Delta_\eta - C_L. \tag{3.4.150}$$

Proof. Since (3.4.133) shows that $J(y,\eta) = R(y) J_0(\eta)$ with $R(y)$ orthogonal, we have

$$\begin{aligned} U^*\left(-\Delta_\lambda\right) U &= -d^{-1/2}\boldsymbol{\nabla} \cdot d^{1/2}\left[J^{-1}(J^{-1})^t\right] d^{1/2}\boldsymbol{\nabla} d^{-1/2} \\ &= -d^{-1/2}\boldsymbol{\nabla} \cdot d^{1/2}\left[J_0^{-1}(J_0^{-1})^t\right] d^{1/2}\boldsymbol{\nabla} d^{-1/2}, \end{aligned} \tag{3.4.151}$$

with $d(y,\eta) = |\det J(y,\eta)|$ and $\boldsymbol{\nabla}$ denoting the gradient with respect to $(y,\eta) \in \mathbb{R}^N$. Recalling the expression (3.4.134) for J_0, we find

$$J_0^{-1} = \begin{pmatrix} A_0^{-1} & 0 \\ -A_1 A_0^{-1} & \mathbb{1} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{1} \end{pmatrix} + \begin{pmatrix} A_0^{-1} & 0 \\ -A_1 A_0^{-1} & 0 \end{pmatrix} =: (1 - \Pi^L_{\nabla,T}) + D. \tag{3.4.152}$$

Since $D(\mathbb{1} - \Pi^L_{\nabla,T}) = (\mathbb{1} - \Pi^L_{\nabla,T}) D^t = 0$, we have

$$J_0^{-1}(J_0^{-1})^t = (\mathbb{1} - \Pi^L_{\nabla,T}) + DD^t \geq \mathbb{1} - \Pi^L_{\nabla,T}. \tag{3.4.153}$$

With (3.4.151) and (3.4.153), we thus obtain

$$\begin{aligned} U^*\left(-\Delta_\lambda\right) U &\geq -d^{-1/2}\boldsymbol{\nabla} \cdot d^{1/2}\left(\mathbb{1} - \Pi^L_{\nabla,T}\right) d^{1/2}\boldsymbol{\nabla} d^{-1/2} \\ &= -\Delta_\eta - (2d)^{-2}|\nabla d|^2 + (2d)^{-1}\Delta d. \end{aligned} \tag{3.4.154}$$

Lemma 3.4.2 guarantees that d and all its derivatives are bounded, and d is bounded away from 0 uniformly in $N > N_L$, $T > 0$ and $\varepsilon \leq \varepsilon_L^1$, leading to (3.4.150). □

In combination, (3.4.148), (3.4.150) and the positivity of M imply that

$$\begin{aligned} j_1 \mathbb{K} j_1 &\geq j_1^2 \inf \operatorname{spec}_{H_0^1(\mathbb{T}_L^3 \times B_\varepsilon^{T,\Lambda})}(U^*\mathbb{K}U) && (3.4.155) \\ &\geq j_1^2 \left(e_L - \frac{N}{2\alpha^2} - O(\varepsilon\Lambda^{-h}) - O(\alpha^{-4}) + \inf \operatorname{spec}_{L^2(\mathbb{R}^N)}\left[-\frac{1}{4\alpha^4}\Delta_\eta + \langle \eta | M | \eta \rangle \right] \right) \\ &= j_1^2 \left(e_L - \frac{1}{2\alpha^2}(N - \operatorname{Tr}\left(M^{1/2}\right)) - O(\varepsilon\Lambda^{-h}) - O(\alpha^{-4}) \right). && (3.4.156) \end{aligned}$$

Note that since we are taking $\Lambda \gg \alpha^{4/5}$, $\varepsilon \ll 1$ and $h > 0$ was arbitrary, picking $h = 5$ allows to absorb the error term $O(\varepsilon\Lambda^{-h})$ in the error term $O(\alpha^{-4})$. Recalling the definition of M given in (3.4.147), we have

$$\operatorname{Tr}\left(M^{1/2}\right) = \operatorname{Tr}\left[\sqrt{(\Pi - \Pi^{L}_{\nabla,T})(\mathbb{1} - K_L - \varepsilon C_L J_L)(\Pi - \Pi^{L}_{\nabla,T})}\right]. \tag{3.4.157}$$

With $\{t_j\}_{j=1}^{N-3}$ an orthonormal basis of $\operatorname{ran}(\Pi - \Pi^{L}_{\nabla,T})$ of eigenfunctions of $(\Pi - \Pi^{L}_{\nabla,T})(\mathbb{1} - K_L - \varepsilon C_L J_L)(\Pi - \Pi^{L}_{\nabla,T})$, we can write

$$\begin{aligned}\operatorname{Tr}\left(M^{1/2}\right) &= \sum_{j=1}^{N-3} \langle t_j|\mathbb{1} - K_L - \varepsilon C_L J_L|t_j\rangle^{1/2} \\ &= \sum_{j=1}^{N-3}\left[\langle t_j|\mathbb{1} - K_L|t_j\rangle^{1/2} - \frac{\varepsilon C_L}{2\xi_j^{1/2}}\langle t_j|J_L|t_j\rangle\right]\end{aligned} \tag{3.4.158}$$

for some $\{\xi_j\}_{j=1}^{N-3}$ satisfying

$$c_L \leq \langle t_j|\mathbb{1} - K_L - \varepsilon C_L J_L|t_j\rangle \leq \xi_j \leq \langle t_j|\mathbb{1} - K_L|t_j\rangle \leq 1 \tag{3.4.159}$$

for T and Λ large enough and ε small enough, where we used (3.4.149) for the lower bound. Using the concavity of the square root and the trace class property of J_L, we conclude that

$$\operatorname{Tr}\left(M^{1/2}\right) \geq \sum_{j=1}^{N-3}\langle t_j|\sqrt{\mathbb{1} - K_L}|t_j\rangle - \varepsilon C_L \operatorname{Tr}(J_L) = \operatorname{Tr}\left[(\Pi - \Pi^{L}_{\nabla,T})\sqrt{\mathbb{1} - K_L}\right] - \varepsilon C_L. \tag{3.4.160}$$

Since $\varphi_L \in C^\infty$ and recalling (3.4.107), for an arbitrary $h > 0$ we can bound

$$\|\Pi^{L}_{\nabla} - \Pi^{L}_{\nabla,T}\| \lesssim_L \min\{\Lambda, T\}^{-h} = T^{-h}, \tag{3.4.161}$$

which also implies the same estimate for the trace-norm of the difference of Π^{L}_{∇} and $\Pi^{L}_{\nabla,T}$, both operators being of rank 3. Recalling that Π^{L}_{∇} projects onto $\ker(\mathbb{1} - K_L)$, we finally obtain

$$\operatorname{Tr}\left(M^{1/2}\right) \geq \operatorname{Tr}\left[\Pi\sqrt{\mathbb{1} - K_L}\right] - O(\varepsilon) - O(T^{-h}). \tag{3.4.162}$$

The error term $O(T^{-h})$ forces $T \to \infty$ as $\alpha \to \infty$, but allows T to grow with an arbitrarily small power of α. By picking h to be sufficiently large we can absorb it in the error term $O(\varepsilon)$.

We obtain the final lower bound

$$\begin{aligned}j_1\mathbb{K}j_1 &\geq j_1^2\left[e_L - \frac{1}{2\alpha^2}\operatorname{Tr}\left[\Pi(\mathbb{1} - (\mathbb{1} - K_L)^{1/2})\right] - O(\varepsilon\alpha^{-2}) - O(\alpha^{-4})\right] \\ &\geq j_1^2\left[e_L - \frac{1}{2\alpha^2}\operatorname{Tr}\left[(\mathbb{1} - (\mathbb{1} - K_L)^{1/2})\right] - O(\varepsilon\alpha^{-2}) - O(\alpha^{-4})\right].\end{aligned} \tag{3.4.163}$$

Bounds on $j_2\mathbb{K}j_2$

We recall Corollary 3.2.1, which implies that, for any $\varphi \in L^2_{\mathbb{R}}(\mathbb{T}^3_L)$,

$$\mathcal{F}_L(\varphi) \geq e_L + \inf_{y\in\mathbb{T}^3_L}\langle\varphi - \varphi^y_L|B|\varphi - \varphi^y_L\rangle, \tag{3.4.164}$$

where B acts in k-space as the multiplication by

$$B(k) = \begin{cases} 1 & \text{for } k = 0, \\ 1 - (1 + \kappa'|k|)^{-1} & \text{for } k \neq 0. \end{cases} \tag{3.4.165}$$

Note that $B - \eta W_T > 0$ for $\eta > 0$ small enough (independently of T). Moreover, for any φ in the support of j_2 and any $y \in \mathbb{T}^3_L$,

$$\langle \varphi - \varphi^y_L | W_T | \varphi - \varphi^y_L \rangle \geq \varepsilon^2/4. \tag{3.4.166}$$

Therefore, on the support of j_2, we have

$$\mathcal{F}_L(\varphi) \geq e_L + \inf_{y \in \mathbb{T}^3_L} \langle \varphi - \varphi^y_L | B - \eta W_T | \varphi - \varphi^y_L \rangle + \eta \varepsilon^2/4. \tag{3.4.167}$$

By the Cauchy–Schwarz inequality, using that all the operators involved commute, we have

$$\begin{aligned} \langle \varphi - \varphi^y_L | B - \eta W_T | \varphi - \varphi^y_L \rangle \geq\ & \langle \varphi | (\mathbb{1} - W_\gamma^{1/2})(B - \eta W_T) | \varphi \rangle \\ & + \langle \varphi_L | (\mathbb{1} - W_\gamma^{-1/2})(B - \eta W_T) | \varphi_L \rangle \end{aligned} \tag{3.4.168}$$

for any $\gamma > 0$. Note that the right hand side is independent of y. Since $\varphi_L \in C^\infty(\mathbb{T}^3_L)$, the Fourier coefficients of φ_L satisfy

$$(1 + |k|^2)^{5/2} |(\varphi_L)_k|^2 \leq C_{L,t} \gamma^{-t} \quad \text{for} \quad |k| \geq \gamma \tag{3.4.169}$$

for any $t > 0$. Using the positivity of $B - \eta W_T$ we can bound

$$\begin{aligned} \langle \varphi_L | (\mathbb{1} - W_\gamma^{-1/2})(\mathbb{B} - \eta W_T) | \varphi_L \rangle &\geq - \sum_{\substack{k \in \frac{2\pi}{L}\mathbb{Z}^3 \\ |k| > \gamma}} (B(k) - \eta W_T(k))(1 + |k|^2)^{1/2} |(\varphi_L)_k|^2 \\ &= - \sum_{\substack{k \in \frac{2\pi}{L}\mathbb{Z}^3 \\ |k| > \gamma}} \frac{(B(k) - \eta W_T(k))}{(1 + |k|^2)^2} (1 + |k|^2)^{5/2} |(\varphi_L)_k|^2 \\ &\geq -C_{L,t} \gamma^{-t} \sum_{\substack{k \in \frac{2\pi}{L}\mathbb{Z}^3 \\ |k| > \gamma}} \frac{1}{(1 + |k|^2)^2} \gtrsim_L \gamma^{-t-1}. \end{aligned} \tag{3.4.170}$$

Therefore we conclude, using the positivity of $\mathbb{1} - W_{\gamma_\beta}^{1/2}$ and of $B - \eta W_T$, that

$$\begin{aligned} & j_2 \mathbb{K} j_2 \\ & \geq j_2^2 \inf \operatorname{spec} \left[e_L - \frac{N}{2\alpha^2} + \frac{\eta \varepsilon^2}{4} - O(\gamma^{-t-1}) - \frac{1}{4\alpha^4} \Delta_\lambda + \langle \varphi | (\mathbb{1} - W_\gamma^{1/2})(B - \eta W_T) | \varphi \rangle \right] \\ & = j_2^2 \left(e_L + \frac{\eta \varepsilon^2}{4} - O(\gamma^{-t-1}) - \frac{1}{2\alpha^2} \operatorname{Tr} \left[\Pi \left(\mathbb{1} - \sqrt{(\mathbb{1} - W_\gamma^{1/2})(B - \eta W_T)} \right) \right] \right). \end{aligned} \tag{3.4.171}$$

We need to estimate the behavior in $N = \operatorname{rank} \Pi$, T and γ of the trace appearing in the last equation, which equals

$$\begin{aligned} & \operatorname{Tr} \left[\Pi \left(\mathbb{1} - \sqrt{(\mathbb{1} - W_\gamma^{1/2})(B - \eta W_T)} \right) \right] \\ & = \sum_{\substack{k \in \frac{2\pi}{L}\mathbb{Z}^3 \\ |k| \leq \Lambda}} \left(1 - \sqrt{(1 - W_\gamma(k)^{1/2})(B(k) - \eta W_T(k))} \right). \end{aligned} \tag{3.4.172}$$

The contribution to the sum from $|k| \leq \max\{\gamma, T\}$ can be bounded by $C(L\max\{\gamma, T\})^3$. For $|k| > \max\{\gamma, T\}$, $W_\gamma(k) = W_T(k) = (1+|k|^2)^{-1}$, and the coefficient under the square root in the last line of (3.4.172) behaves asymptotically for large momenta as $1-|k|^{-1}$. Hence, recalling (3.4.102), we conclude that

$$\operatorname{Tr}\left[\Pi\left(\mathbb{1} - \sqrt{(\mathbb{1} - W_\gamma^{1/2})(B - \eta W_T)}\right)\right] \leq O\left(\max\{\gamma, T\}^3\right) + O(\Lambda^2). \tag{3.4.173}$$

Because of (3.4.107), the first term on the right hand side is negligible compared to the second if we choose γ to equal α to some small enough power. Because t was arbitrary, we thus arrive at

$$j_2 \mathbb{K} j_2 \geq j_2^2 \left(e_L + \frac{\eta\varepsilon^2}{4} - O(\alpha^{-2}\Lambda^2)\right). \tag{3.4.174}$$

Therefore, if

$$\varepsilon \geq C_L \alpha^{-1}\Lambda \tag{3.4.175}$$

for a sufficiently large constant C_L, we conclude that for sufficiently large α and Λ

$$j_2 \mathbb{K} j_2 \geq j_2^2 e_L. \tag{3.4.176}$$

Proof of Theorem 3.2.2, lower bound

By combining the results (3.4.163) and (3.4.176) of the previous two subsections with (3.4.109) and (3.4.116), we obtain

$$\begin{aligned} \mathbb{K} &\geq j_1 \mathbb{K} j_1 + j_2 \mathbb{K} j_2 + O(\alpha^{-4}\varepsilon^{-2}) \\ &\geq j_1^2 \left[e_L - \frac{1}{2\alpha^2}\operatorname{Tr}\Big[(\mathbb{1} - (\mathbb{1} - K_L)^{1/2})\Big] + O(\varepsilon\alpha^{-2}) + O(\alpha^{-4})\right] + j_2^2 e_L + O(\alpha^{-4}\varepsilon^{-2}) \\ &\geq e_L - \frac{1}{2\alpha^2}\operatorname{Tr}\Big[(\mathbb{1} - (\mathbb{1} - K_L)^{1/2})\Big] + O(\varepsilon\alpha^{-2}) + O(\alpha^{-4}) + O(\alpha^{-4}\varepsilon^{-2}) \end{aligned} \tag{3.4.177}$$

under the constraint (3.4.175). With Proposition 3.4.3 we can thus conclude that

$$\begin{aligned} \inf\operatorname{spec}\mathbb{H}_L &\geq \inf\operatorname{spec}\mathbb{H}_L^\Lambda + O(\Lambda^{-5/2}) + O(\alpha^{-1}\Lambda^{-3/2}) + O(\alpha^{-2}\Lambda^{-1}) \\ &\geq \inf\operatorname{spec}\mathbb{K} + O(\Lambda^{-5/2}) + O(\alpha^{-1}\Lambda^{-3/2}) + O(\alpha^{-2}\Lambda^{-1}) \\ &\geq e_L - \frac{1}{2\alpha^2}\operatorname{Tr}\Big[(\mathbb{1} - (\mathbb{1} - K)^{1/2})\Big] + O(\varepsilon\alpha^{-2}) + O(\alpha^{-4}) + O(\alpha^{-4}\varepsilon^{-2}) \\ &\quad + O(\Lambda^{-5/2}) + O(\alpha^{-1}\Lambda^{-3/2}) + O(\alpha^{-2}\Lambda^{-1}). \end{aligned} \tag{3.4.178}$$

To minimize the error terms under the constraint (3.4.175), we pick $\varepsilon \sim \alpha^{-1/7}$ and $\Lambda \sim \alpha^{6/7}$, which yields the claimed estimate

$$\inf\operatorname{spec}\mathbb{H}_L \geq e_L - \frac{1}{2\alpha^2}\operatorname{Tr}\Big[(\mathbb{1} - (\mathbb{1} - K_L)^{1/2})\Big] + O(\alpha^{-15/7}). \tag{3.4.179}$$

This concludes the proof of the lower bound, and hence the proof of Theorem 3.2.2.

CHAPTER 4

Persistence of the Spectral Gap for the Landau–Pekar Equations

This Chapter contains the work

- Dario Feliciangeli, Simone Rademacher, and Robert Seiringer. Persistence of the spectral gap for the Landau–Pekar equations. *Letters in Mathematical Physics*, 111(1):1–19, 2021.

Abstract

The Landau–Pekar equations describe the dynamics of a strongly coupled polaron. Here we provide a class of initial data for which the associated effective Hamiltonian has a uniform spectral gap for all times. For such initial data, this allows us to extend the results on the adiabatic theorem for the Landau–Pekar equations and their derivation from the Fröhlich model obtained in previous works to larger times.

4.1 Introduction and Main Results

The Landau–Pekar equations [66] provide an effective description of the dynamics for a strongly coupled polaron, modeling an electron moving in an ionic crystal. The strength of the interaction of the electron with its self-induced polarization field is described by a coupling parameter $\alpha > 0$. In this system of coupled differential equations, the time evolution of the electron wave function $\psi_t \in H^1(\mathbb{R}^3)$ is governed by a Schrödinger equation with respect to an effective Hamiltonian h_{φ_t} depending on the polarization field $\varphi_t \in L^2(\mathbb{R}^3)$, which evolves according to a classical field equation. Motivated by the recent work in [73, 87, 74], we are interested in initial data for which the Hamiltonian h_{φ_t} possesses a uniform spectral gap (independent of t and α) above the infimum of its spectrum.

The Landau–Pekar equations are of the form

$$\begin{aligned} i\partial_t \psi_t &= h_{\varphi_t}\psi_t \\ i\alpha^2 \partial_t \varphi_t &= \varphi_t + \sigma_{\psi_t} \end{aligned} \tag{4.1.1}$$

with

$$h_\varphi = -\Delta + V_\varphi, \quad V_\varphi(x) = 2(2\pi)^{3/2}\,\mathrm{Re}\,[(-\Delta)^{-1/2}\varphi](x), \quad \sigma_\psi(x) = (2\pi)^{3/2}\left[(-\Delta)^{-1/2}|\psi|^2\right](x). \tag{4.1.2}$$

For initial data $(\psi_0, \varphi_0) \in H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$, (5.1.1) is well-posed for all times $t \in \mathbb{R}$ (see [38] or Lemma 4.2.1 below).

For $(\psi, \varphi) \in H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ with $\|\psi\|_2 = 1$, the energy functional corresponding to the Landau–Pekar equations is defined as

$$\mathcal{G}(\psi, \varphi) = \langle \psi, h_\varphi \psi \rangle + \|\varphi\|_2^2. \tag{4.1.3}$$

One readily checks that for solutions of (5.1.1), $\mathcal{G}(\psi_t, \varphi_t)$ is independent of t [38, Lemma 2.1], and the same holds for $\|\psi_t\|_2$. We also define

$$\mathcal{E}(\psi) = \inf_{\varphi \in L^2(\mathbb{R}^3)} \mathcal{G}(\psi, \varphi), \qquad \mathcal{F}(\varphi) = \inf_{\substack{\psi \in H^1(\mathbb{R}^3) \\ \|\psi\|_2 = 1}} \mathcal{G}(\psi, \varphi). \tag{4.1.4}$$

These three functionals are known as Pekar functionals and we shall discuss some of their properties in Section 4.2. It follows from the work in [76] that there exist $(\psi_{\mathrm{P}}, \varphi_{\mathrm{P}}) \in H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ with $\|\psi_{\mathrm{P}}\|_2 = 1$, called Pekar minimizers, realizing

$$\inf_{\psi, \varphi} \mathcal{G}(\psi, \varphi) = \mathcal{G}(\psi_{\mathrm{P}}, \varphi_{\mathrm{P}}) = \mathcal{E}(\psi_{\mathrm{P}}) = \mathcal{F}(\varphi_{\mathrm{P}}) = e_{\mathrm{P}} < 0\,, \tag{4.1.5}$$

and $(\psi_{\mathrm{P}}, \varphi_{\mathrm{P}})$ is unique up to symmetries (i.e., translations and multiplication of ψ_{P} by a constant phase factor). We also note that the Hamiltonian $h_{\varphi_{\mathrm{P}}}$ has a spectral gap above its ground state energy, i.e., $\Lambda(\varphi_{\mathrm{P}}) > 0$, where we denote for general $\varphi \in L^2(\mathbb{R}^3)$

$$\Lambda(\varphi) = \inf_{\substack{\lambda \in \mathrm{spec}(h_\varphi) \\ \lambda \neq e(\varphi)}} |\lambda - e(\varphi)| \quad \text{with} \quad e(\varphi) = \inf \mathrm{spec}\, h_\varphi\,. \tag{4.1.6}$$

In the following we consider solutions (ψ_t, φ_t) to the Landau–Pekar equations (5.1.1) with initial data (ψ_0, φ_0) such that its energy $\mathcal{G}(\psi_0, \varphi_0)$ is sufficiently close to e_{P}, and show that for such initial data the Hamiltonian h_{φ_t} possesses a uniform spectral gap above the infimum of its spectrum for all times $t \in \mathbb{R}$ and any coupling constant $\alpha > 0$. This is the content of the following Theorem.

Theorem 4.1.1. *For any $0 < \Lambda < \Lambda(\varphi_{\mathrm{P}})$ there exists $\varepsilon_\Lambda > 0$ such that if (ψ_t, φ_t) is the solution of the Landau–Pekar equations* (5.1.1) *with initial data $(\psi_0, \varphi_0) \in H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ with $\|\psi_0\|_2 = 1$ and $\mathcal{G}(\psi_0, \varphi_0) \leq e_{\mathrm{P}} + \varepsilon_\Lambda$, then*

$$\Lambda(\varphi_t) \geq \Lambda \quad \text{for all} \quad t \in \mathbb{R},\, \alpha > 0. \tag{4.1.7}$$

Theorem 4.1.1 is proved in Section 4.3. It provides a class of initial data for the Landau–Pekar equations for which the Hamiltonian h_{φ_t} has a uniform spectral gap for all times $t \in \mathbb{R}$. The existence of initial data with this particular property is of relevance for recent work [73, 87, 74] on the adiabatic theorem for the Landau–Pekar equations, and on their derivation from the Fröhlich model (where the polarization is described as a quantum field instead). For this particular initial data, the results obtained there can then be extended in the following way:

Adiabatic theorem. Due to the separation of time scales in (5.1.1), the Landau–Pekar equations decouple adiabatically for large α (see [73] or also [39] for an analogous one-dimensional model). To be more precise, in [73] the initial phonon state function is assumed to satisfy

$$\varphi_0 \in L^2(\mathbb{R}^3) \quad \text{with} \quad e(\varphi_0) = \inf \operatorname{spec} h_{\varphi_0} < 0, \tag{4.1.8}$$

which implies that h_{φ_0} has a spectral gap and that there exists a unique positive and normalized ground state ψ_{φ_0} of h_{φ_0}. Under this assumption, denoting by (ψ_t, φ_t) the solution of the Landau–Pekar equations (5.1.1) with initial data $(\psi_{\varphi_0}, \varphi_0)$, [73, Thm. II.1 & Rem. II.3] proves that there exist constants $C, T > 0$ (depending on φ_0) such that

$$\|\psi_t - e^{-i\int_0^t ds\, e(\varphi_s)}\psi_{\varphi_t}\|_2^2 \leq C\alpha^{-4} \quad \text{for all} \quad |t| \leq T\alpha^2, \tag{4.1.9}$$

where ψ_{φ_t} denotes the unique positive and normalized ground state of h_{φ_t}. The restriction on $|t|$ in (4.1.9) is due to the need of ensuring that the spectral gap of the effective Hamiltonian h_{φ_t} does not become too small for initial data satisfying (4.1.8), which is only proven (in [73, Lemma II.1]) for times $|t| \leq T\alpha^2$. Nevertheless, *assuming* that there exists $\Lambda > 0$ such that $\Lambda(\varphi_t) > \Lambda$ for all times $t \in \mathbb{R}$, the adiabatic theorem in [73, Thm. II.1] allows to approximate ψ_t by $e^{-i\int_0^t ds\, e(\varphi_s)}\psi_{\varphi_t}$ for all times $|t| \ll \alpha^4$. This raises the question about initial data for which the existence of a spectral gap of order one holds true for longer times, and Theorem 4.1.1 answers this question. In fact, by suitably adjusting the phase factor, we can prove the following stronger result.

Corollary 4.1.1. *Let $\varphi_0 \in L^2(\mathbb{R}^3)$ be such that*

$$\mathcal{F}(\varphi_0) \leq e_{\mathrm{P}} + \varepsilon \tag{4.1.10}$$

for sufficiently small $\varepsilon > 0$. Then h_{φ_0} has a ground state ψ_{φ_0}. Let (ψ_t, φ_t) be the solution to the Landau–Pekar equations (5.1.1) *with initial data $(\psi_{\varphi_0}, \varphi_0)$ and define*

$$\nu(s) = -\alpha^{-4}\langle \psi_{\varphi_s}, V_{\mathrm{Im}\,\varphi_s} R_{\varphi_s}^3 V_{\mathrm{Im}\,\varphi_s}\psi_{\varphi_s}\rangle \quad \textit{and} \quad \widetilde{\psi}_t = e^{i\int_0^t ds (e(\varphi_s)+\nu(s))}\psi_t, \tag{4.1.11}$$

where $R_{\varphi_s} = q_s(h_{\varphi_s} - e(\varphi_s))^{-1}q_s$ with $q_s = 1 - |\psi_{\varphi_s}\rangle\langle\psi_{\varphi_s}|$. Then, there exists a $C > 0$ (independent of φ_0 and α) such that

$$\|\widetilde{\psi}_t - \psi_{\varphi_t}\|_2^2 \leq C\varepsilon\alpha^{-4}\left(1 + \alpha^{-2}|t|\right)e^{C\alpha^{-4}|t|}. \tag{4.1.12}$$

Our proof in Section 4.3 shows that the smallness condition on ε in Corollary 4.1.1 can be made explicit in terms of properties of φ_{P}. It also shows that $\min_{\theta\in[0,2\pi)} \|e^{i\theta}\psi_t - \psi_{\varphi_t}\|_2^2 \leq C\varepsilon$ for all times t, independently of α. The bound (4.1.12) improves upon this for large α as long as $\alpha^{-4}|t|e^{C\alpha^{-4}|t|} \ll \alpha^2$ and hence, in particular, for $|t| \lesssim \alpha^4$.

Effective dynamics for the Fröhlich Hamiltonian. As already mentioned, the Landau–Pekar equations provide an effective description of the dynamics for a strongly coupled polaron. Its true dynamics is described by the Fröhlich Hamiltonian [47] H_α acting on $L^2(\mathbb{R}^3) \otimes \mathcal{F}$, the tensor product of the Hilbert space $L^2(\mathbb{R}^3)$ for the electron and the bosonic Fock space $\mathcal{F}$ for the phonons. We refer to [73, 74] for a detailed definition. Pekar product states of the form $\psi_t \otimes W(\alpha^2\varphi_t)\Omega$, with (ψ_t, φ_t) a solution of the Landau–Pekar equations, W the Weyl operator and Ω the Fock space vacuum, were proven in [73, Thm. II.2] to approximate the dynamics defined by the Fröhlich Hamiltonian H_α for times $|t| \ll \alpha^2$. Recently, it was shown in [74] that in order to obtain a norm approximation valid for times of order α^2, one needs to implement correlations among phonons, which are captured by a suitable Bogoliubov dynamics acting on the Fock space of the phonons only. In fact, considering initial data satisfying (4.1.8), [74, Theorem I.3] proves that there exist constants $C, T > 0$ (depending on φ_0) such that

$$\|e^{-iH_\alpha t}\psi_{\varphi_0}\otimes W(\alpha^2\varphi_0)\Omega - e^{-i\int_0^t ds\,\omega(s)}\psi_t\otimes W(\alpha^2\varphi_t)\Upsilon_t\|_{L^2(\mathbb{R}^3)\otimes\mathcal{F}} \leq C\alpha^{-1} \quad \text{for all} \quad |t| \leq T\alpha^2, \tag{4.1.13}$$

where $\omega(s) = \alpha^2 \operatorname{Im}\langle\varphi_s, \partial_s\varphi_s\rangle + \|\varphi_s\|_2^2$ and Υ_t is the solution of the dynamics of a suitable Bogoliubov Hamiltonian on $\mathcal{F}$ (see [74, Definition I.2] for a precise definition). As for the adiabatic theorem discussed above, the restriction to times $|t| \leq T\alpha^2$ results from the need of a spectral gap of h_{φ_t} of order one (compare with [74, Remark I.4]), which under the sole assumption (4.1.8) is guaranteed by [73, Lemma II.1] only for $|t| \leq T\alpha^2$. Theorem 4.1.1 now provides a class of initial data for which the above norm approximation holds true for all times of order α^2, in the following sense.

Corollary 4.1.2. *Let $\varphi_0 \in L^2(\mathbb{R}^3)$ be such that*

$$\mathcal{F}(\varphi_0) \leq e_{\mathrm{P}} + \varepsilon \tag{4.1.14}$$

for sufficiently small $\varepsilon > 0$. Then h_{φ_0} has a ground state ψ_{φ_0}. Let (ψ_t, φ_t) be the solution to the Landau–Pekar equations (5.1.1) *with initial data $(\psi_{\varphi_0}, \varphi_0)$. Then there exists a $C > 0$ (independent of φ_0 and α) such that*

$$\|e^{-iH_\alpha t}\psi_{\varphi_0}\otimes W(\alpha^2\varphi_0)\Omega - e^{-i\int_0^t ds\,\omega(s)}\psi_t\otimes W(\alpha^2\varphi_t)\Upsilon_t\|_{L^2(\mathbb{R}^3)\otimes\mathcal{F}} \leq C\alpha^{-1}e^{C\alpha^{-2}|t|}. \tag{4.1.15}$$

Again, the smallness condition on ε in Corollary 4.1.2 can be made explicit in terms of properties of φ_{P}. Corollary 4.1.2 is an immediate consequence of Theorem 4.1.1 and the method of proof in [74], as explained in [74, Remark I.4].

4.2 Properties of the Spectral Gap and the Pekar Functionals

Throughout the paper, we use the symbol C for generic constants, and their value might change from one occurrence to the next.

4.2.1 Preliminary Lemmas

We begin by stating some preliminary Lemmas we shall need throughout the following discussion.

Lemma 4.2.1 (Lemma 2.1 in [38]). *For any $(\psi_0, \varphi_0) \in H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$, there is a unique global solution (ψ_t, φ_t) of the Landau–Pekar equations* (5.1.1)*. Moreover, $\|\psi_0\|_2 = \|\psi_t\|_2$, $\mathcal{G}(\psi_0, \varphi_0) = \mathcal{G}(\psi_t, \varphi_t)$ for all $t \in \mathbb{R}$ and there exists a constant $C > 0$ such that*

$$\|\psi_t\|_{H^1(\mathbb{R}^3)} \leq C, \quad \|\varphi_t\|_2 \leq C \tag{4.2.1}$$

for all $\alpha > 0$ and all $t \in \mathbb{R}$.

The following Lemma collects some properties of V_φ and σ_ψ (see also [73, Lemma III.2] and [74, Lemma II.2]).

Lemma 4.2.2. *There exists $C > 0$ such that for every $\varphi \in L^2(\mathbb{R}^3)$ and $\psi \in H^1(\mathbb{R}^3)$*

$$\|V_\varphi\|_6 \leq C\|\varphi\|_2 \quad \text{and} \quad \|V_\varphi \psi\|_2 \leq C\|\varphi\|_2\|\psi\|_{H^1(\mathbb{R}^3)}. \tag{4.2.2}$$

Moreover, there exists $C > 0$ such that for all $\psi_1, \psi_2 \in H^1(\mathbb{R}^3)$

$$\|\sigma_{\psi_1} - \sigma_{\psi_2}\|_2 \leq C\left(\|\psi_1\|_2 + \|\psi_2\|_2\right) \min_{\theta\in[0,2\pi)} \|e^{i\theta}\psi_1 - \psi_2\|_{H^1(\mathbb{R}^3)}. \tag{4.2.3}$$

Proof. The first two inequalities follow immediately from [73, Lemma III.2] and [74, Lemma II.2]. For the last inequality, we note that $\sigma_\psi = \sigma_{e^{i\theta}\psi}$ for arbitrary $\theta \in \mathbb{R}$. Hence, it is enough to prove the result for $\theta = 0$. We write the difference

$$\begin{aligned} \widehat{\sigma}_{\psi_1}(k) - \widehat{\sigma}_{\psi_2}(k) &= |k|^{-1}\left(\langle \psi_1, e^{-ik\cdot}\psi_1\rangle - \langle \psi_2, e^{-ik\cdot}\psi_2\rangle\right) \\ &= |k|^{-1}\left(\langle \psi_1 - \psi_2, e^{-ik\cdot}\psi_1\rangle + \langle \psi_2, e^{-ik\cdot}(\psi_1-\psi_2)\rangle\right). \end{aligned} \tag{4.2.4}$$

where $\widehat{\sigma}_\psi(k) = (2\pi)^{-3/2}\int dx\, e^{-ik\cdot x}\sigma_\psi(x)$ denotes the Fourier transform of σ_ψ. Thus,

$$\|\sigma_{\psi_1} - \sigma_{\psi_2}\|_2^2 \leq 2\int dk \frac{1}{|k|^2}\left(|\langle \psi_1 - \psi_2, e^{-ik\cdot}\psi_1\rangle|^2 + |\langle \psi_2, e^{-ik\cdot}(\psi_1-\psi_2)\rangle|^2\right). \tag{4.2.5}$$

For the first term, we write

$$\int \frac{dk}{|k|^2}|\langle \psi_1 - \psi_2, e^{-ik\cdot}\psi_1\rangle|^2 = C\int \frac{dx\,dy}{|x-y|}(\psi_1-\psi_2)(x)\overline{(\psi_1-\psi_2)(y)}\,\overline{\psi_1(x)}\psi_1(y). \tag{4.2.6}$$

The Hardy-Littlewood-Sobolev inequality implies that

$$\int \frac{dk}{|k|^2}|\langle \psi_1 - \psi_2, e^{-ik\cdot}\psi_1\rangle|^2 \leq C\|\psi_1\overline{(\psi_1-\psi_2)}\|_{6/5}^2 \leq C\|\psi_1-\psi_2\|_3^2\|\psi_1\|_2^2, \tag{4.2.7}$$

and we obtain with the Sobolev inequality that

$$\int \frac{dk}{|k|^2}|\langle \psi_1 - \psi_2, e^{-ik\cdot}\psi_1\rangle|^2 \leq C\|\psi_1-\psi_2\|_{H^1(\mathbb{R}^3)}^2\|\psi_1\|_2^2. \tag{4.2.8}$$

The second term of (4.2.5) can be bounded in a similar way, and we obtain the desired estimate. □

We recall the definition of the resolvent

$$R_\varphi = q_{\psi_\varphi}\left(h_\varphi - e(\varphi)\right)^{-1} q_{\psi_\varphi}, \tag{4.2.9}$$

where $q_{\psi_\varphi} = 1 - |\psi_\varphi\rangle\langle\psi_\varphi|$. In the following Lemma we collect useful estimates on R_φ.

Lemma 4.2.3. *There exists $C > 0$ such that*

$$\|R_\varphi\| = \Lambda(\varphi)^{-1}, \quad \|\left(-\Delta+1\right)^{1/2} R_\varphi^{1/2}\| \leq C(1 + \|\varphi\|_2\|R_\varphi^{1/2}\|) \tag{4.2.10}$$

for any $\varphi \in L^2(\mathbb{R}^3)$ with $e(\varphi) < 0$.

Proof. The first identity for the norm of the resolvent follows immediately from the definition of the spectral gap $\Lambda(\varphi)$ in (4.1.6). For $\psi \in L^2(\mathbb{R}^3)$ we have

$$\|\left(-\Delta+1\right)^{1/2} R_\varphi^{1/2}\psi\|_2^2 = \langle \psi, R_\varphi^{1(2}\left(-\Delta+1\right) R_\varphi^{1/2}\psi\rangle. \tag{4.2.11}$$

It follows from Lemma 4.2.2 that there exists $C > 0$ such that

$$\begin{aligned} \|\left(-\Delta+1\right)^{1/2} R_\varphi^{1/2}\psi\|_2^2 &\leq C\,\langle \psi, R_\varphi^{1/2}\left(h_\varphi + C\|\varphi\|_2^2\right) R_\varphi^{1/2}\psi\rangle \\ &= C\,\|q_{\psi_\varphi}\psi\|_2^2 + C\left(C\|\varphi\|_2^2 + e(\varphi)\right)\|R_\varphi^{1/2}\psi\|_2^2. \end{aligned} \tag{4.2.12}$$

Since $e(\varphi) < 0$ this implies the desired estimate. □

4.2.2 Perturbative properties of ground states and of the spectral gap

Since the essential spectrum of h_φ is $\mathbb{R}_+$, the assumption $e(\varphi) < 0$ guarantees the existence of a ground state (denoted by ψ_φ) and of a spectral gap $\Lambda(\varphi) > 0$ of h_φ. In the next two Lemmas we investigate the behavior of $\Lambda(\varphi)$ and ψ_φ under L^2-perturbations of φ.

Lemma 4.2.4. *Let φ_0 satisfy* (4.1.8)*, and let $0 < \Lambda < \Lambda(\varphi_0)$. Then, there exists $\delta_\Lambda > 0$ (depending, besides Λ, only on the spectrum of h_{φ_0} and $\|\varphi_0\|_2$) such that*

$$\Lambda(\varphi) \geq \Lambda \quad \text{for all} \quad \varphi \in L^2(\mathbb{R}^3) \quad \text{with} \quad \|\varphi - \varphi_0\|_2 \leq \delta_\Lambda. \tag{4.2.13}$$

Proof. By definition of the spectral gap

$$\Lambda(\varphi) = e_1(\varphi) - e(\varphi), \tag{4.2.14}$$

where $e(\varphi)$ denotes the ground state energy of h_φ, and $e_1(\varphi)$ its first excited eigenvalue if it exists, or otherwise $e_1(\varphi) = 0$ (which is the bottom of the essential spectrum). By the min-max principle we can write

$$e_1(\varphi) = \inf_{\substack{A \subset L^2(\mathbb{R}^3) \\ \dim A = 2}} \sup_{\substack{\psi \in A \\ \|\psi\|_2 = 1}} \langle \psi, h_\varphi \psi \rangle. \tag{4.2.15}$$

For $\psi \in H^1(\mathbb{R}^3)$ with $\|\psi\|_2 = 1$ we find with Lemma 4.2.2

$$\begin{aligned} \langle \psi, h_\varphi \psi \rangle &= \langle \psi, h_{\varphi_0} \psi \rangle + \langle \psi, V_{\varphi - \varphi_0} \psi \rangle \\ &\leq \langle \psi, h_{\varphi_0} \psi \rangle + C \|\varphi - \varphi_0\|_2 \|\psi\|^2_{H^1(\mathbb{R}^3)}. \end{aligned} \tag{4.2.16}$$

Moreover, for $\varepsilon > 0$,

$$\|\psi\|^2_{H^1(\mathbb{R}^3)} = \langle \psi, h_{\varphi_0} \psi \rangle - \langle \psi, V_{\varphi_0} \psi \rangle + 1 \leq \langle \psi, h_{\varphi_0} \psi \rangle + \varepsilon \|\psi\|^2_{H^1(\mathbb{R}^3)} + C\varepsilon^{-1} \|\varphi_0\|_2^2 + 1. \tag{4.2.17}$$

Hence, choosing $\varepsilon = 1/2$, we find

$$\|\psi\|^2_{H^1(\mathbb{R}^3)} \leq 2 \langle \psi, h_{\varphi_0} \psi \rangle + C(\|\varphi_0\|_2^2 + 1). \tag{4.2.18}$$

Thus, if $\|\varphi - \varphi_0\|_2 \leq \delta$, we have

$$\langle \psi, h_\varphi \psi \rangle \leq (1 + C\delta) \langle \psi, h_{\varphi_0} \psi \rangle + C\delta(\|\varphi_0\|_2^2 + 1), \tag{4.2.19}$$

and similarly

$$\langle \psi, h_\varphi \psi \rangle \geq (1 - C\delta) \langle \psi, h_{\varphi_0} \psi \rangle - C\delta(\|\varphi_0\|_2^2 + 1). \tag{4.2.20}$$

Since $e(\varphi_0), e(\varphi_1) \leq 0$, we therefore find

$$\Lambda(\varphi) \geq \Lambda(\varphi_0) - C\delta \left(e(\varphi_0) + e_1(\varphi_0) + 2(\|\varphi_0\|_2^2 + 1) \right) \geq \Lambda(\varphi_0) - 2C\delta(\|\varphi_0\|_2^2 + 1) > \Lambda \tag{4.2.21}$$

for sufficiently small $\delta = \delta_\Lambda > 0$. □

Lemma 4.2.5. *Let φ_0 satisfy* (4.1.8)*, and let $\varphi \in L^2(\mathbb{R}^3)$ with*

$$\|\varphi - \varphi_0\| \leq \delta_{\varphi_0} \tag{4.2.22}$$

for sufficiently small $\delta_{\varphi_0} > 0$. Then, there exists a unique positive and normalized ground state ψ_φ of h_φ. Moreover, there exists $C > 0$ (independent of φ) such that

$$\|\psi_{\varphi_0} - \psi_\varphi\|_{H^1(\mathbb{R}^3)} \leq C \|\varphi - \varphi_0\|_2. \tag{4.2.23}$$

Proof. We write

$$\psi_\varphi - \psi_{\varphi_0} = \int_0^1 d\mu\, \partial_\mu \psi_{\varphi_\mu}, \tag{4.2.24}$$

with $\varphi_\mu = \varphi_0 + \mu(\varphi - \varphi_0)$. Note that ψ_{φ_μ} is well defined for all $\mu \in [0,1]$, since

$$\|\varphi_\mu - \varphi_0\|_2 = \mu\|\varphi - \varphi_0\|_2 \leq \mu\delta_{\varphi_0} \leq \delta_{\varphi_0} \tag{4.2.25}$$

and therefore Lemma 4.2.4 guarantees the existence of a spectral gap

$$\Lambda(\varphi_\mu) \geq \Lambda > 0 \tag{4.2.26}$$

for sufficiently small δ_{φ_0}, uniformly in $\mu \in [0,1]$. First order perturbation theory yields

$$\partial_\mu \psi_{\varphi_\mu} = R_{\varphi_\mu} V_{\varphi_0 - \varphi} \psi_{\varphi_\mu} \tag{4.2.27}$$

and it follows from Lemma 4.2.2 that

$$\begin{aligned} \|\psi_{\varphi_0} - \psi_\varphi\|_{H^1(\mathbb{R}^3)} &\leq \int_0^1 d\mu\, \|R_{\varphi_\mu} V_{\varphi - \varphi_0} \psi_{\varphi_\mu}\|_{H^1(\mathbb{R}^3)} \\ &\leq C \int_0^1 d\mu\, \|\,(-\Delta + 1)^{1/2}\, R_{\varphi_\mu}^{1/2}\|^2\, \|\varphi - \varphi_0\|_2. \end{aligned} \tag{4.2.28}$$

Lemma 4.2.3 shows that

$$\|\,(-\Delta + 1)^{1/2}\, R_{\varphi_\mu}\| \leq C\left(1 + \|\varphi_\mu\|_2 \|R_{\varphi_\mu}\|\right). \tag{4.2.29}$$

Since $\|\varphi_\mu\|_2 \leq \|\varphi_0\|_2 + \mu\|\varphi - \varphi_0\|_2 \leq \|\varphi_0\|_2 + \delta_{\varphi_0}$, the bound (4.2.26) implies that the right-hand side of (4.2.29) is bounded independently of μ. Hence the desired estimate (4.2.23) follows. □

4.2.3 Pekar Functionals

Recall the definition of the Pekar Functionals $\mathcal{G}$, $\mathcal{E}$ and $\mathcal{F}$ in (5.2.1) and (4.1.4), and note that

$$\mathcal{G}(\psi, \varphi) = \mathcal{E}(\psi) + \|\varphi + \sigma_\psi\|_2^2. \tag{4.2.30}$$

As was shown in [76], $\mathcal{E}$ admits a unique *strictly positive and radially symmetric* minimizer, which is smooth and will be denoted by ψ_{P}. Moreover, the set of all minimizers of $\mathcal{E}$ coincides with

$$\Theta(\psi_{\mathrm{P}}) = \{e^{i\theta}\psi_{\mathrm{P}}(\,\cdot\, - y)\,|\,\theta \in [0, 2\pi),\, y \in \mathbb{R}^3\}. \tag{4.2.31}$$

This clearly implies that the set of minimizers of $\mathcal{F}$ coincides with

$$\Omega(\varphi_{\mathrm{P}}) = \{\varphi_{\mathrm{P}}(\,\cdot\, - y)\,|\,y \in \mathbb{R}^3\} \quad \text{with} \quad \varphi_{\mathrm{P}} = -\sigma_{\psi_{\mathrm{P}}}. \tag{4.2.32}$$

In the following we prove quadratic lower bounds for the Pekar Functionals $\mathcal{E}$ and $\mathcal{F}$. The key ingredients are the results obtained in [70]. In particular, these results allow to infer, using standard arguments, the following Lemma 4.2.6, which provides the quadratic lower bounds for $\mathcal{E}$. (We spell out its proof for completeness in the Appendix; a very similar proof in a slightly different setting is also given in [41]). Based on the bound for $\mathcal{E}$, it is then quite straightforward to obtain the quadratic lower bound for $\mathcal{F}$ in the subsequent Lemma 4.2.7.

Lemma 4.2.6 (Quadratic Bounds for $\mathcal{E}$)**.** *There exists a positive constant κ such that, for any L^2-normalized $\psi \in H^1(\mathbb{R}^3)$,*

$$\mathcal{E}(\psi) - e_{\mathrm{P}} \geq \kappa \min_{\substack{y\in\mathbb{R}^3 \\ \theta\in[0,2\pi)}} \|\psi - e^{i\theta}\psi_{\mathrm{P}}(\,\cdot\, - y)\|^2_{H^1(\mathbb{R}^3)} = \kappa\,\mathrm{dist}^2_{H^1(\mathbb{R}^3)}(\psi, \Theta(\psi_{\mathrm{P}})). \tag{4.2.33}$$

Lemma 4.2.7 (Quadratic Bounds for $\mathcal{F}$)**.** *There exists a positive constant τ such that, for any $\varphi \in L^2(\mathbb{R}^3)$,*

$$\mathcal{F}(\varphi) - e_{\mathrm{P}} \geq \tau \min_{y\in\mathbb{R}^3} \|\varphi - \varphi_{\mathrm{P}}(\,\cdot\, - y)\|_2^2 = \tau\,\mathrm{dist}^2_{L^2(\mathbb{R}^3)}(\varphi, \Omega(\varphi_{\mathrm{P}})). \tag{4.2.34}$$

Proof. Recalling that

$$\mathcal{F}(\varphi) = \inf_{\substack{\|\psi\|_2=1 \\ \psi\in H^1(\mathbb{R}^3)}} \mathcal{G}(\psi,\varphi) \tag{4.2.35}$$

our claim trivially follows by showing that for any L^2-normalized $\psi \in H^1(\mathbb{R}^3)$ and $\varphi \in L^2(\mathbb{R}^3)$

$$\mathcal{G}(\psi,\varphi) - e_{\mathrm{P}} \geq \tau\ \mathrm{dist}^2_{L^2(\mathbb{R}^3)}(\varphi, \Omega(\varphi_{\mathrm{P}})). \tag{4.2.36}$$

For any such ψ let $y^* \in \mathbb{R}^3$ and $\theta^* \in [0, 2\pi)$ be such that

$$\|\psi - e^{i\theta^*}\psi_{\mathrm{P}}(\,\cdot\, - y^*)\|^2_{H^1(\mathbb{R}^3)} = \mathrm{dist}^2_{H^1(\mathbb{R}^3)}(\psi, \Theta(\psi_{\mathrm{P}})), \tag{4.2.37}$$

and denote $e^{i\theta^*}\psi_{\mathrm{P}}(\,\cdot\, - y^*)$ by ψ^*_{P}. By using the previous Lemma 4.2.6, the fact that ψ and ψ^*_{P} are L^2-normalized, (4.2.3) and completing the square, we obtain for, some positive $\kappa^* > 0$,

$$\begin{aligned}
\mathcal{G}(\psi,\varphi) - e_{\mathrm{P}} &= \mathcal{E}(\psi) - e_{\mathrm{P}} + \|\varphi + \sigma_\psi\|_2^2 \geq \kappa\|\psi - \psi^*_{\mathrm{P}}\|^2_{H^1(\mathbb{R}^3)} + \|\varphi + \sigma_\psi\|_2^2 \\
&\geq \kappa^*\|\sigma_\psi - \sigma_{\psi^*_{\mathrm{P}}}\|_2^2 + \|\varphi + \sigma_\psi\|_2^2 \\
&= \|(1+\kappa^*)^{1/2}(\sigma_{\psi^*_{\mathrm{P}}} - \sigma_\psi) - (1+\kappa^*)^{-1/2}(\varphi + \sigma_{\psi^*_{\mathrm{P}}})\|_2^2 + \frac{\kappa^*}{1+\kappa^*}\|\varphi + \sigma_{\psi^*_{\mathrm{P}}}\|_2^2 \\
&\geq \frac{\kappa^*}{1+\kappa^*}\|\varphi - \varphi_{\mathrm{P}}(\,\cdot\, - y^*)\|_2^2 \geq \frac{\kappa^*}{1+\kappa^*}\,\mathrm{dist}^2_{L^2(\mathbb{R}^3)}(\varphi, \Omega(\varphi_{\mathrm{P}})).
\end{aligned} \tag{4.2.38}$$

This completes the proof of (4.2.36), and hence of the Lemma, with $\tau = \kappa^*/(1+\kappa^*)$. □

Remark 4.2.1. *The two previous quadratic bounds on $\mathcal{E}$ and $\mathcal{F}$ clearly imply, together with* (4.1.4)*, that, for any L^2-normalized $\psi \in H^1(\mathbb{R}^3)$ and any $\varphi \in L^2(\mathbb{R}^3)$, having low energy guarantees closeness to the surfaces of minimizers $\Theta(\psi_{\mathrm{P}})$ and $\Omega(\varphi_{\mathrm{P}})$, i.e.*

$$\mathcal{G}(\psi,\varphi) \leq e_{\mathrm{P}}+\varepsilon \quad \Rightarrow \quad \mathcal{E}(\psi), \mathcal{F}(\varphi) \leq e_{\mathrm{P}}+\varepsilon \quad \Rightarrow \quad \mathrm{dist}^2_{H^1}(\psi, \Theta(\psi_{\mathrm{P}})), \mathrm{dist}^2_{L^2}(\varphi, \Omega(\varphi_{\mathrm{P}})) \leq C\varepsilon\,. \tag{4.2.39}$$

Finally, we exploit the previous estimate to obtain the following Lemma. It states that for couples (ψ, φ) which have low energy ψ is close to ψ_φ, the ground state of h_φ, and φ is close to $-\sigma_{\psi_\varphi}$, in the following sense.

Lemma 4.2.8. *Let $\varepsilon > 0$ be sufficiently small, $\psi \in H^1(\mathbb{R}^3)$ be L^2-normalized, $\varphi \in L^2(\mathbb{R}^3)$ and let (ψ, φ) be such that*

$$\mathcal{G}(\psi,\varphi) \leq e_{\mathrm{P}} + \varepsilon\,. \tag{4.2.40}$$

Then h_φ has a positive ground state ψ_φ, and there exists $C > 0$ (independent of (ψ, φ)) such that

$$\min_{\theta\in[0,2\pi)} \|\psi - e^{i\theta}\psi_\varphi\|^2_{H^1(\mathbb{R}^3)} \leq C\varepsilon, \tag{4.2.41}$$

$$\|\varphi + \sigma_{\psi_\varphi}\|_2^2 \leq C\varepsilon. \tag{4.2.42}$$

Proof. Since $\mathcal{F}(\varphi) \leq \mathcal{G}(\psi, \varphi)$ for any L^2-normalized $\psi \in H^1(\mathbb{R}^3)$, Lemma 4.2.7 implies that for any $\delta > 0$ there exists $\varepsilon_\delta > 0$ such that $\operatorname{dist}_{L^2}(\varphi, \Omega(\varphi_{\mathrm{P}})) \leq \delta$ whenever $\mathcal{G}(\psi, \varphi) \leq e_{\mathrm{P}} + \varepsilon_\delta$. Moreover, by Lemma 4.2.4, there exists $\bar{\delta} > 0$ such that if $\operatorname{dist}_{L^2}(\varphi, \Omega(\varphi_{\mathrm{P}})) \leq \bar{\delta}$ then ψ_φ exists. We then pick $\varepsilon = \varepsilon_{\bar{\delta}}$ and this guarantees that under the hypothesis of the Lemma ψ_φ is well defined.

Using Lemmas 4.2.6 and 4.2.7, the assumption (4.2.40) implies that there exist y_1 and y_2 such that

$$\min_{\theta \in [0.2\pi)} \|\psi - e^{i\theta}\psi_{\mathrm{P}}(\,\cdot\, - y_1)\|_{H^1(\mathbb{R}^3)}^2 \leq C\varepsilon, \quad \|\varphi - \varphi_{\mathrm{P}}(\,\cdot\, - y_2)\|_2^2 \leq C\varepsilon. \tag{4.2.43}$$

Moreover, since

$$e_{\mathrm{P}} + \varepsilon \geq \mathcal{G}(\psi, \varphi) = \mathcal{E}(\psi) + \|\varphi + \sigma_\psi\|_2^2 \geq e_{\mathrm{P}} + \|\varphi + \sigma_\psi\|_2^2, \tag{4.2.44}$$

we also have

$$\|\varphi + \sigma_\psi\|_2^2 \leq \varepsilon. \tag{4.2.45}$$

In combination, the second bound in (4.2.43) and (4.2.45) imply

$$\|\varphi_{\mathrm{P}}(\,\cdot\, - y_2) + \sigma_\psi\|_2^2 \leq C\varepsilon. \tag{4.2.46}$$

Moreover, with the aid of (4.2.3) and the first bound in (4.2.43), we obtain

$$\|\varphi_{\mathrm{P}}(\,\cdot\, - y_1) + \sigma_\psi\|_2^2 = \|\sigma_{\psi_{\mathrm{P}}(\,\cdot\,-y_1)} - \sigma_\psi\|_2^2 \leq C \min_{\theta \in [0,2\pi)} \|\psi - e^{i\theta}\psi_{\mathrm{P}}(\,\cdot\, - y_1)\|_{H^1}^2 \leq C\varepsilon. \tag{4.2.47}$$

By putting the second equation in (4.2.43), (4.2.46) and (4.2.47) together, we can hence conclude that

$$\|\varphi - \varphi_{\mathrm{P}}(\,\cdot\, - y_1)\|_2 \leq \|\varphi - \varphi_{\mathrm{P}}(\,\cdot\, - y_2)\|_2 + \|\varphi_{\mathrm{P}}(\,\cdot\, - y_2) + \sigma_\psi\|_2 + \|\sigma_\psi + \varphi_{\mathrm{P}}(\,\cdot\, - y_1)\|_2 \leq C\varepsilon^{1/2}. \tag{4.2.48}$$

Therefore, using Lemma 4.2.5, we obtain

$$\begin{aligned} \|\psi - e^{i\theta}\psi_\varphi\|_{H^1} &\leq \|\psi - e^{i\theta}\psi_{\mathrm{P}}(\,\cdot\, - y_1)\|_{H^1} + \|\psi_{\mathrm{P}}(\,\cdot\, - y_1) - \psi_\varphi\|_{H^1} \\ &= \|\psi - e^{i\theta}\psi_{\mathrm{P}}(\,\cdot\, - y_1)\|_{H^1} + \|\psi_{\varphi_{\mathrm{P}}(\,\cdot\,-y_1)} - \psi_\varphi\|_{H^1} \\ &\leq \|\psi - e^{i\theta}\psi_{\mathrm{P}}(\,\cdot\, - y_1)\|_{H^1} + C\|\varphi_{\mathrm{P}}(\,\cdot\, - y_1) - \varphi\|_2 \,. \end{aligned} \tag{4.2.49}$$

This yields (4.2.41) after taking the infimum over $\theta \in [0, 2\pi)$ and using (4.2.48) and the first bound in (4.2.43). To prove (4.2.42), we use (4.2.45), (4.2.3), the normalization of ψ and ψ_φ and (4.2.41) to obtain

$$\|\varphi + \sigma_{\psi_\varphi}\|_2 \leq \|\varphi + \sigma_\psi\|_2 + \|\sigma_\psi - \sigma_{\psi_\varphi}\|_2 \leq \varepsilon^{1/2} + C \min_{\theta \in [0,2\pi)} \|\psi - e^{i\theta}\psi_\varphi\|_{H^1} \leq C\varepsilon^{1/2}. \tag{4.2.50}$$

□

4.3 Proof of the Main Results

The conservation of $\mathcal{G}$ along solutions of the Landau–Pekar equations allows to apply the tools developed in Section 4.2 to get results valid for all times. This will in particular allow us to prove the results stated in Section 4.1. When combined with energy conservation, Remark 4.2.1 shows that we can estimate the distance to the sets of Pekar minimizers of solutions of the Landau–Pekar equations only in terms of the energy of their initial data. Since $\Omega(\varphi_{\mathrm{P}})$ contains only real-valued functions this yields bounds on the L^2-norm of the imaginary part of φ_t. That is, there exists a $C > 0$ such that if (ψ_t, φ_t) solves the Landau–Pekar equations (5.1.1) with initial data (ψ_0, φ_0), then

$$\min_{\substack{y\in\mathbb{R}^3\\ \theta\in[0,2\pi)}} \|\psi_t - e^{i\theta}\psi_{\mathrm{P}}(\,\cdot\,-y)\|^2_{H^1(\mathbb{R}^3)} \leq C(\mathcal{G}(\psi_0,\varphi_0)-e_{\mathrm{P}}), \quad \|\operatorname{Im}\,\varphi_t\|_2^2 \leq C(\mathcal{G}(\psi_0,\varphi_0)-e_{\mathrm{P}}),$$
$$\min_{y\in\mathbb{R}^3}\|\operatorname{Re}\,\varphi_t - \varphi_{\mathrm{P}}(\,\cdot\,-y)\|_2^2 \leq C(\mathcal{G}(\psi_0,\varphi_0)-e_{\mathrm{P}}) \tag{4.3.1}$$

for all $t\in\mathbb{R}$ and $\alpha>0$. It is then straightforward to obtain a proof of Theorem 4.1.1.

Proof of Theorem 4.1.1. Let $0<\Lambda<\Lambda(\varphi_{\mathrm{P}})$ and let (ψ_t,φ_t) denote the solution to the Landau–Pekar equations with initial data (ψ_0,φ_0) satisfying $\mathcal{G}(\psi_0,\varphi_0)\leq e_{\mathrm{P}}+\varepsilon_\Lambda$. From (4.3.1) we deduce that for any $t\in\mathbb{R}$ there exists $y_t\in\mathbb{R}^3$ such that

$$\|\varphi_t - \varphi_{\mathrm{P}}(\,\cdot\,-y_t)\|_2^2 \leq C\varepsilon_\Lambda \tag{4.3.2}$$

for some $C>0$. Since the spectrum of $h_{\varphi_{\mathrm{P}}(\,\cdot\,-y)}$ and $\|\varphi_{\mathrm{P}}(\,\cdot\,-y)\|_2$ are independent of $y\in\mathbb{R}^3$, Theorem 4.1.1 now follows immediately from Lemma 4.2.4 by taking $\varepsilon_\Lambda = C^{-1}\delta_\Lambda^2$, where δ_Λ is the same as in Lemma 4.2.4. □

Conservation of energy also allows to extend the validity of Lemma 4.2.8 for all times. If (ψ_t,φ_t) solves (5.1.1) with initial data (ψ_0,φ_0) satisfying $\mathcal{G}(\psi_0,\varphi_0)\leq e_{\mathrm{P}}+\varepsilon$ for a sufficiently small ε, then ψ_{φ_t} is well defined for all times and

$$\min_{\theta\in[0,2\pi)}\|\psi_t - e^{i\theta}\psi_{\varphi_t}\|^2_{H^1(\mathbb{R}^3)} \leq C\varepsilon, \quad \|\varphi_t+\sigma_{\psi_{\varphi_t}}\|_2^2\leq C\varepsilon. \tag{4.3.3}$$

Moreover, Theorem 4.1.1 implies that for all times $\Lambda(\varphi_t)\geq\Lambda$ for a suitable $\Lambda>0$. It thus follows from Lemmas 4.2.1 and 4.2.3 that for some $C>0$

$$\|R_{\varphi_t}\|\leq C \quad \text{and} \quad \|(-\Delta+1)^{1/2}R_{\varphi_t}^{1/2}\|\leq C \quad \text{for all} \quad t\in\mathbb{R}, \tag{4.3.4}$$

where as above $R_{\varphi_t} = q_t\left(h_{\varphi_t}-e(\varphi_t)\right)^{-1}q_t$ and $q_t = 1-p_t = 1-|\psi_{\varphi_t}\rangle\langle\psi_{\varphi_t}|$.

With these preparations, we are now ready to prove Corollary 4.1.1.

Proof of Corollary 4.1.1. The proof follows closely the ideas of the proof of [73, Theorem II.1], hence we allow ourselves to be a bit sketchy at some points and refer to [73] for more details. It follows from the Landau–Pekar equations (5.1.1) that

$$\alpha^2\partial_t V_{\varphi_t} = V_{\operatorname{Im}\,\varphi_t}, \quad \alpha^2\partial_t V_{\operatorname{Im}\,\varphi_t} = -V_{\operatorname{Re}\,\varphi_t+\sigma_{\psi_t}}. \tag{4.3.5}$$

Lemmas 4.2.1–4.2.3 imply, together with (4.3.1), that there exists $C>0$ such that

$$\|R_{\varphi_t}V_{\operatorname{Im}\,\varphi_t}\|^2\leq C\varepsilon \quad \text{for all} \quad t\in\mathbb{R}. \tag{4.3.6}$$

In the same way, by the triangle inequality, Lemma 4.2.2 and (4.3.3), there exists $C>0$ such that

$$\|R_{\varphi_t}V_{\operatorname{Re}\,\varphi_t+\sigma_{\psi_t}}\|^2 \leq C\min_{\theta\in(0,2\pi]}\|\psi_t-e^{i\theta}\psi_{\varphi_t}\|^2_{H^1(\mathbb{R}^3)}+C\|\operatorname{Re}\,\varphi_t+\sigma_{\psi_{\varphi_t}}\|_2^2\leq C\varepsilon \quad \text{for all} \quad t\in\mathbb{R}. \tag{4.3.7}$$

Moreover, it follows from

$$\alpha^2 \partial_t \psi_{\varphi_t} = -R_{\varphi_t} V_{\mathrm{Im}\,\varphi_t} \psi_{\varphi_t} \tag{4.3.8}$$

that

$$\alpha^2 \partial_t R_{\varphi_t} = p_t V_{\mathrm{Im}\,\varphi_t} R^2_{\varphi_t} + R^2_{\varphi_t} V_{\mathrm{Im}\,\varphi_t} p_t - R_{\varphi_t} \left(V_{\mathrm{Im}\,\varphi_t} - \langle \psi_{\varphi_t}, V_{\mathrm{Im}\,\varphi_t} \psi_{\varphi_t} \rangle \right) R_{\varphi_t} \tag{4.3.9}$$

(see [73, Lemma IV.2]) and by the same arguments as above that

$$\| \left(-\Delta + 1\right)^{1/2} \partial_t R_{\varphi_t} \left(-\Delta + 1\right)^{1/2} \| \leq C \varepsilon^{1/2} \alpha^{-2} \quad \text{for all} \quad t \in \mathbb{R}. \tag{4.3.10}$$

Recall the definitions of $\widetilde{\psi}_t$ and ν in (4.1.11). The same computations as in [73, Eqs. (58)–(65)], using

$$q_t\, e^{i \int_0^t ds\, e(\varphi_s)} \psi_t = i\, R_{\varphi_t}\, \partial_t\, e^{i \int_0^t ds\, e(\varphi_s)} \psi_t \tag{4.3.11}$$

and integration by parts, lead to

$$\begin{aligned}
\|\widetilde{\psi}_t - \psi_{\varphi_t}\|_2^2 = {} & 2\alpha^{-2}\, \mathrm{Im}\, \langle \widetilde{\psi}_t,\, R^2_{\varphi_t} V_{\mathrm{Im}\,\varphi_t} \psi_{\varphi_t} \rangle & \text{(4.3.12a)} \\
& + 2\alpha^{-2} \int_0^t ds\, \nu(s)\, \mathrm{Re} \langle \widetilde{\psi}_s,\, R^2_{\varphi_s} V_{\mathrm{Im}\,\varphi_s} \psi_{\varphi_s} \rangle & \text{(4.3.12b)} \\
& + 2\alpha^{-4} \int_0^t ds\, \mathrm{Im} \langle \widetilde{\psi}_s,\, R_{\varphi_s} \left(R_{\varphi_s} V_{\mathrm{Im}\,\varphi_s} \right)^2 \psi_{\varphi_s} \rangle & \text{(4.3.12c)} \\
& + 2\alpha^{-4} \int_0^t ds\, \mathrm{Im} \langle \widetilde{\psi}_s,\, R^2_{\varphi_s} V_{\mathrm{Re}\,\varphi_s + \sigma_{\psi_s}} \psi_{\varphi_s} \rangle & \text{(4.3.12d)} \\
& - 2\alpha^{-2} \int_0^t ds\, \left(\mathrm{Im} \langle \widetilde{\psi}_s,\, \left(\partial_s R^2_{\varphi_s} \right) V_{\mathrm{Im}\,\varphi_s} \psi_{\varphi_s} \rangle + \alpha^2 \nu(s)\, \mathrm{Im} \langle \widetilde{\psi}_s,\, \psi_{\varphi_s} \rangle \right). & \text{(4.3.12e)}
\end{aligned}$$

The difference to the calculations in [73] are the additional terms (4.3.12b) and the second term in (4.3.12e) resulting from the phase ν. While (4.3.12b) is, as we show below, only a subleading error term, the phase in (4.3.12e) leads to a crucial cancellation. This cancellation allows to integrate by parts once more, and finally results in the improved estimate in Corollary 4.1.1.

We shall now estimate the various terms in (4.3.12). Since $\|q_t \widetilde{\psi}_t\|_2 \leq \|\widetilde{\psi}_t - \psi_{\varphi_t}\|_2$, we find for the first term using (4.3.4) and (4.3.6)

$$|\text{(4.3.12a)}| \leq C \alpha^{-2} \varepsilon^{1/2} \|\widetilde{\psi}_t - \psi_{\varphi_t}\|_2 \leq \delta \|\widetilde{\psi}_t - \psi_{\varphi_t}\|_2^2 + C \delta^{-1} \alpha^{-4} \varepsilon \tag{4.3.13}$$

for arbitrary $\delta > 0$. Moreover, we have $|\nu(s)| \leq C\alpha^{-4}\varepsilon$ for all $s \in \mathbb{R}$, and find for the second term

$$|\text{(4.3.12b)}| \leq C \alpha^{-6} \varepsilon^{3/2} \int_0^t ds\, \|\widetilde{\psi}_s - \psi_{\varphi_s}\|_2\,. \tag{4.3.14}$$

For the third term, we integrate by parts using (4.3.11) once more, with the result that

$$\begin{aligned}
\text{(4.3.12c)} = {} & -2\alpha^{-4}\, \mathrm{Re}\, \langle \widetilde{\psi}_t,\, R^2_{\varphi_t} \left(R_{\varphi_t} V_{\mathrm{Im}\,\varphi_t} \right)^2 \psi_{\varphi_t} \rangle + 2\alpha^{-4} \int_0^t ds\, \nu(s)\, \mathrm{Im}\, \langle \widetilde{\psi}_s, R^2_{\varphi_s} \left(R_{\varphi_s} V_{\mathrm{Im}\,\varphi_s} \right)^2 \psi_{\varphi_s} \rangle \\
& + 2\alpha^{-4} \int_0^t ds\, \mathrm{Re}\, \langle \widetilde{\psi}_s,\, \partial_s \left(R^2_{\varphi_s} \left(R_{\varphi_s} V_{\mathrm{Im}\,\varphi_s} \right)^2 \psi_{\varphi_s} \right) \rangle. \qquad \text{(4.3.15)}
\end{aligned}$$

The first two terms can be bounded in the same way as (4.3.12a) and (4.3.12b). For the third term, note that the r.h.s. of the inner product depends on time s through φ_s only, hence its time derivative leads to another factor of α^{-2}. With (4.3.5), (4.3.8) and (4.3.9) we compute its time derivative. From the time derivative of the resolvent in (4.3.9), we obtain one term for which the projection p_s hits $\widetilde{\psi}_s$ on the l.h.s. of the inner product, in which case we can only bound $\|p_s\widetilde{\psi}_s\|_2 \leq 1$. For the remaining terms, we use $\|q_s\widetilde{\psi}_s\|_2 \leq \|\widetilde{\psi}_s - \psi_{\varphi_s}\|_2$ instead. With the same arguments as above and (4.3.7), we obtain

$$|(4.3.12c)| \leq \delta\|\widetilde{\psi}_t - \psi_{\varphi_t}\|_2^2 + C\delta^{-1}\alpha^{-8}\varepsilon^2 + C\alpha^{-6}\varepsilon\int_0^t ds\,\|\widetilde{\psi}_s - \psi_{\varphi_s}\|_2 + C\alpha^{-6}\varepsilon^{3/2}|t| \quad (4.3.16)$$

for any $\delta > 0$. For the forth term (4.3.12d), we first split

$$(4.3.12d) = 2\alpha^{-4}\int_0^t ds\,\left(\mathrm{Im}\,\langle\widetilde{\psi}_s,\, R_{\varphi_s}^2 V_{\sigma_{\psi_s}-\sigma_{\psi_{\varphi_s}}}\psi_{\varphi_s}\rangle + \mathrm{Im}\,\langle\widetilde{\psi}_s,\, R_{\varphi_s}^2 V_{\mathrm{Re}\,\varphi_s+\sigma_{\psi_{\varphi_s}}}\psi_{\varphi_s}\rangle\right). \quad (4.3.17)$$

Lemmas 4.2.1–4.2.3 and (4.3.4) imply that we can bound $\|R_{\varphi_s}^2 V_{\sigma_{\psi_s}-\sigma_{\psi_{\varphi_s}}}\| \leq C\|\widetilde{\psi}_s - \psi_{\varphi_s}\|_2$ in the first term. For the second term, we observe that the r.h.s. of the inner product depends on s again only through φ_s, whose time derivative is of order α^{-2}. We thus again use (4.3.11) and integration by parts, and proceed as above. For the calculation, we need to bound the time derivative of $\sigma_{\psi_{\varphi_s}}$, which can be done with the aid [74, Lemma II.4], with the result that $\|\partial_s\sigma_{\psi_{\varphi_s}}\|_2 \leq C\varepsilon^{1/2}\alpha^{-2}$. Altogether, this shows that

$$\begin{aligned}|(4.3.12d)| \leq{}& C\alpha^{-4}\int_0^t ds\,\|\widetilde{\psi}_s - \psi_{\varphi_s}\|_2^2 + \delta\|\widetilde{\psi}_t - \psi_{\varphi_t}\|_2^2 + C\delta^{-1}\alpha^{-8}\varepsilon \\ &+ C\alpha^{-6}\varepsilon^{1/2}\int_0^t ds\,\|\widetilde{\psi}_s - \psi_{\varphi_s}\|_2 + C\alpha^{-6}\varepsilon|t| \end{aligned} \quad (4.3.18)$$

for any $\delta > 0$. For the last term, we compute using (4.3.9)

$$\begin{aligned}(4.3.12e) ={}& -6\alpha^{-4}\int_0^t ds\;\mathrm{Im}\langle\widetilde{\psi}_s,\, R_{\varphi_s}^3 V_{\mathrm{Im}\,\varphi_s} p_s V_{\mathrm{Im}\,\varphi_s}\psi_{\varphi_s}\rangle \\ &+ 2\alpha^{-4}\int_0^t ds\;\mathrm{Im}\langle\widetilde{\psi}_s,\, \left(R_{\varphi_s}^2 V_{\mathrm{Im}\,\varphi_s} R_{\varphi_s} + R_{\varphi_s} V_{\mathrm{Im}\,\varphi_s} R_{\varphi_s}^2\right) V_{\mathrm{Im}\,\varphi_s}\psi_{\varphi_s}\rangle. \end{aligned} \quad (4.3.19)$$

Note that the phase $\nu(s)$ cancels the contribution of $\partial_s R_{\varphi_s}$ projecting onto ψ_{φ_s} (the first term of (4.3.9)). This cancellation is important, since the integration by parts argument using (4.3.11) would not be applicable to this term. It can be applied to all the terms in (4.3.19), however, proceeding as above, with the result that

$$|(4.3.12e)| \leq \delta\|\widetilde{\psi}_t - \psi_{\varphi_t}\|_2^2 + C\delta^{-1}\alpha^{-8}\varepsilon^2 + C\alpha^{-6}\varepsilon\int_0^t ds\,\|\widetilde{\psi}_s - \psi_{\varphi_s}\|_2 + C\alpha^{-6}\varepsilon^{3/2}|t| \quad (4.3.20)$$

for any $\delta > 0$.

Collecting the bounds in (4.3.13), (4.3.14), (4.3.16), (4.3.18) and (4.3.20), Eq. (4.3.12) shows that

$$\begin{aligned}\|\widetilde{\psi}_t - \psi_{\varphi_t}\|_2^2 &\leq C\alpha^{-4}\varepsilon + C\alpha^{-6}\varepsilon^{1/2}\int_0^t ds\,\|\widetilde{\psi}_s - \psi_{\varphi_s}\|_2 + C\alpha^{-4}\int_0^t ds\,\|\widetilde{\psi}_s - \psi_{\varphi_s}\|_2^2 + C\alpha^{-6}\varepsilon|t| \\ &\leq C\alpha^{-4}\varepsilon + C\alpha^{-4}\int_0^t ds\,\|\widetilde{\psi}_s - \psi_{\varphi_s}\|_2^2 + C\alpha^{-6}\varepsilon|t| \end{aligned} \quad (4.3.21)$$

for $\alpha \gtrsim 1$ and $\varepsilon \lesssim 1$. A Gronwall type argument finally yields the desired bound (4.1.12). □

4.4 Appendix: Proof of Lemma 4.2.6

In this appendix we give the proof of Lemma 4.2.6. As already mentioned, the result follows from the work in [70] by standard arguments. We follow closely the proof given in [41] of a corresponding result in the slightly different setting of a confined polaron.

Proof of Lemma 4.2.6. **Step 1**: For any L^2-normalized $\psi \in H^1(\mathbb{R}^3)$, there exists $\bar{\theta} \in [0, 2\pi)$ and $\bar{y} \in \mathbb{R}^3$ such that

$$\|e^{i\bar{\theta}}\psi(\,\cdot\, - \bar{y}) - \psi_{\mathrm{P}}\|_2 = \min_{y,\theta} \|e^{i\theta}\psi(\,\cdot\, - y) - \psi_{\mathrm{P}}\|_2. \tag{4.4.1}$$

By invariance of $\mathcal{E}$ under translations and changes of phase, it is then sufficient to show that for any L^2-normalized ψ such that

$$\|\psi - \psi_{\mathrm{P}}\|_2 = \min_{y,\theta} \|\psi - e^{i\theta}\psi_{\mathrm{P}}(\,\cdot\, - y)\|_2, \tag{4.4.2}$$

the inequality

$$\mathcal{E}(\psi) - e_{\mathrm{P}} \geq \kappa \|\psi - \psi_{\mathrm{P}}\|^2_{H^1(\mathbb{R}^3)} \tag{4.4.3}$$

holds (for some $\kappa > 0$ independent of ψ). In fact, this is stronger than the desired bound (4.2.33). We henceforth only work with L^2-normalized ψ satisfying (4.4.2), and denote $\delta = \psi - \psi_{\mathrm{P}}$. Observe that any ψ satisfying (4.4.2) also satisfies

$$\langle \psi | \psi_{\mathrm{P}} \rangle \geq 0, \quad \langle \psi | \partial_i \psi_{\mathrm{P}} \rangle = 0 \text{ for } i = 1, 2, 3. \tag{4.4.4}$$

Step 2: We first prove the quadratic lower bound (4.4.3) locally around ψ_{P} for any L^2-normalized ψ satisfying (4.4.2). By straightforward computations, using that

$$\|\delta\|_2^2 = 2 - 2\,\langle \psi_{\mathrm{P}} | \psi \rangle = -2\,\langle \psi_{\mathrm{P}} | \delta \rangle \tag{4.4.5}$$

since both ψ_{P} and ψ are L^2-normalized, we obtain

$$\mathcal{E}(\psi) - e_{\mathrm{P}} = \mathsf{Hess}_{\psi_{\mathrm{P}}}(\delta) + O(\|\delta\|^3_{H^1(\mathbb{R}^3)}), \tag{4.4.6}$$

with

$$\begin{aligned} \mathsf{Hess}_{\psi_{\mathrm{P}}}(\delta) &= \langle \mathrm{Im}\ \delta | Q L_- Q | \mathrm{Im}\ \delta \rangle + \langle \mathrm{Re}\ \delta | Q L_+ Q | \mathrm{Re}\ \delta \rangle\,, \\ Q &= 1 - |\psi_{\mathrm{P}}\rangle \langle \psi_{\mathrm{P}}|\,, \\ L_- &= h_{\varphi_{\mathrm{P}}} - e(\varphi_{\mathrm{P}}), \\ L_+ &= L_- - 4X, \\ X &= (2\pi)^3 \psi_{\mathrm{P}} (-\Delta)^{-1} \psi_{\mathrm{P}}\,, \end{aligned} \tag{4.4.7}$$

where in the last formula for X, ψ_{P} has to be understood as a multiplication operator.

The Euler–Lagrange equation for the minimization of $\mathcal{E}$ reads $L_- \psi_{\mathrm{P}} = 0$, and since L_- is a Schrödinger operator and ψ_{P} is strictly positive, L_- has 0 as its lowest eigenvalue, and a gap above. Therefore we have

$$Q L_- Q \geq \kappa_1 Q \tag{4.4.8}$$

for some $\kappa_1 > 0$. Moreover, it was shown in [70] that the kernel of L_+ coincides with $\mathrm{span}_{i=1,2,3}\{\partial_i \psi_{\mathrm{P}}\}$ and from this we can infer the existence of a $\kappa_2 > 0$ such that

$$Q L_+ Q \geq \kappa_2 Q' \quad \text{with } Q' = Q - \sum_{i=1}^{3} \|\partial_i \psi_{\mathrm{P}}\|_2^{-2}\, |\partial_i \psi_{\mathrm{P}}\rangle \langle \partial_i \psi_{\mathrm{P}}|\,. \tag{4.4.9}$$

Recall that $Q'\delta = Q\delta$ by assumption on ψ and orthogonality of $\psi_{\rm P}$ to its partial derivatives. With $\kappa' = \min\{\kappa_1, \kappa_2\}$ we thus have

$$\text{Hess}_{\psi_{\rm P}}(\delta) \geq \kappa_1 \|Q \operatorname{Im} \delta\|_2^2 + \kappa_2 \|Q' \operatorname{Re} \delta\|_2^2 \geq \kappa' \|Q\delta\|_2^2. \tag{4.4.10}$$

Using again (4.4.5) we see that

$$\|Q\delta\|_2^2 = \|\delta\|_2^2 - \langle \psi_{\rm P} | \delta \rangle^2 = \|\delta\|_2^2 \left(1 - \frac{1}{4}\|\delta\|_2^2\right) \geq \frac{1}{2}\|\delta\|_2^2, \tag{4.4.11}$$

which finally implies that

$$\text{Hess}_{\psi_{\rm P}}(\delta) \geq \frac{\kappa'}{2}\|\delta\|_2^2. \tag{4.4.12}$$

We now want to improve this bound to include the full H^1-norm of δ. Using the regularity of $\psi_{\rm P}$ it is rather straightforward to show that

$$\begin{aligned} L_- = QL_-Q &\geq -\Delta - C\,, \\ QL_+Q &\geq -\Delta - C \end{aligned} \tag{4.4.13}$$

which implies, that

$$\text{Hess}_{\psi_{\rm P}}(\delta) \geq \|\delta\|_{H^1}^2 - C\|\delta\|_2^2. \tag{4.4.14}$$

By interpolating between (4.4.12) and (4.4.14), we finally obtain

$$\text{Hess}_{\psi_{\rm P}}(\delta) \geq \frac{\kappa'}{\kappa' + 2C}\|\delta\|_{H^1}^2 = \kappa''\|\delta\|_{H^1}^2. \tag{4.4.15}$$

In combination with (4.4.6), we conclude that

$$\mathcal{E}(\psi) - e_{\rm P} \geq \kappa''\|\delta\|_{H^1}^2 - C\|\delta\|_{H^1}^3 \tag{4.4.16}$$

for any L^2-normalized ψ satisfying (4.4.2), which shows that (4.4.3) holds for $\|\delta\|_{H^1}$ sufficiently small.

Step 3: We now extend the previous local bound to show that (4.4.3) holds globally. Suppose by contradiction that there does not exist a universal κ such that (4.4.3) holds. Then there exists a sequence ψ_n of L^2-normalized functions satisfying (4.4.2) such that

$$\mathcal{E}(\psi_n) \leq e_{\rm P} + \frac{1}{n}\|\psi_n - \psi_{\rm P}\|_{H^1}^2 \leq \frac{2}{n}\|\psi_n\|_{H^1}^2 + C\,. \tag{4.4.17}$$

One readily checks that

$$\mathcal{E}(\psi_n) \geq \frac{1}{2}\|\psi_n\|_{H^1}^2 - C\,, \tag{4.4.18}$$

hence ψ_n must be bounded in $H^1(\mathbb{R}^3)$. Again using (4.4.17), we conclude that ψ_n must be a minimizing sequence for $\mathcal{E}$. It was proven in [76] that any minimizing sequence converges in $H^1(\mathbb{R}^3)$ to a minimizer of $\mathcal{E}$, i.e., an element of $\Theta(\psi_{\rm P})$ in (4.2.31), and since ψ_n satisfies (4.4.2) this implies that $\psi_n \xrightarrow{H^1} \psi_{\rm P}$. This yields a contradiction, since we already know by (4.4.16) that locally the bound (4.4.3) holds. □

CHAPTER 5

Effective Mass of the Polaron via Landau–Pekar Equations

This Chapter contains the work

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Abstract

We provide a definition of the effective mass for the classical polaron described by the Landau–Pekar equations. It is based on a novel variational principle, minimizing the energy functional over states with given (initial) velocity. The resulting formula for the polaron's effective mass agrees with the prediction by Landau and Pekar [66].

5.1 Introduction

The polaron is a model of an electron interacting with its self-induced polarization field of the underlying crystal. The description of the polarization as a quantum field corresponds to the Fröhlich model [47]. In the classical approximation, on the other hand, the dynamics of a polaron is described by the Landau–Pekar (LP) equations. For $(\psi_t, \varphi_t) \in H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$, where ψ_t is the electron wave function and φ_t denotes the phonon field, these equations read in suitable units

$$\begin{aligned} i\partial_t \psi_t &= h_{\varphi_t} \psi_t, \\ i\alpha^2 \partial_t \varphi_t &= \varphi_t + \sigma_{\psi_t}, \end{aligned} \tag{5.1.1}$$

where h_φ is the Schrödinger operator

$$h_\varphi = -\Delta + V_\varphi \tag{5.1.2}$$

with potential

$$V_\varphi(x) = 2(2\pi)^{3/2}\, \mathrm{Re}\,[(-\Delta)^{-1/2}\varphi](x) = 4(2\pi)^{5/2}|x|^{-2} * \mathrm{Re}\ \varphi, \tag{5.1.3}$$

and

$$\sigma_\psi(x) = (2\pi)^{3/2}\left[(-\Delta)^{-1/2}|\psi|^2\right](x) = 2(2\pi)^{5/2}|x|^{-2} * |\psi|^2. \tag{5.1.4}$$

The parameter $\alpha > 0$ quantifies the strength of the coupling of the electron's charge to the polarization field.

The LP equations can be derived from the dynamics generated by the (quantum) Fröhlich Hamiltonian for suitable initial states in the strong coupling limit $\alpha \to \infty$ [74] (see also [40, 38, 56, 73, 87] for earlier results on this problem). One of the outstanding open problems concerns the polaron's effective mass [81, 109, 111]: due to the interaction with the polarization field, the electron effectively becomes heavier and behaves like a particle with a larger mass. This mass increases with the coupling α, and is expected to diverge as α^4 as $\alpha \to \infty$. A precise asymptotic formula was obtained by Landau and Pekar [66] based on the classical approximation, and hence it is natural to ask to what extent the derivation of the LP equations in [74] allows to draw conclusions on the effective mass problem.

It is, however, far from obvious how to rigorously obtain the effective mass even on the classical level, i.e., from the LP equations (5.1.1). A heuristic derivation, reviewed in Section 5.4.1 below, considers traveling wave solutions of (5.1.1) for non-zero velocity $v \in \mathbb{R}^3$, and expands the corresponding energy for small v. The existence of such solutions remains unclear, however, and we in fact conjecture that no such solutions exist for non-zero v. This is related to the fact the energy functional corresponding to (5.1.1) (given in Eq. (5.2.1) below) does not dominate the total momentum, and a computation of the ground state energy as a function of the (conserved) total momentum would simply yield a constant function (corresponding to an infinite effective mass). Due to the vanishing of the sound velocity in the medium, a moving electron can be expected to be slowed down to zero speed by emitting radiation. (See [49, 50] for the study of a similar effect in a model of a classical particle coupled to a field.)

In this paper, we provide a novel definition of the effective mass for the LP equations. We shall argue that all low energy states have a well-defined notion of (initial) velocity, and hence we can minimize the energy functional among states with given velocity. Expanding the resulting energy-velocity relation for small velocity gives a definition of the effective mass, which coincides with the prediction by Landau and Pekar [66].

5.1.1 Structure of the paper

In Section 5.2, we explain our rigorous approach to derive the energy-velocity relation of the system, allowing for a precise definition and computation of the effective mass. After introducing some notation and recalling fundamental properties of the Pekar energy functional in Section 5.2.1, we identify in Section 5.2.2 a set of initial data for the LP equations for which it is possible to define the position, and consequently the velocity, at any time. We then arrive at an energy-velocity relation by defining $E(v)$ in Section 5.2.3 as the minimal energy among all admissible initial states of fixed initial velocity v. Finally, in Section 5.2.4 we state our main result, an expansion of $E(v)$ for small velocities v, allowing for the computation the effective mass of the system.

Section 5.3 contains the proof of our main result, Theorem 5.2.1.

In Section 5.4 we discuss the formal approach to the effective mass via traveling waves. Moreover, we investigate an alternative definition of the effective mass, through an alternative notion of velocity of low-energy states.

5.2 Main Results

5.2.1 Preliminaries

We start by introducing further notation and recalling some known results. The classical energy functional corresponding to the Landau–Pekar equations (5.1.1) is defined on $H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ as

$$\mathcal{G}(\psi, \varphi) = \langle \psi, h_\varphi \psi \rangle + \|\varphi\|_2^2 \quad \text{for} \quad \|\psi\|_2 = 1. \tag{5.2.1}$$

Equipped with the symplectic form $\frac{1}{2i}\int d\psi \wedge d\bar{\psi} + \frac{\alpha^2}{2i}\int d\varphi \wedge d\bar{\varphi}$, it defines a dynamical system leading to the LP equations (5.1.1). Moreover, $\mathcal{G}$ is conserved along solutions of (5.1.1).

It was proved in [76] that the Pekar ground state energy

$$\min \mathcal{G}(\psi, \varphi) =: e_{\mathrm{P}} \tag{5.2.2}$$

is attained for the Pekar minimizers $(\psi_{\mathrm{P}}, \varphi_{\mathrm{P}})$, which are radial functions in $C^\infty(\mathbb{R}^3)$ satisfying $\psi_{\mathrm{P}} > 0$, $\varphi_{\mathrm{P}} = -\sigma_{\psi_{\mathrm{P}}}$ and $\psi_{\mathrm{P}} = \psi_{\varphi_{\mathrm{P}}}$, where ψ_φ denotes the ground state of h_φ whenever it exists. Moreover, this minimizer is unique up to the symmetries of the problem, i.e., translation-invariance and multiplication of ψ by a phase. We shall denote

$$H_{\mathrm{P}} = h_{\varphi_{\mathrm{P}}} - \mu_{\mathrm{P}} \quad \text{with} \quad \mu_{\mathrm{P}} = \inf \operatorname{spec} h_{\varphi_{\mathrm{P}}}. \tag{5.2.3}$$

Associated to $\mathcal{G}$, there are the two functionals

$$\mathcal{E}(\psi) := \inf_{\varphi \in L^2(\mathbb{R}^3)} \mathcal{G}(\psi, \varphi), \quad \mathcal{F}(\varphi) := \inf_{\substack{\psi \in H^1(\mathbb{R}^3) \\ \|\psi\|_2 = 1}} \mathcal{G}(\psi, \varphi) \tag{5.2.4}$$

and clearly $e_{\mathrm{P}} = \min \mathcal{G}(\psi, \varphi) = \min \mathcal{E}(\psi) = \min \mathcal{F}(\varphi)$. We also define the manifolds of minimizers

$$\mathcal{M}_{\mathcal{G}} := \{(\psi, \varphi) \,|\, \mathcal{G}(\psi, \varphi) = e_{\mathrm{P}}\}, \ \mathcal{M}_{\mathcal{E}} := \{\psi \,|\, \mathcal{E}(\psi) = e_{\mathrm{P}}\}, \ \mathcal{M}_{\mathcal{F}} := \{\varphi \,|\, \mathcal{F}(\varphi) = e_{\mathrm{P}}\}. \tag{5.2.5}$$

The results in [76] imply that we can write these in terms of the Pekar minimizers $(\psi_{\mathrm{P}}, \varphi_{\mathrm{P}})$ as

$$\begin{aligned} \mathcal{M}_{\mathcal{G}} &= \{(e^{i\theta}\psi_{\mathrm{P}}^y, \varphi_{\mathrm{P}}^y) \,|\, \theta \in [0, 2\pi),\, y \in \mathbb{R}^3\}, \\ \mathcal{M}_{\mathcal{E}} &= \{e^{i\theta}\psi_{\mathrm{P}}^y \,|\, \theta \in [0, 2\pi),\, y \in \mathbb{R}^3\}, \\ \mathcal{M}_{\mathcal{F}} &= \{\varphi_{\mathrm{P}}^y \,|\, y \in \mathbb{R}^3\} \end{aligned} \tag{5.2.6}$$

where $f^y := f(\cdot - y)$ for any function f. Furthermore, it can be deduced from the results in [70] that the energy functionals $\mathcal{F}$ and $\mathcal{E}$ are both coercive (see [35, Lemmas 2.6 and 2.7]), i.e., there exists $C > 0$ such that

$$\mathcal{F}(\varphi) \geq e_{\mathrm{P}} + C \operatorname{dist}^2_{L^2}(\varphi, \mathcal{M}_{\mathcal{F}}), \quad \mathcal{E}(\psi) \geq e_{\mathrm{P}} + C \operatorname{dist}^2_{H^1}(\psi, \mathcal{M}_{\mathcal{E}}). \tag{5.2.7}$$

The following Lemma on properties of the projection onto the manifold $\mathcal{M}_{\mathcal{F}}$ will be important for our analysis below. Its proof will be given in Section 5.5.

Lemma 5.2.1. *There exists $\delta > 0$ such that the L^2-projection onto $\mathcal{M}_{\mathcal{F}}$, is well-defined (i.e., unique) on*

$$(\mathcal{M}_{\mathcal{F}})_\delta := \{\varphi \in L^2(\mathbb{R}^3) \mid \operatorname{dist}_{L^2}(\varphi, \mathcal{M}_{\mathcal{F}}) \leq \delta\}. \tag{5.2.8}$$

For any $\varphi \in (\mathcal{M}_{\mathcal{F}})_\delta$, we define $z_\varphi \in \mathbb{R}^3$ via

$$P_{L^2}^{\mathcal{M}_{\mathcal{F}}}(\varphi) = \varphi_{\mathrm{P}}^{z_\varphi} \, . \tag{5.2.9}$$

Then z_φ is a differentiable function from $(\mathcal{M}_{\mathcal{F}})_\delta$ to $\mathbb{R}^3$ and its partial derivative in the direction $\eta \in L^2(\mathbb{R}^3)$ is given by

$$\partial_t z_{\varphi+t\eta} \restriction_{t=0} = A_\varphi^{-1} \langle \mathrm{Re}\, \eta | \nabla \varphi_P^{z_\varphi} \rangle, \tag{5.2.10}$$

where A is the invertible matrix defined for any $\varphi \in (\mathcal{M}_{\mathcal{F}})_\delta$ by $A_{i,j} := -\mathrm{Re}\langle \varphi | \partial_i \partial_j \varphi_P^{z_\varphi} \rangle$.

Remark 5.2.1. *Likewise, it can be shown that the H^1- (resp. L^2-) projection onto $\mathcal{M}_{\mathcal{E}}$ have similar properties: There exists $\delta > 0$ such that the H^1- (resp. the L^2-) projection onto $\mathcal{M}_{\mathcal{E}}$*

$$P_{H^1}^{\mathcal{M}_{\mathcal{E}}}(\psi) = e^{i\theta_\psi} \psi_{\mathrm{P}}^{y_\psi}, \quad \left(\text{resp. } P_{L^2}^{\mathcal{M}_{\mathcal{E}}}(\psi) = e^{i\theta'_\psi} \psi_{\mathrm{P}}^{y'_\psi} \right) \tag{5.2.11}$$

is well-defined on the set $(\mathcal{M}_{\mathcal{E}})_\delta^{H^1} := \{\psi \in L^2(\mathbb{R}^3) \mid \mathrm{dist}_{H^1}(\psi, \mathcal{M}_{\mathcal{E}}) \leq \delta\}$ (resp. $(\mathcal{M}_{\mathcal{E}})_\delta^{L^2} := \{\psi \in L^2(\mathbb{R}^3) \mid \mathrm{dist}_{L^2}(\psi, \mathcal{M}_{\mathcal{E}}) \leq \delta\}$) and the functions y_ψ, θ_ψ (resp. y'_ψ, θ'_ψ) defined through (5.2.11) *are differentiable functions from $(\mathcal{M}_{\mathcal{E}})_\delta^{H^1}$ (resp. $(\mathcal{M}_{\mathcal{E}})_\delta^{L^2}$) to $\mathbb{R}/(2\pi\mathbb{Z})$ and $\mathbb{R}^3$.*

5.2.2 Position and velocity of solutions

In this section, we give a meaning to the notion of position, and therefore velocity, for solutions of the Landau–Pekar equations (at least for a class of initial data). There is a natural way of defining, given ψ_t, the position of the electron at time t, which is simply given by

$$\mathsf{X}_{\mathsf{el}}(t) := \langle \psi_t | x | \psi_t \rangle \, . \tag{5.2.12}$$

This yields, by straightforward computations using (5.1.1), that

$$\mathsf{V}_{\mathsf{el}}(t) := \frac{d}{dt} \mathsf{X}_{\mathsf{el}}(t) = 2 \langle \psi_t | -i\nabla | \psi_t \rangle \, . \tag{5.2.13}$$

Note that (5.2.13) is always well-defined for $\psi \in H^1(\mathbb{R}^3)$, even although (5.2.12) not necessarily is.

For the phonon field, the situation is more complicated as φ cannot be interpreted as a probability distribution over positions. This calls for a different approach. By (5.2.7), Lemma 5.2.1 and the conservation of $\mathcal{G}$ along solutions of (5.1.1), we know that there exists δ^* such that for any initial condition (ψ_0, φ_0) such that

$$\mathcal{G}(\psi_0, \varphi_0) \leq e_{\mathrm{P}} + \delta^*, \tag{5.2.14}$$

φ_t admits a unique L^2-projection $\varphi_{\mathrm{P}}^{z(t)}$ onto $\mathcal{M}_{\mathcal{F}}$ for all times. We use this to define

$$\mathsf{X}_{\mathsf{ph}}(t) := z(t), \quad \mathsf{V}_{\mathsf{ph}} := \frac{d}{dt} \mathsf{X}_{\mathsf{ph}}(t) = \dot{z}(t). \tag{5.2.15}$$

Note that $\mathsf{X}_{\mathsf{ph}}(t)$ is indeed differentiable by Lemma 5.2.1 and the differentiability of the LP dynamics. At this point, for any initial data satisfying (5.2.14), we have a well-defined notion of position and velocity for all times, admittedly in a much less explicit form for the phonon field.

5.2.3 Initial conditions of velocity v

For any $v \in \mathbb{R}^3$ (or at least for $|v|$ sufficiently small), we are now interested in considering all initial conditions (ψ_0, φ_0) whose solutions have instantaneous velocity v at $t = 0$ (both in the electron and in the phonon coordinate) and to then minimize the functional $\mathcal{G}$ over such states. This will give us an explicit relation between the energy and the velocity of the system, allowing us to define the effective mass of the polaron in the classical setting defined by the Landau–Pekar equations.

Note that by radial symmetry of the problem only the absolute value of the velocity, and not its direction, affects our analysis. Hence, for $v \in \mathbb{R}$, we consider initial conditions (ψ_0, φ_0) such that

(i) $(\psi_0, \varphi_0) \in H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ with $\|\psi_0\|_2 = 1$ and such that (5.2.14) is satisfied,

(ii) $\mathsf{V}_{\mathsf{el}}(0) = \mathsf{V}_{\mathsf{ph}}(0) = v(1,0,0)$.

The set of admissible initial conditions of velocity $v \in \mathbb{R}$ can hence be compactly written as

$$I_v := \{(\psi_0, \varphi_0) \,|\, \text{(i), (ii) are satisfied}\}. \tag{5.2.16}$$

We will show below that it is non-empty for small enough v.

5.2.4 Expansion of the energy

In order to compute the effective mass of the polaron, we now minimize the energy $\mathcal{G}$ over the set I_v. To this end, we define the energy

$$E(v) := \inf_{(\psi_0,\varphi_0)\in I_v} \mathcal{G}(\psi_0, \varphi_0). \tag{5.2.17}$$

The following theorem gives an expansion of $E(v)$ for sufficiently small velocities v. Its proof will be given in Section 5.3.

Theorem 5.2.1. *As $v \to 0$ we have*

$$E(v) = e_{\mathrm{P}} + v^2 \left(\frac{1}{4} + \frac{\alpha^4}{3} \|\nabla \varphi_{\mathrm{P}}\|_2^2 \right) + O(v^3). \tag{5.2.18}$$

Since the kinetic energy of a particle of mass m and velocity v equals $mv^2/2$, (5.2.18) identifies the effective mass of the system as

$$m_{\mathsf{eff}} = \lim_{v \to 0} \frac{E(v) - e_{\mathrm{P}}}{v^2/2} = \frac{1}{2} + \frac{2\alpha^4}{3} \|\nabla \varphi_{\mathrm{P}}\|_2^2. \tag{5.2.19}$$

The first term $1/2$ is simply the bare mass of the election, while the second term $\frac{2\alpha^4}{3}\|\nabla \varphi_{\mathrm{P}}\|_2^2$ corresponds to the additional mass acquired through the interaction with the phonon field, and agrees with the prediction in [66].

Remark 5.2.2 (Traveling waves)**.** *The heuristic computations contained in the physics literature concerning m_{eff} [1, 66] all rely, in one way or another, on the existence of traveling* *wave solutions of the LP equations of velocity v (at least for sufficiently small velocity), i.e. solutions with initial data (ψ_v, φ_v) such that*

$$(\psi_t(x), \varphi_t(x)) = (e^{-ie_v t}\psi_v(x-vt), \varphi_v(x-vt)) \tag{5.2.20}$$

for suitable $e_v \in \mathbb{R}$. Such solutions would allow to define the energy of the system at velocity v as $E^{TW}(v) = \mathcal{G}(\psi_v, \varphi_v)$, and a perturbative calculation (discussed in Section 5.4.1 below) yields indeed

$$\lim_{v\to 0} \frac{E^{TW}(v) - e_{\mathrm{P}}}{v^2/2} = \frac{1}{2} + \frac{2\alpha^4}{3}\|\nabla\varphi_{\mathrm{P}}\|^2, \tag{5.2.21}$$

in agreement with (5.2.19)*. Unfortunately, this approach turns out to be only formal, and we conjecture traveling wave solutions to not exist for any $\alpha > 0$, $v > 0$.*

Remark 5.2.3. *In Section 5.2.2, we used the standard approach from quantum mechanics to define the electron's position* (5.2.12) *and velocity* (5.2.13)*. We could, instead, use also for the electron a similar approach to the one we use for the phonon field (i.e.* (5.2.15)*) through the projection onto the manifold of minimizers $\mathcal{M}_{\mathcal{E}}$. A natural question is whether one obtains the same effective mass using this different notion of position. In Section 5.4.2, we show that, in fact, this alternate definition yields a different effective mass equal to*

$$\widetilde{m}_{\mathit{eff}} = \frac{2\|\nabla\psi_{\mathrm{P}}\|_2^4}{3\|\nabla\varphi_{\mathrm{P}}\|_2^2} + \frac{2\alpha^4}{3}\|\nabla\varphi_{\mathrm{P}}\|_2^2. \tag{5.2.22}$$

This coincides with (5.2.19) *and* (5.2.21) *for large α (hence still confirming the prediction in [66]), but differs in the $O(1)$ term. In fact, as we discuss in Section 5.4.2, one has $\widetilde{m}_{\mathit{eff}} < m_{\mathit{eff}}$.*

5.3 Proof of Theorem 5.2.1

Let us denote $\delta_1 = \psi_0 - \psi_{\mathrm{P}}$ and $\delta_2 = \varphi_0 - \varphi_{\mathrm{P}}$. Expanding $\mathcal{G}$ in (5.2.1) and using that $\varphi_{\mathrm{P}} = -\sigma_{\psi_{\mathrm{P}}}$ we find

$$\begin{aligned}\mathcal{G}(\psi_0, \varphi_0) &= \mathcal{G}(\psi_{\mathrm{P}} + \delta_1, \varphi_{\mathrm{P}} + \delta_2) \\ &= e_{\mathrm{P}} + 2\langle\psi_{\mathrm{P}}|\, h_{\varphi_{\mathrm{P}}}\, |\mathrm{Re}\,\delta_1\rangle \\ &\quad + \langle\delta_1|h_{\varphi_{\mathrm{P}}}|\delta_1\rangle + 2\langle\mathrm{Re}\,\delta_1|\, V_{\delta_2}\, |\psi_{\mathrm{P}}\rangle + \|\delta_2\|_2^2 + \langle\delta_1|V_{\delta_2}|\delta_1\rangle\,. \end{aligned} \tag{5.3.1}$$

Since ψ_0 is normalized, we have

$$1 = \|\psi_0\|_2^2 = \|\psi_{\mathrm{P}} + \delta_1\|_2^2 = 1 + \|\delta_1\|_2^2 + 2\langle\psi_{\mathrm{P}}|\mathrm{Re}\,\delta_1\rangle \iff 2\langle\psi_{\mathrm{P}}|\mathrm{Re}\,\delta_1\rangle = -\|\delta_1\|_2^2. \tag{5.3.2}$$

Hence

$$2\langle\psi_{\mathrm{P}}|\, h_{\varphi_{\mathrm{P}}}\, |\mathrm{Re}\,\delta_1\rangle = 2\mu_{\mathrm{P}}\langle\psi_{\mathrm{P}}|\mathrm{Re}\,\delta_1\rangle = -\mu_{\mathrm{P}}\|\delta_1\|_2^2, \tag{5.3.3}$$

and using $\|V_{\delta_2}\delta_1\|_2 \leq C\|\delta_2\|_2\,\|\delta_1\|_{H^1}$ (see, e.g., [73, Lemma III.2]) we arrive at

$$\mathcal{G}(\psi_0, \varphi_0) = e_{\mathrm{P}} + \langle\delta_1|H_{\mathrm{P}}|\delta_1\rangle + 2\langle\mathrm{Re}\,\delta_1|\, V_{\delta_2}\, |\psi_{\mathrm{P}}\rangle + \|\delta_2\|_2^2 + O(\|\delta_2\|_2\|\delta_1\|_{H^1}^2). \tag{5.3.4}$$

By completing the square, we have

$$\begin{aligned}&\| \operatorname{Re} \delta_2\|_2^2 + 2 \langle \operatorname{Re} \delta_1 |\, V_{\delta_2} \,| \psi_{\mathrm{P}} \rangle \\ &= \| \operatorname{Re} \delta_2 + 2(2\pi)^{3/2}(-\Delta)^{-1/2}(\psi_{\mathrm{P}} \operatorname{Re} \delta_1)\|_2^2 - 4(2\pi)^3 \langle \operatorname{Re} \delta_1 | \psi_{\mathrm{P}} (-\Delta)^{-1} \psi_{\mathrm{P}} | \operatorname{Re} \delta_1 \rangle \end{aligned} \tag{5.3.5}$$

and therefore

$$\begin{aligned}\mathcal{G}(\psi_0, \varphi_0) = e_{\mathrm{P}} + &\ \langle \operatorname{Im} \psi_0 | H_{\mathrm{P}} | \operatorname{Im} \psi_0 \rangle + \| \operatorname{Im} \varphi_0\|_2^2 \\ &+ \| \operatorname{Re} \delta_2 + 2(2\pi)^{3/2}(-\Delta)^{-1/2}(\psi_{\mathrm{P}} \operatorname{Re} \delta_1)\|_2^2 \\ &+ \langle \operatorname{Re} \delta_1 | H_{\mathrm{P}} - 4X_{\mathrm{P}} | \operatorname{Re} \delta_1 \rangle + O(\|\delta_2\|_2 \|\delta_1\|_{H^1}^2), \end{aligned} \tag{5.3.6}$$

where X_{P} is the operator with integral kernel $X_{\mathrm{P}}(x,y) := (2\pi)^3 \psi_{\mathrm{P}}(x)(-\Delta)^{-1}(x,y)\psi_{\mathrm{P}}(y)$. Since X_{P} is bounded, and $\|P_{\psi_{\mathrm{P}}} \operatorname{Re} \delta_1\| = \|\delta_1\|_2^2/2$ by (5.3.2) (with $P_{\psi_{\mathrm{P}}} = |\psi_{\mathrm{P}}\rangle\langle\psi_{\mathrm{P}}|$ the rank one projection onto ψ_{P}), we also have

$$\begin{aligned}\mathcal{G}(\psi_0, \varphi_0) = e_{\mathrm{P}} + &\ \langle \operatorname{Im} \psi_0 | H_{\mathrm{P}} | \operatorname{Im} \psi_0 \rangle + \| \operatorname{Im} \varphi_0\|_2^2 \\ &+ \| \operatorname{Re} \delta_2 + 2(2\pi)^{3/2}(-\Delta)^{-1/2}(\psi_{\mathrm{P}} \operatorname{Re} \delta_1)\|_2^2 \\ &+ \langle \operatorname{Re} \delta_1 | Q(H_{\mathrm{P}} - 4X)Q | \operatorname{Re} \delta_1 \rangle + O(\|\delta_2\|_2 \|\delta_1\|_{H^1}^2) + O(\|\delta_1\|_{L^2}^3), \end{aligned} \tag{5.3.7}$$

where $Q = \mathbb{1} - P_{\psi_{\mathrm{P}}}$.

Upper Bound: For sufficiently small v, we use as a trial state

$$(\bar{\psi}_0, \bar{\varphi}_0) = \Big(f_v \psi_{\mathrm{P}} + i g_v H_{\mathrm{P}}^{-1} \partial_1 \psi_{\mathrm{P}},\ \varphi_{\mathrm{P}} + i v \alpha^2 \partial_1 \varphi_{\mathrm{P}} \Big) \tag{5.3.8}$$

with $f_v, g_v > 0$ given by

$$f_v^2 := \frac{2v^2 \|H_{\mathrm{P}}^{-1} \partial_1 \psi_{\mathrm{P}}\|_2^2}{1 - \sqrt{1 - 4v^2 \|H_{\mathrm{P}}^{-1} \partial_1 \psi_{\mathrm{P}}\|_2^2}},\ g_v^2 := \frac{1 - \sqrt{1 - 4v^2 \|H_{\mathrm{P}}^{-1} \partial_1 \psi_{\mathrm{P}}\|_2^2}}{2 \|H_{\mathrm{P}}^{-1} \partial_1 \psi_{\mathrm{P}}\|_2^2}. \tag{5.3.9}$$

Note that $\partial_1 \psi_{\mathrm{P}}$ is orthogonal to ψ_{P}, hence $H_{\mathrm{P}}^{-1} \partial_1 \psi_{\mathrm{P}}$ is well-defined. We begin by showing that (5.3.8) is an element of the set of admissible initial data I_v in (5.2.16). To prove that $(\bar{\psi}_0, \bar{\varphi}_0)$ satisfies (i), we only need to check that $\bar{\psi}_0$ is normalized (which follows easily from (5.3.9)) as the condition (5.2.14) will follow a posteriori from the energy bound we shall derive. We now proceed to show that $(\bar{\psi}_0, \bar{\varphi}_0)$ satisfies (ii). For the electron, using that $H_{\mathrm{P}}^{-1} \partial_j \psi_{\mathrm{P}} = -x_j \psi_{\mathrm{P}}/2$ (which can be checked by applying H_P and using that $[H_P, x_1] = -2\partial_1$) and consequently that

$$\langle \partial_i \psi_{\mathrm{P}} |\, H_{\mathrm{P}}^{-1} \,| \partial_j \psi_{\mathrm{P}} \rangle = \delta_{ij}/4 \tag{5.3.10}$$

since ψ_{P} is radial, we can conclude that

$$-2 \left\langle \bar{\psi}_0 \middle| i\partial_j \middle| \bar{\psi}_0 \right\rangle = 4 f_v g_v \langle H_{\mathrm{P}}^{-1} \partial_1 \psi_{\mathrm{P}} | \partial_j \psi_{\mathrm{P}} \rangle = v \delta_{j1}, \tag{5.3.11}$$

i.e., that $\mathsf{V}_{\mathsf{el}}(0) = v(1,0,0)$, as required.

For the phonons, we first note that $\mathsf{X}_{\mathsf{ph}}(0) = 0$, since $\operatorname{Re} \bar{\varphi}_0 = \varphi_{\mathrm{P}}$. Next, we derive a relation for the velocity of the phonons $\mathsf{V}_{\mathsf{ph}}(t) = \dot{z}(t)$ in terms of their position $\mathsf{X}_{\mathsf{ph}}(t) = z(t)$ for general time t. Since

$$\min_z \|\varphi_t - \varphi_{\mathrm{P}}^z\|_2^2 = \|\varphi_t - \varphi_{\mathrm{P}}^{z(t)}\|_2^2, \tag{5.3.12}$$

the position $z(t)$ necessarily has to satisfy

$$\mathrm{Re}\left\langle \varphi_t \middle| (u\cdot\nabla)\varphi_{\mathrm{P}}^{z(t)}\right\rangle = 0 \quad \text{for all} \quad u\in\mathbb{S}^2 \iff \mathrm{Re}\,\varphi_t \perp \mathrm{span}\{\nabla\varphi_{\mathrm{P}}^{z(t)}\}. \tag{5.3.13}$$

Differentiating (5.3.13) w.r.t. time, using (5.1.1) and evaluating the resulting expression at $t=0$, we arrive at

$$\begin{aligned} 0 &= \mathrm{Re}\left\langle -i\alpha^{-2}(u\cdot\nabla)(\bar{\varphi}_0+\sigma_{\bar{\psi}_0}) \middle| \varphi_{\mathrm{P}}\right\rangle - \mathrm{Re}\left\langle (\dot{z}(0)\cdot\nabla)\bar{\varphi}_0 | (u\cdot\nabla)\varphi_{\mathrm{P}}\right\rangle \\ &= \left\langle -\alpha^{-2}\,\mathrm{Im}\,\bar{\varphi}_0 \middle| (u\cdot\nabla)\varphi_{\mathrm{P}}\right\rangle - \left\langle (\dot{z}(0)\cdot\nabla)\,\mathrm{Re}\,\bar{\varphi}_0 | (u\cdot\nabla)\varphi_{\mathrm{P}}\right\rangle \\ &= -\left\langle v\partial_1\varphi_{\mathrm{P}} | (u\cdot\nabla)\varphi_{\mathrm{P}}\right\rangle - \left\langle (\dot{z}(0)\cdot\nabla)\varphi_{\mathrm{P}} | (u\cdot\nabla)\varphi_{\mathrm{P}}\right\rangle, \end{aligned} \tag{5.3.14}$$

which the velocity $\dot{z}(0)$ has to satisfy for all $u\in\mathbb{S}^2$, given its position $\mathsf{X}_{\mathsf{ph}}(0)=z(0)=0$. By invertibility of the coefficient matrix, (5.3.14) has the unique solution $\dot{z}(0)=v(1,0,0)$, and we indeed conclude that $\mathsf{V}_{\mathsf{ph}}(0)=v(1,0,0)$.

We now evaluate $\mathcal{G}(\bar{\psi}_0,\bar{\varphi}_0)$. Since $f_v=1+O(v^2), g_v=v+O(v^3)$, using (5.3.7) and (5.3.10) we find

$$E(v)\le\mathcal{G}(\bar{\psi}_0,\bar{\varphi}_0)=e_{\mathrm{P}}+v^2\left(\frac{1}{4}+\alpha^4\|\partial_1\varphi_{\mathrm{P}}\|_2^2\right)+O(v^3) \tag{5.3.15}$$

verifying on the one hand (5.2.14) for sufficiently small v, and on the other hand the r.h.s. of (5.2.18) as an upper bound on $E(v)$ (using that φ_{P} is radial).

Lower Bound: We first observe that to derive a lower bound on $E(v)$ we can w.l.o.g. restrict to initial conditions (ψ_0,φ_0) satisfying additionally

$$P_{L^2}^{\mathcal{M}_{\mathcal{E}}}(\psi_0)>0, \tag{5.3.16}$$

$$\mathsf{X}_{\mathsf{ph}}(0)=0. \tag{5.3.17}$$

This simply follows from the invariance of $\mathcal{G}$ under translations (of both ψ and φ) and under changes of phase of ψ. Moreover, by the upper bound derived in the first step of this proof and the coercivity of $\mathcal{E}$ and $\mathcal{F}$ in (5.2.7), we conclude that it is sufficient to minimize over elements of I_v such that $\mathrm{dist}_{H^1}(\psi_0,\mathcal{M}_{\mathcal{E}})=O(v)=\mathrm{dist}_{L^2}(\varphi_0,\mathcal{M}_{\mathcal{F}})$ for small v. Since the L^2-projection of φ_0 is φ_{P} by (5.3.17), it immediately follows that $\|\delta_2\|_2=O(v)$. We now proceed to show that necessarily also $\|\delta_1\|_{H^1}=O(v)$. Let $y',y\in\mathbb{R}^3$ and $\theta\in[0,2\pi)$ be such that

$$P_{L^2}^{\mathcal{M}_{\mathcal{E}}}(\psi_0)=\psi_{\mathrm{P}}^{y'},\quad P_{H^1}^{\mathcal{M}_{\mathcal{E}}}(\psi_0)=e^{i\theta}\psi_{\mathrm{P}}^{y}, \tag{5.3.18}$$

where we recall that the L^2-projection is assumed to be positive by (5.3.16). Combining the upper bound derived in the first step with [**?** , Eq. (53)], we get

$$\|\varphi_0-\varphi_{\mathrm{P}}^y\|_2^2\le C\left(\mathcal{G}(\psi_0,\varphi_0)-e_{\mathrm{P}}\right)\le Cv^2. \tag{5.3.19}$$

There exist $\delta,C_1,C_2>0$ such that

$$\|\varphi_{\mathrm{P}}-\varphi_{\mathrm{P}}^y\|_2\ge\begin{cases}C_1|y|\|\nabla\varphi_{\mathrm{P}}\|_2, & |y|\le\delta\\ C_2 & |y|>\delta\end{cases}, \tag{5.3.20}$$

and this allows to conclude that $|y|=O(v)$. In other words, assuming centering w.r.t. to translations in the phonon coordinate (i.e. (5.3.17)) forces, at low energies, also the centering w.r.t. translations in the electron coordinate, at least approximately. At this point, it is also easy to verify that $\theta = O(v)$ (and, as an aside, that $|y'| = O(v)$), since, by the upper bound derived in the first step and the coercivity of $\mathcal{E}$, we have

$$\|\psi_{\rm P}^{y'} - e^{i\theta}\psi_{\rm P}^{y}\|_2 \leq \|\psi_{\rm P}^{y'} - \psi_0\|_2 + \|e^{i\theta}\psi_{\rm P}^{y} - \psi_0\|_2 = O(v). \tag{5.3.21}$$

In particular, we conclude that

$$\|\delta_1\|_{H^1} \leq \|e^{i\theta}\psi_{\rm P}^{y} - \psi_0\|_{H^1} + \|\psi_{\rm P} - e^{i\theta}\psi_{\rm P}^{y}\|_{H^1} = O(v). \tag{5.3.22}$$

Using again (5.3.7) and that $Q(H_{\rm P} - 4X_{\rm P})Q \geq 0$, we conclude that for any $(\psi_0, \varphi_0) \in I_v$ satisfying (5.3.16) and (5.3.17), as well as $\mathcal{G}(\psi_0, \varphi_0) \leq e_{\rm P} + O(v^2)$, we have

$$\mathcal{G}(\psi_0, \varphi_0) \geq e_{\rm P} + \langle \operatorname{Im}\psi_0 | H_{\rm P} | \operatorname{Im}\psi_0 \rangle + \|\operatorname{Im}\varphi_0\|_2^2 + O(v^3). \tag{5.3.23}$$

By arguing as in (5.3.14), we see that the conditions $\mathsf{X}_{\mathsf{ph}}(0) = 0$ and $\mathsf{V}_{\mathsf{ph}}(0) = v$ imply that

$$P_{\nabla\varphi_{\rm P}}(\operatorname{Im}\varphi_0 + v\alpha^2\partial_1 \operatorname{Re}\varphi_0) = 0, \tag{5.3.24}$$

where $P_{\nabla\varphi_{\rm P}}$ denotes the projection onto the span of $\partial_j\varphi_{\rm P}$, $1 \leq j \leq 3$. Since $P_{\nabla\varphi_{\rm P}}\partial_1$ is a bounded operator, and $\|\delta_2\|_2 = O(v)$, we find

$$\|\operatorname{Im}\varphi_0\|_2^2 \geq \|P_{\nabla\varphi_{\rm P}} \operatorname{Im}\varphi_0\|_2^2 = v^2\alpha^4\|\partial_1\varphi_{\rm P} + P_{\nabla\varphi_{\rm P}}\partial_1 \operatorname{Re}\delta_2\|_2^2 \geq v^2\alpha^4\|\partial_1\varphi_{\rm P}\|_2^2 - O(v^3). \tag{5.3.25}$$

We are left with giving a lower bound on $\langle \operatorname{Im}\psi_0 | H_{\rm P} | \operatorname{Im}\psi_0 \rangle$, under the condition that

$$2\langle \psi_0 | -i\nabla | \psi_0 \rangle = 4\langle \operatorname{Im}\psi_0 | \nabla \operatorname{Re}\psi_0 \rangle = v(1,0,0). \tag{5.3.26}$$

We already argued in (5.3.22) that $\|\psi_0 - \psi_{\rm P}\|_{H^1} = O(v)$, and therefore

$$4\langle \operatorname{Im}\psi_0 | \nabla\psi_{\rm P} \rangle = v(1,0,0) + O(v^2). \tag{5.3.27}$$

Completing the square, we find

$$\begin{aligned}\langle \operatorname{Im}\psi_0 | H_{\rm P} | \operatorname{Im}\psi_0 \rangle = &\ \langle H_{\rm P}\operatorname{Im}\psi_0 - v\partial_1\psi_{\rm P} | H_{\rm P}^{-1} | H_{\rm P}\operatorname{Im}\psi_0 - v\partial_1\psi_{\rm P} \rangle \\ &+ 2v\langle \operatorname{Im}\psi_0 | \partial_1\psi_{\rm P} \rangle - v^2\langle \partial_1\psi_{\rm P} | H_{\rm P}^{-1} | \partial_1\psi_{\rm P} \rangle \\ \geq &\ 2v\langle \operatorname{Im}\psi_0 | \partial_1\psi_{\rm P} \rangle - v^2\langle \partial_1\psi_{\rm P} | H_{\rm P}^{-1} | \partial_1\psi_{\rm P} \rangle .\end{aligned} \tag{5.3.28}$$

From the constraint (5.3.27) and (5.3.10), it thus follows that

$$\langle \operatorname{Im}\psi_0 | H_{\rm P} | \operatorname{Im}\psi_0 \rangle \geq \frac{v^2}{4} + O(v^3). \tag{5.3.29}$$

By combining (5.3.23), (5.3.25) and (5.3.29), we arrive at the final lower bound

$$E(v) \geq e_{\rm P} + v^2\left(\frac{1}{4} + \alpha^4\|\partial_1\varphi_{\rm P}\|_2^2\right) + O(v^3). \tag{5.3.30}$$

Again, since $\varphi_{\rm P}$ is radial, this is of the desired form, and hence the proof is complete. □

5.4 Further Considerations

In this section, we carry out the details related to Remarks 5.2.2 and 5.2.3.

5.4.1 Effective mass through traveling wave solutions

A possible way of formalizing the derivation of the effective mass in [1, 66] relies on traveling wave solutions of the Landau–Pekar equations. A traveling wave of velocity $v \in \mathbb{R}^3$ is a solution (ψ_t, φ_t) of (5.1.1) of the form

$$(\psi_t, \varphi_t) = (e^{-ie_v t}\psi_v^{\mathsf{TW}}(\cdot - vt), \varphi_v^{\mathsf{TW}}(\cdot - vt)) \tag{5.4.1}$$

for all $t \in \mathbb{R}$, with $e_v \in \mathbb{R}$ defining a suitable phase factor. As before, by rotation invariance we can restrict our attention to velocities of the form $v(1,0,0)$ with $v \in \mathbb{R}$ in the following.

Note that in the case $\alpha = 0$, where $\varphi_t = -\sigma_{\psi_t}$ for all $t \in \mathbb{R}$, the LP equations simplify to a non-linear Schrödinger equation (also known as Choquard equation). In this case, a traveling wave is given by $\psi_v^{\mathsf{TW}}(x) = e^{ix_1 v/2}\psi_{\mathrm{P}}(x)$ with $e_v = \mu_{\mathrm{P}} + \frac{v^2}{4}$, and its energy can be computed to be

$$\mathcal{G}\left(\psi_v^{\mathsf{TW}}, -\sigma_{\psi_v^{\mathsf{TW}}}\right) = e_{\mathrm{P}} + \frac{v^2}{4}, \tag{5.4.2}$$

yielding an effective mass $m = 1/2$ at $\alpha = 0$. For the case $\alpha > 0$, on the other hand, we conjecture that there are no traveling wave solutions of the form (5.4.1).

Conjecture 5.4.1. *For $\alpha > 0$, there are no solutions to the LP equations* (5.1.1) *of the form* (5.4.1) *with $v \neq 0$.*

If one *assumes* the existence of traveling wave solutions, at least for small v, one can predict an effective mass that agrees with our formula (5.2.19), as we shall now demonstrate. From the LP equations (5.1.1) one easily sees that a traveling wave solution needs to satisfy

$$\begin{aligned} -iv\partial_1\psi_v^{\mathsf{TW}} &= \left(h_{\varphi_v^{\mathsf{TW}}} + e_v\right)\psi_v^{\mathsf{TW}} \\ -i\alpha^2 v\partial_1\varphi_v^{\mathsf{TW}} &= \varphi_v^{\mathsf{TW}} + \sigma_{\psi_v^{\mathsf{TW}}}. \end{aligned} \tag{5.4.3}$$

We shall denote by $E^{\mathsf{TW}}(v)$ the energy of the traveling wave as a function of the velocity $v \in \mathbb{R}$, i.e.

$$E^{\mathsf{TW}}(v) := \mathcal{G}(\psi_v^{\mathsf{TW}}, \varphi_v^{\mathsf{TW}}). \tag{5.4.4}$$

In the following, we assume that $e_v = \mu_{\mathrm{P}} + O(v^2)$ and that the traveling wave is of the form

$$(\psi_v^{\mathsf{TW}}, \varphi_v^{\mathsf{TW}}) = \left(\frac{\psi_{\mathrm{P}} + v\xi_v}{\|\psi_{\mathrm{P}} + v\xi_v\|_2}, \varphi_{\mathrm{P}} + v\eta_v\right), \tag{5.4.5}$$

with both ξ_v and η_v bounded in v and converging to some (ξ, η) as $v \to 0$. In other words, we assume that the traveling waves have a suitable differentiability in v, at least for small v, and converge to the standing wave solution $(e^{-i\mu_{\mathrm{P}}t}\psi_{\mathrm{P}}, \varphi_{\mathrm{P}})$ for $v = 0$. W.l.o.g. we may also assume that ξ_v is orthogonal to ψ_{P}.

We can then use that

$$\frac{1}{\|\psi_{\mathrm{P}} + v\xi_v\|_2^2} = 1 - v^2\frac{\|\xi_v\|_2^2}{\|\psi_{\mathrm{P}} + v\xi_v\|_2^2} = 1 - v^2\|\xi\|_2^2 + o(v^2) \tag{5.4.6}$$

in order to linearize the traveling wave equations (5.4.1), obtaining that (ξ, η) solves

$$\begin{pmatrix} i\partial_1\psi_{\mathrm{P}} \\ i\alpha^2\partial_1\varphi_{\mathrm{P}} \end{pmatrix} = \begin{pmatrix} H_{\mathrm{P}} & 2(2\pi)^{3/2}\psi_{\mathrm{P}}(-\Delta)^{-1/2}\,\mathrm{Re} \\ 2(2\pi)^{3/2}(-\Delta)^{-1/2}\psi_{\mathrm{P}}\,\mathrm{Re} & 1 \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix}, \tag{5.4.7}$$

where $H_{\mathrm{P}} = h_{\varphi_{\mathrm{P}}} - \mu_{\mathrm{P}}$, as defined in (5.2.3). Splitting into real and imaginary parts, we equivalently find

$$H_{\mathrm{P}}\,\mathrm{Im}\,\xi = \partial_1\psi_{\mathrm{P}} \tag{5.4.8}$$
$$\mathrm{Im}\,\eta = \alpha^2\partial_1\varphi_{\mathrm{P}} \tag{5.4.9}$$
$$H_{\mathrm{P}}\,\mathrm{Re}\,\xi + 2(2\pi)^{3/2}\psi_{\mathrm{P}}\,(-\Delta)^{-1/2}\,\mathrm{Re}\,\eta = 0 \tag{5.4.10}$$
$$2(2\pi)^{3/2}\,(-\Delta)^{-1/2}\,\psi_{\mathrm{P}}\,\mathrm{Re}\,\xi + \mathrm{Re}\,\eta = 0. \tag{5.4.11}$$

Combining (5.4.10) and (5.4.11) gives $(H_{\mathrm{P}} - 4X_{\mathrm{P}})\,\mathrm{Re}\,\xi = 0$, with X_{P} defined after (5.3.6). It was shown in [70] that the kernel of $H_{\mathrm{P}} - 4X_{\mathrm{P}}$ is spanned by $\nabla\psi_{\mathrm{P}}$, hence $\mathrm{Re}\,\xi \in \mathrm{span}\{\nabla\psi_{\mathrm{P}}\}$. Eq, (5.4.11) then implies that $\mathrm{Re}\,\eta \in \mathrm{span}\{\nabla\varphi_{\mathrm{P}}\}$.

Using these equations and (5.4.6) in the expansion (5.3.7), it is straightforward to obtain

$$E^{\mathsf{TW}}(v) = e_{\mathrm{P}} + v^2\left(\frac{1}{4} + \alpha^4\|\partial_1\varphi_{\mathrm{P}}\|_2^2\right) + o(v^2), \tag{5.4.12}$$

which agrees with (5.4.2) for the case $\alpha = 0$, and also with (5.2.18) to leading order in v. In particular, (5.2.21) holds.

5.4.2 Effective mass with alternative definition for the electron's velocity

In this Section, we discuss a different approach to the definition of the effective mass. This approach is based on an alternative way of defining the electron's position and velocity. While in Section 5.2.2 we use the standard definition from quantum mechanics, here we use a definition similar to the one of the phonons' position and velocity (5.2.15). For this purpose, we recall Remark 5.2.1 and that δ^* has been chosen such that the condition $\mathcal{E}(\psi_0) \leq \mathcal{G}(\psi_0, \varphi_0) \leq e_{\mathrm{P}} + \delta^*$ ensures that for all times there exists a unique L^2-projection $e^{i\theta(t)}\psi_{\mathrm{P}}^{y(t)}$ of ψ_t onto the manifold $\mathcal{M}_{\mathcal{E}}$. Then, we define the electron's position and velocity by

$$\widetilde{\mathsf{X}}_{\mathsf{el}}(t) = y(t), \quad \widetilde{\mathsf{V}}_{\mathsf{el}}(t) = \dot{y}(t). \tag{5.4.13}$$

Similarly to the conditions (i) and (ii) in Section 5.2.2, we define the set of admissible initial data as

$$\widetilde{I}_v = \{(\psi_0, \varphi_0)\,|\,\text{(i),(ii') are satisfied}\} \tag{5.4.14}$$

where

(ii') $\widetilde{\mathsf{V}}_{\mathsf{el}}(t) = \mathsf{V}_{\mathsf{ph}}(0) = v(1, 0, 0)$.

Note that we are leaving the parameter $\dot{\theta}(0)$ free, which in this case is also relevant. In other words, we have

$$\widetilde{I}_v = \cup_{\kappa\in\mathbb{R}}\widetilde{I}_{v,\kappa}, \tag{5.4.15}$$

where

$$\widetilde{I}_{v,\kappa} = \{(\psi_0, \varphi_0) \,|\, \text{(i),(ii') are satisfied and } \dot{\theta}(0) = \kappa\}. \tag{5.4.16}$$

Minimizing now the energy over all states of the set $\widetilde{I}_v$

$$\widetilde{E}(v) := \inf_{(\psi_0,\varphi_0)\in\widetilde{I}_v} \mathcal{G}(\psi_0, \varphi_0), \tag{5.4.17}$$

leads to an energy expansion in v that differs from the one of Theorem 5.2.1 in its second order.

Proposition 5.4.1. *As $v \to 0$, we have*

$$\widetilde{E}(v) = e_{\mathrm{P}} + v^2 \left(\frac{\|\nabla\psi_{\mathrm{P}}\|_2^4}{3\|\nabla\varphi_{\mathrm{P}}\|_2^2} + \frac{\alpha^4}{3}\|\nabla\varphi_{\mathrm{P}}\|_2^2 \right) + O(v^3). \tag{5.4.18}$$

The energy expansion in (5.4.18) leads to the effective mass

$$\widetilde{m}_{\mathsf{eff}} = \lim_{v\to 0} \frac{\widetilde{E}(v) - e_{\mathrm{P}}}{v^2/2} = \frac{2\|\nabla\psi_{\mathrm{P}}\|_2^4}{3\|\nabla\varphi_{\mathrm{P}}\|_2^2} + \frac{2\alpha^4}{3}\|\nabla\varphi_{\mathrm{P}}\|_2^2 \tag{5.4.19}$$

which agrees with (5.2.19) and (5.2.21) in leading order for large α only (and thus still confirms the Landau–Pekar prediction [66]), but differs in the $O(1)$ term. In fact, it turns out that $\widetilde{m}_{\mathsf{eff}} < m_{\mathsf{eff}}$ with m_{eff} defined in (5.2.21).

This follows from the observation that the trial state

$$(\widetilde{\psi}_0, \widetilde{\varphi}_0) = \left(\frac{f_v\psi_{\mathrm{P}} + ivH_{\mathrm{P}}^{-1}\partial_1\psi_{\mathrm{P}}}{\|f_v\psi_{\mathrm{P}} + ivH_{\mathrm{P}}^{-1}\partial_1\psi_{\mathrm{P}}\|}, \varphi_{\mathrm{P}} + iv\alpha^2\partial_1\varphi_{\mathrm{P}} \right) \tag{5.4.20}$$

with $f_v = \frac{1}{2}\left(1 + \sqrt{1 - v^2/(4\|\partial_1\psi_{\mathrm{P}}\|_2^2)}\right)$ (which coincides up to terms of order v^2 with the trial state (5.3.8)) is an element of $\widetilde{I}_{v,\bar{\kappa}}$ for $\bar{\kappa} = -\mu_{\mathrm{P}} + 4\|\partial_1\psi_{\mathrm{P}}\|_2^2(f_v - 1)$ and is such that $\mathcal{G}(\widetilde{\psi}_0, \widetilde{\varphi}_0) = e_{\mathrm{P}} + m_{\mathsf{eff}}\, v^2/2 + O(v^3)$. Thus, $\widetilde{m}_{\mathsf{eff}} \leq m_{\mathsf{eff}}$ and equality holds if and only if equality (up to terms $o(v^2)$) holds in (5.4.36). This is the case if and only if

$$Q_{\psi_{\mathrm{P}}}\left(\operatorname{Im}\widetilde{\psi}_0 - cv\partial_1\psi_{\mathrm{P}}\right) = o(v). \tag{5.4.21}$$

Using (5.4.20), equality holds if and only if

$$0 = H_{\mathrm{P}}^{-1}\partial_1\psi_P - c\partial_1\psi_{\mathrm{P}} = -\left(x_1/2 + c\partial_1\right)\psi_{\mathrm{P}} \tag{5.4.22}$$

i.e. , recalling the radiality of ψ_{P}, if and only if ψ_{P} is a Gaussian with variance $\sigma^2 = 1/(2c)$. Since ψ_{P} satisfies the Euler–Lagrange equation

$$H_{\mathrm{P}}\psi_{\mathrm{P}} = 0 \iff V_{\varphi_{\mathrm{P}}}\psi_{\mathrm{P}} = (-\Delta + \mu_P)\psi_{\mathrm{P}}, \tag{5.4.23}$$

it cannot be a Gaussian and therefore $\tilde{m}_{\mathsf{eff}} < m_{\mathsf{eff}}$.

We present only a sketch of the proof of Proposition 5.4.1, since it uses very similar arguments as the proof of Theorem 5.2.1.

Sketch of Proof of Proposition 5.4.1. **Upper bound**: We use the alternative trial state

$$(\widetilde{\psi}_0, \widetilde{\varphi}_0) = \left(\frac{f_v \psi_{\mathrm{P}} + ivc\partial_1 \psi_{\mathrm{P}}}{\|f_v \psi_{\mathrm{P}} + ivc\partial_1 \psi_{\mathrm{P}}\|}, \varphi_{\mathrm{P}} + iv\alpha^2 \partial_1 \varphi_{\mathrm{P}} \right), \tag{5.4.24}$$

with

$$f_v := \frac{1 + \sqrt{1 + 4c^2 v^2 \|\partial_1 \psi_{\mathrm{P}}\|^2}}{2}, \quad c := \frac{\|\partial_1 \psi_{\mathrm{P}}\|^2}{\|\partial_1 \varphi_{\mathrm{P}}\|^2}. \tag{5.4.25}$$

With similar arguments as in the previous section, one can verify that $(\widetilde{\psi}_0, \widetilde{\varphi}_0) \in \widetilde{I}_v$, in particular $(\widetilde{\psi}_0, \widetilde{\varphi}_0) \in \widetilde{I}_{v,\kappa}$ with $\kappa = -\mu_{\mathrm{P}} + \frac{-1+\sqrt{1+4c^2v^2\|\partial_1\psi_{\mathrm{P}}\|^2}}{2c}$.

Note that, similarly to (5.3.14), one can derive necessary conditions for the velocities $\dot{y}(0), \dot{\theta}(0)$ (using $\widetilde{\mathsf{X}}_{\mathrm{el}}(0) = 0, \theta(0) = 0$), namely

$$\left\langle [h_{\mathrm{Re}\, \widetilde{\varphi}_0} + \dot{\theta}(0)] \operatorname{Im} \widetilde{\psi}_0 - \dot{y}(0) \cdot \nabla \operatorname{Re} \widetilde{\psi}_0 \middle| (u \cdot \nabla) \psi_{\mathrm{P}} \right\rangle = 0 \quad \text{for all} \quad u \in \mathbb{S}^2 \tag{5.4.26}$$

and

$$\left\langle \psi_{\mathrm{P}} \middle| (h_{\mathrm{Re}\, \widetilde{\varphi}_0} + \dot{\theta}(0)) \operatorname{Re} \widetilde{\psi}_0 + \dot{y}(0) \cdot \nabla \operatorname{Im} \widetilde{\psi}_0 \right\rangle = 0. \tag{5.4.27}$$

Straightforward computations then show that

$$\widetilde{E}(v) \le \mathcal{G}(\widetilde{\psi}_0, \widetilde{\varphi}_0) = e_{\mathrm{P}} + v^2 \left(\frac{\|\partial_1 \psi_{\mathrm{P}}\|_2^4}{\|\partial_1 \varphi_{\mathrm{P}}\|_2^2} + \alpha^4 \|\partial_1 \varphi_{\mathrm{P}}\|_2^2 \right) + O(v^3). \tag{5.4.28}$$

Lower bound: We proceed similarly to the lower bound in the previous section. First, we assume w.l.o.g. that

$$P_{L^2}^{\mathcal{M}_{\mathcal{E}}}(\psi_0) = \psi_{\mathrm{P}}^{y(0)}, \quad P_{L^2}^{\mathcal{M}_{\mathcal{F}}}(\varphi_0) = \varphi_{\mathrm{P}}, \tag{5.4.29}$$

i.e., centering with respect to translations and changes of phase. We can then substitute the two conditions of (ii') and the conditions for $\psi_{\mathrm{P}}^{y(0)}$ (resp. φ_{P}) to be the L^2-projection of ψ_0 (resp. φ_0) onto $\mathcal{M}_{\mathcal{E}}$ (resp. $\mathcal{M}_{\mathcal{F}}$) with their analogue necessary conditions (whose computations proceed along the lines of (5.4.26) and (5.4.27)). With this discussion, we are left with the task of minimizing $\mathcal{G}$ over the set

$$\widetilde{I}'_v := \bigcup_{\kappa \in \mathbb{R}} \widetilde{I}'_{v,\kappa} \tag{5.4.30}$$

with

$$\begin{aligned} \widetilde{I}'_{v,\kappa} := \Big\{ (\psi_0, \varphi_0) \in \widetilde{I}^* \,|\, & P_{\nabla \psi_{\mathrm{P}}^{y(0)}} \left[(h_{\mathrm{Re}\,\varphi_0} + \kappa) \operatorname{Im} \psi_0 - v\partial_1 \operatorname{Re} \psi_0 \right] = 0, \\ & P_{\psi_{\mathrm{P}}^{y(0)}} \left[(h_{\mathrm{Re}\,\varphi_0} + \kappa) \operatorname{Re} \psi_0 + v\partial_1 \operatorname{Im} \psi_0 \right] = 0, \\ & P_{\nabla \varphi_{\mathrm{P}}} (\operatorname{Im} \varphi_0 - v\alpha^2 \partial_1 \operatorname{Re} \varphi_0) = 0 \Big\}. \end{aligned} \tag{5.4.31}$$

and

$$\widetilde{I}^* := \left\{ (\psi_0, \varphi_0) \,|\, \mathcal{G}(\psi_0, \varphi_0) \le e_{\mathrm{P}} + \delta^*, \ \|\psi_0\|_2^2 = 1, \operatorname{Re} \psi_0 \perp \nabla \psi_{\mathrm{P}}^{y(0)}, \operatorname{Re} \varphi_0 \perp \nabla \varphi_{\mathrm{P}} \right\}. \tag{5.4.32}$$

As in the previous section, one can argue by coercivity of $\mathcal{E}$ and $\mathcal{F}$ and the upper bound that it is possible to restrict to initial conditions such that $\|\delta_2\|_2, \|\delta_1\|_{H^1}, y(0)$ are all $O(v)$. Moreover, the second constraint of the r.h.s. of (5.4.31) shows that $\kappa = -\mu_{\rm P} + O(v)$. Thus, we are left with minimizing $\mathcal{G}$ over the set

$$\widetilde{I}''_v := \widetilde{I}'_v \cap \{\kappa + \mu_{\rm P} = O(v),\ \|\delta_1\|_{H^1} = O(v),\ \|\delta_2\|_2 = O(v)\}\,. \tag{5.4.33}$$

The lower bound is proven in the same way as before. But instead of the constraint (5.3.27), this time we need to minimize w.r.t.

$$P_{\nabla\psi_{\rm P}^{y(0)}}\left[(h_{\operatorname{Re}\varphi_0} + \kappa)\operatorname{Im}\psi_0 - v\partial_1 \operatorname{Re}\psi_0\right] = 0. \tag{5.4.34}$$

Since $\kappa + \mu_{\rm P}, y_0, \|\delta_1\|_{H^1}$ and $\|\delta_2\|_2$ are all order v and $\psi_{\rm P} \in C_0^\infty(\mathbb{R}^3)$ (and these facts also allow to infer that $\psi_{\rm P}^{y(0)} = \psi_{\rm P} + O(v)$), the constraint (5.4.34) can be written as

$$\langle \nabla\psi_{\rm P} | H_{\rm P} | \operatorname{Im}\psi_0\rangle = v\|\partial_1\psi_P\|_2^2(1,0,0) + O(v^2). \tag{5.4.35}$$

Denoting $c = \|\partial_1\psi_P\|_2^2/\|\partial_1\varphi_P\|_2^2$, we complete the square

$$\begin{aligned}\langle \operatorname{Im}\psi_0 | H_{\rm P} | \operatorname{Im}\psi_0\rangle =\ & \langle \operatorname{Im}\psi_0 - vc\partial_1\psi_{\rm P} | H_{\rm P} | \operatorname{Im}\psi_0 - vc\partial_1\psi_{\rm P}\rangle \\ & + 2vc\,\langle \operatorname{Im}\psi_0 | H_{\rm P} | \partial_1\psi_{\rm P}\rangle - c^2v^2\,\langle \partial_1\psi_{\rm P} | H_{\rm P} | \partial_1\psi_{\rm P}\rangle \\ \geq\ & 2cv\,\langle \operatorname{Im}\psi_0 | H_{\rm P}\partial_1\psi_{\rm P}\rangle - c^2v^2\,\langle \partial_1\psi_{\rm P} | H_{\rm P} | \partial_1\psi_{\rm P}\rangle\,.\end{aligned} \tag{5.4.36}$$

With the constraint (5.4.34) and $\langle \partial_i\psi_{\rm P} | H_{\rm P} | \partial_j\psi_{\rm P}\rangle = \delta_{i,j}\|\partial_j\varphi_{\rm P}\|_2^2$, we arrive at (5.4.18). □

5.5 Appendix A: Well-posedness and regularity of the projections onto $\mathcal{M}_\mathcal{F}$

Similar arguments to the ones used in the following proof are contained in [33], where the functional $\mathcal{F}$ is investigated in the case of a torus in place of $\mathbb{R}^3$. Remark 5.2.1 on the properties $\mathcal{M}_\mathcal{E}$ can be shown with a similar approach, but we omit its proof.

Proof of Lemma 5.2.1. We need to prove that there exists $\delta > 0$ such that for any $\varphi \in (\mathcal{M}_\mathcal{F})_\delta$ there exists a unique z_φ identifying the projection of φ onto $\mathcal{M}_\mathcal{F}$, and such that z_φ is differentiable at any $\varphi \in (\mathcal{M}_\mathcal{F})_\delta$. As the problem is invariant w.r.t. translations, we can w.l.o.g. restrict to show differentiability at $\varphi_0 \in (\mathcal{M}_\mathcal{F})_\delta$ such that $z_{\varphi_0} = 0$.

We define the function $F : L^2(\mathbb{R}^3) \times \mathbb{R}^3 \to \mathbb{R}^3$ given, component-wise, by

$$F_i(\varphi, z) = \operatorname{Re}\langle \varphi | \partial_i \varphi_P^z\rangle \quad \text{for} \quad i = 1,2,3. \tag{5.5.1}$$

By definition of z_φ, we have $F(\varphi_0, 0) = 0$ and $F(\varphi, z_\varphi) = 0$, for any φ in a sufficiently small neighborhood of φ_0. Hence, we set out to use the implicit function theorem to determine properties of z_φ. Observe that, for any $\eta \in L^2(\mathbb{R}^3)$, $z \in \mathbb{R}^3$ and $i, j \in \{1,2,3\}$, we have

$$\partial_t F_i(\varphi + t\eta, z) = \operatorname{Re}\langle \eta | \partial_i \varphi_P^z\rangle \quad \text{and} \quad \partial_{z_j} F_i(\varphi, z) = -\operatorname{Re}\langle \varphi | \partial_i\partial_j \varphi_P^z\rangle\,. \tag{5.5.2}$$

Since $\varphi_P \in C^\infty(\mathbb{R}^3)$, the map $(\mathcal{M}_\mathcal{F})_\delta \ni \varphi \mapsto \det\left(\frac{\partial F_i}{\partial z_j}(\varphi, z)\right)_{i,j=1,\dots,3}$ is continuous w.r.t the L^2-norm and, by radiality of φ_P,

$$\det\left(\frac{\partial F_i}{\partial z_j}(\varphi_P, 0)\right)_{i,j=1,\dots,3} = \frac{1}{9}\|\nabla\varphi_P\|_2^2 > 0\,. \tag{5.5.3}$$

Thus, it follows that det $\left(\frac{\partial F_i}{\partial z_j}(\varphi_0, 0)\right)_{i,j=1,\ldots,3} > 0$, uniformly in φ_0 for sufficiently small $\delta > 0$. By the implicit function theorem, there exists a unique differentiable $z_\varphi : (\mathcal{M}_\mathcal{F})_\delta \to \mathbb{R}^3$ whose partial derivative in the direction $\eta \in L^2(\mathbb{R}^3)$ at φ_0 is given by

$$\partial_t z_{\varphi_0+t\eta} \restriction_{t=0} = \left[\left(\frac{\partial F_i}{\partial z_j}(\varphi_0, z_{\varphi_0})\right)_{i,j=1,\ldots,3}\right]^{-1} \mathrm{Re}\langle \eta | \partial_i \varphi_P^{z_{\varphi_0}} \rangle \ . \tag{5.5.4}$$

□

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APPENDIX A

A Non-Commutative Entropic Optimal Transport Approach to Quantum Composite Systems at Positive Temperature

This Appendix contains the work

- Dario Feliciangeli, Augusto Gerolin, and Lorenzo Portinale. A non-commutative entropic optimal transport approach to quantum composite systems at positive temperature. *arXiv preprint arXiv:2106.11217*, 2021.

Abstract

This paper establishes new connections between many-body quantum systems, One-body Reduced Density Matrices Functional Theory (1RDMFT) and Optimal Transport (OT), by interpreting the problem of computing the ground-state energy of a finite dimensional composite quantum system at positive temperature as a non-commutative entropy regularized Optimal Transport problem. We develop a new approach to fully characterize the dual-primal solutions in such non-commutative setting. The mathematical formalism is particularly relevant in quantum chemistry: numerical realizations of the many-electron ground state energy can be computed via a non-commutative version of Sinkhorn algorithm. Our approach allows to prove convergence and robustness of this algorithm, which, to our best knowledge, were unknown even in the two marginal case. Our methods are based on careful a priori estimates in the dual problem, which we believe to be of independent interest. Finally, the above results are extended in 1RDMFT setting, where bosonic or fermionic symmetry conditions are enforced on the problem.

A.1 Introduction

In this work we are interested in studying the ground state energy of a finite dimensional composite quantum system at positive temperature. In particular, we focus on the problem of minimizing the energy of the composite system *conditionally* to the knowledge of the states of all its subsystems.

The first motivation for this study is physical: it is useful to understand how one could infer the state of a composite system when one only has experimental access to the measurement of the states of its subsystems. The second motivation is mathematical: indeed this problem can be cast as a non-commutative optimal transport problem, therefore showcasing how several ideas and concepts introduced in the commutative setting carry through to the non-commutative framework. Finally, a third motivation comes from the fact that one-body reduced density matrix functional theory, which is of interest on its own, can be framed as a special case of our setting.

Let us consider a composite system with N subsystems, each with state space given by the complex Hilbert space $\mathfrak{h}_j$ of dimension $d_j < \infty$, for $j = 1, \dots, N$, and denote the state space of the composite system $\mathfrak{h} := \mathfrak{h}_1 \otimes \mathfrak{h}_2 \otimes \cdots \otimes \mathfrak{h}_N$ (with dimension $d = d_1 \cdot d_2 \cdot \ldots d_N$). Further denote by H the Hamiltonian to which the whole system is subject and suppose that $\mathrm{H} = \mathrm{H}_0 + \mathrm{H}_{\mathsf{int}}$, where H_0 is the non-interacting part of the Hamiltonian, i.e. $\mathrm{H}_0 = \bigoplus_{j=1}^N \mathrm{H}_j := \mathrm{H}_1 \otimes \mathbb{1} \cdots \otimes \mathbb{1} + \mathbb{1} \otimes \mathrm{H}_2 \otimes \mathbb{1} \cdots \otimes \mathbb{1} + \cdots + \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes \mathrm{H}_N$ with H_j acting on $\mathfrak{h}_j$, and $\mathrm{H}_{\mathsf{int}}$ is its interacting part. Finally, suppose to have knowledge of the states $\boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_N)$ of the N subsystems, where each γ_j is a density matrix over $\mathfrak{h}_j$.

Then the energy of the composite system at temperature $\varepsilon > 0$ is given by

$$\begin{aligned}\inf_{\Gamma \mapsto \boldsymbol{\gamma}} \left\{ \mathrm{Tr}(H\Gamma) + \varepsilon S(\Gamma) \right\} &= \sum_{j=1}^N \mathrm{Tr}(H_j \gamma_j) + \mathfrak{F}^\varepsilon(\boldsymbol{\gamma}) \\ &:= \sum_{j=1}^N \mathrm{Tr}(H_j \gamma_j) + \inf_{\Gamma \mapsto \boldsymbol{\gamma}} \left\{ \mathrm{Tr}(\mathrm{H}_{\mathsf{int}}\, \Gamma) + \varepsilon S(\Gamma) \right\}, \end{aligned} \tag{A.1.1}$$

where the shorthand notation $\Gamma \mapsto \boldsymbol{\gamma}$ denotes the set of density matrices over $\mathfrak{h}$ with j-th marginal equal to γ_j, and $S(\Gamma) := \mathrm{Tr}\left(\Gamma \log(\Gamma)\right)$ is the opposite of the Von Neumann entropy of Γ (note that we prefer to adopt the mathematical sign convention).

Our approach for the study of $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma})$ borrows ideas from optimal transport and convex analysis, and takes the following observation as a starting point: the minimization appearing in $\mathfrak{F}^\varepsilon$ can be cast as a non-commutative entropic optimal transport problem. Indeed, one looks for an optimal non-commutative coupling Γ, with fixed non-commutative marginals (i.e. partial traces) $\boldsymbol{\gamma}$, which minimizes the sum of a transport cost (given by $\mathrm{Tr}(\mathrm{H}_{\mathsf{int}}\, \Gamma)$) and an entropic term. In light of this interpretation, setting the quantum problem at positive temperature ε corresponds to consider an entropic optimal transport problem with parameter ε.

Guided by this viewpoint, we first show that $\mathfrak{F}^\varepsilon$ has a dual formulation (see Theorem A.2.1 (i)), i.e. that the constrained minimization appearing in its definition is in duality with an unconstrained maximization problem (defined in (A.2.2)). We can then consider any vector $(U_1^\varepsilon, \dots, U_N^\varepsilon)$ of self-adjoint matrices which is a maximizer in the dual functional of $\mathfrak{F}^\varepsilon$, whose existence and uniqueness up to trivial transformations we prove in Theorem A.2.1(ii). We refer to such U_i^ε-s as *Kantorovich potentials* and show in Theorem A.2.1(iii) that the unique minimizer Γ^ε realizing $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma})$ can be written in terms of them as

$$\Gamma^\varepsilon = \exp\left(\frac{\bigoplus_{i=1}^N U_i^\varepsilon - \mathrm{H}_{\mathsf{int}}}{\varepsilon} \right), \tag{A.1.2}$$

in the case of all the γ_j-s having trivial kernels (in the general case a very similar formula holds). In this setting, $\mathfrak{F}^\varepsilon$ is continuous and its functional derivative can be computed in terms of the *Kantorovich potentials* as

$$\frac{\mathrm{d}\mathfrak{F}^\varepsilon}{\mathrm{d}\gamma_i}(\boldsymbol{\gamma}) = U_i^\varepsilon, \quad \text{for all} \quad i = 1, \dots, N, \tag{A.1.3}$$

as we show in Proposition A.2.1.

Furthermore, we introduce the Non-Commutative Sinkhorn algorithm to compute the optimizer realizing $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma})$. This algorithm exploits the shape of the minimizer obtained in (A.1.2), in order to construct a sequence $\Gamma^{(k)}$ of density matrices converging to Γ^ε of the form

$$\Gamma^{(k)} = \exp\left(\frac{\bigoplus_{i=1}^N U_i^{(k)} - \mathrm{H}_{\text{int}}}{\varepsilon}\right), \tag{A.1.4}$$

where the vector $(U_1^{(k)}, \dots, U_N^{(k)})$ is iteratively updated by progressively imposing that $\Gamma^{(k)}$ has at least one correct marginal. We prove the convergence and the robustness of this algorithm in Section A.5.

It is important to note that studying $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma})$, i.e. the constrained minimization at fixed marginals, can also help solving the unconstrained minimization of the Hamiltonian H at positive temperature ε. Indeed, denoting by $\mathfrak{P}(\mathfrak{h})$ the set of density matrices over $\mathfrak{h}$, then

$$E^\varepsilon(\mathrm{H}) := \inf_{\Gamma\in\mathfrak{P}(\mathfrak{h})} \{\mathrm{Tr}(\mathrm{H}\,\Gamma) + \varepsilon S(\Gamma)\} = \inf_{\boldsymbol{\gamma}} \left\{\sum_{j=1}^N \mathrm{Tr}(\mathrm{H}_j\,\gamma_j) + \mathfrak{F}^\varepsilon(\boldsymbol{\gamma})\right\}. \tag{A.1.5}$$

Combining (A.1.3) and (A.1.5) allows to write down the Euler–Lagrange equation of (A.1.5) recovering its optimizer, i.e. the Gibbs state constructed with H at temperature ε.

Our work is not the first to try to extend the theory of optimal transport to the non-commutative setting. One of the first attempts was carried out by E. Carlen and J. Maas [16], followed by many others (e.g. [11, 13, 14, 20, 18, 26, 25, 88, 90, 98, 99]). There is an important distinction to be made here. Commutative optimal transport can be cast *equivalently* as a static coupling problem or as a dynamical optimization problem. On the other hand, in the non-commutative setting it is not clear what is the relation (if any) between the two interpretations. This singles out a big difference between works that consider the dynamical formulation of commutative optimal transport as a starting point (e.g. [11, 16, 20, 18, 88, 90, 98, 99]) and the ones which instead focus on its static formulation (e.g. [24, 51, 71, 108, 123]).

This paper adopts an even different approach. We consider as a starting point the Entropic regularization of optimal transport (which is to be considered as an extension of static optimal transport, see e.g. the survey [72] and references therein) and introduce its non-commutative counterpart. We carry out this program by extending the method developed in [28, 29, 53]. See also Section A.5 for a detailed explanation of the multimarginal Sinkhorn algorithm in the commutative setting, as studied in [28].

In the work [13], the authors study the case of $\varepsilon = 0$ temperature and prove a duality result for the non-commutative problem in the very same spirit of the Kantorovich duality for the classical Monge problem. The recent work [121] studies the entropic quantum optimal transport problem as well, adopting, in constrast to our static approach, a dynamical formulation. Therein, the author proves a dynamical duality result at positive and zero temperature. To the best of our knowledge, the present work is the first complete analysis of the quantum entropic transport problem in the static framework.

As for the Sinkhorn Algorithm, another concept which we borrow from the commutative setting and extend to the quantum one, its convergence in the commutative setting was first established in the $N = 2$ marginal case [46, 110] for discrete measures and in [104] for continuous measures (see also [19]). In the multi-marginal setting, convergence guarantees were obtained for the discrete case in [21, 63] and for continuous measures in [28, 29]. Other variants of the Sinkhorn algorithm for (unbalanced) tensor-valued measures or matrix optimal mass transport have been studied in [98, 105] and do not apply to our setting. In the context of Computational Optimal Transport, the entropic regularization and the Sinkhorn algorithm was introduced in [24, 51].

Enforcing Symmetry Constraints: One-body Reduced Density Matrix Functional Theory

We conclude this introduction by briefly discussing the case in which symmetry conditions are enforced on the problem, either bosonic or fermionic, which we can also treat (see Section A.2.3). In this case, (A.1.1) makes sense only for $\mathfrak{h}_j = \mathfrak{h}_0$ for all $j = 1, \dots, N$ and $\boldsymbol{\gamma} = (\gamma, \dots, \gamma)$ (i.e. the underlying Hilbert spaces and the marginals must all be the same) and its study can be framed in the context of One-body Reduced Density Matrix Functional Theory (1RDMFT), introduced in 1975 by Gilbert [55] as an extension of the Hohenberg-Kohn (Levy-Lieb) formulation of Density Functional Theory (DFT) [62, 75, 77]. In the last decades, DFT and 1RDMFT have been standard methods for numerical electronic structure calculations and are to be considered a major breakthrough in fields ranging from materials science to chemistry and biochemistry.
In both these theories one tries to approximate a complicated N-particle quantum system by studying one-particle objects, namely one-body densities in the case of DFT and one-body reduced density matrices in the case of 1RDM-FT, by using a two-steps minimization analogous to the one introduced in (A.1.5).

It is interesting to see that the well-known Pauli principle (see e.g. [79, Theorem 3.2]) , which provides necessary and sufficient conditions for γ to be the one-reduced density matrix of an N-body antisymmetric density matrix, finds a variational interpretation in our discussion. Indeed, in the antisymmetric case we show (see Proposition A.2.2) that γ satisfies the Pauli principle (resp. satisfies the Pauli principle *strictly*) if and only if the supremum of the dual functional of $\mathfrak{F}^{\varepsilon}$ is finite (resp. is attained), as it is to be expected.

Other extensions of DFT have been considered, including Mermin's Thermal Density Functional Theory [86], Spin DFT [118], and Current DFT [117]. Physical and computational aspects of 1RDM-FT have been investigated in [7, 6, 5, 12, 85, 93, 96, 97, 102, 106, 116]. A framework for 1RDM for Bosons at zero temperature was recently introduced in [9] (see also [54] and references therein for a recent review). In particular, the first exchange-correlation energy in density-matrix functional theory was introduced by Müller [93], leading to mathematical results [42, 45].

Organisation of the paper

The paper is divided as follows: in Section A.2 we introduce the framework, the main definitions, and present our main results Theorem A.2.1, Theorem A.2.2, and Theorem A.2.3. In Section

A.3 we introduce and develop the technical tools needed to prove our main results, in particular we define the notion of non-commutative (H,ε)-transform (see Section A.3.1) and prove a stability and differentiability result for the primal problem in Proposition A.2.1. In Section A.4, Section A.5, and Section A.6 we build upon Section A.3 and prove our main results, respectively, Theorem A.2.1, Theorem A.2.2, and Theorem A.2.3.

A.2 Contributions and Statements of the Main Results

The main contributions of this work consist in

- Theorem A.2.1, which represents a duality result for the functional $\mathfrak{F}^\varepsilon$ (whose definition is recalled below in equation (A.2.1)). Theorem A.2.1 also includes the characterization of the optimizers of $\mathfrak{F}^\varepsilon$ (and of its dual functional).
- The introduction of a non-commutative Sinkhorn algorithm, which can be used to compute the aforementioned optimizers. We also prove convergence and robustness of this algorithm in Theorem A.2.2.
- The introduction a non-commutative notion of (H,ε)-transform and the proof of suitable a priori estimates in Section A.3, which turns out to be crucial in the proof of Theorem A.2.1 and Theorem A.2.2. Consequently, we are also able to show stability and differentiability of $\mathfrak{F}^\varepsilon(\cdot)$ in Proposition A.2.1.
- The generalization of Theorem A.2.1 to the case of bosonic or fermionic systems, stated in Theorem A.2.3. This also allows to give an interesting variational characterization of the Pauli exclusion principle (see Proposition A.2.2).

We now proceed to introduce our setting and state our main contributions in mathematical rigorous terms.

A.2.1 Duality and Minimization of $\mathfrak{F}^\varepsilon$

We recall that in this case we simply work with a general composite system, with no symmetry constraints enforced. For $d \in \mathbb{N}$, we shall denote by $\mathcal{M}^d = \mathcal{M}^d(\mathbb{C})$ the set of all $d \times d$ complex matrices, by $\mathcal{S}^d$ the hermitian elements of $\mathcal{M}^d$, and by $\mathcal{S}^d_{\geq}$ (respectively $\mathcal{S}^d_{>}$) the set of all the positive semidefinite (resp. positive definite) elements of $\mathcal{S}^d$. With a slight abuse of notation, we denote by Tr the trace operator on $\mathcal{M}_d$ for any dimension d. Furthemore, for any Hilbert space $\mathfrak{h}$, we denote by $\mathfrak{P}(\mathfrak{h})$ the set of *density matrices* over $\mathfrak{h}$, namely the positive self-adjoint operators with trace one. For simplicity, we shall also use the notation $\mathfrak{P}^d = \mathfrak{P}(\mathbb{C}^d)$. For every $N \in \mathbb{N}$ we adopt the notation $[N] := \{1, ..., N\}$.

Our main object of study is the minimisation problem for $N \in \mathbb{N}$, $i \in [N]$, $\gamma_i \in \mathfrak{P}^{d_i}$, $\mathrm{H} \in \mathcal{S}^{\boldsymbol{d}}$

$$\mathfrak{F}^\varepsilon(\boldsymbol{\gamma}) = \inf\Big\{\mathrm{Tr}(\mathrm{H}\,\Gamma) + \varepsilon\,\mathrm{Tr}(\Gamma\log\Gamma) \ : \ \Gamma \in \mathfrak{P}^{\boldsymbol{d}} \text{ and } \Gamma \mapsto \boldsymbol{\gamma}\Big\}, \qquad \text{(A.2.1)}$$

where $d_i \in \mathbb{N}$, $\boldsymbol{d} := \prod_{i=1}^N d_i$, $\boldsymbol{\gamma} := (\gamma_i)_{i\in[N]}$, and $\Gamma \mapsto \boldsymbol{\gamma}$ means that the i-th marginal (A.3.2) of Γ is equal to γ_i. This coincides with the Definition of $\mathfrak{F}^\varepsilon$ given in (A.1.1).

The natural space to work with is given by $\mathcal{O} := \otimes_{i=1}^N \Big(\ker\gamma_i\Big)^\perp$ where for simplicity we set $\hat{d}_i := (d_i - \dim\ker\gamma_i)$ and $\hat{\mathbf{d}} := \prod_{i=1}^N \hat{d}_i$. We also denote by $\mathrm{H}_\mathcal{O}$ the restriction of H to the subspace $\mathcal{O}$. The corresponding dual problem is defined as

$$\mathfrak{D}^{\varepsilon}(\boldsymbol{\gamma}) = \sup\left\{ \sum_{i=1}^{N} \mathrm{Tr}(U_i\gamma_i) - \varepsilon\,\mathrm{Tr}\left(\exp\left[\frac{\bigoplus_{i=1}^{N} U_i - \mathrm{H}_{\mathcal{O}}}{\varepsilon}\right]\right) \ :\ U_i \in \mathcal{S}^{\hat{d}_i} \right\} + \varepsilon\,, \quad \text{(A.2.2)}$$

where $\bigoplus$ denotes the Kronecker sum (A.3.3).

Our first result is a duality result and serves also as a characterization of the minimizers in (A.2.1). Note that, throughout the whole paper, when no confusion can arise, we shall use the slightly imprecise notation $\alpha\mathbb{1} = \alpha$ for $\alpha \in \mathbb{C}$.

Theorem A.2.1 (Duality)**.** *Let $\varepsilon > 0$, $N \in \mathbb{N}$, and $\mathrm{H} \in \mathcal{S}^{\boldsymbol{d}}$. For fixed $\boldsymbol{\gamma} = (\gamma_i \in \mathfrak{P}^{d_i})_{i\in[N]}$, consider the primal and dual problems $\mathfrak{F}^{\varepsilon}(\boldsymbol{\gamma})$, $\mathfrak{D}^{\varepsilon}(\boldsymbol{\gamma})$ as in* (A.2.1), (A.2.2) *respectively. We then have that*

(i) the primal and dual problems coincide, thus $\mathfrak{F}^{\varepsilon}(\boldsymbol{\gamma}) = \mathfrak{D}^{\varepsilon}(\boldsymbol{\gamma})$.

(ii) $\mathfrak{D}^{\varepsilon}(\boldsymbol{\gamma})$ admits a maximizer $\{U_i^{\varepsilon} \in \mathcal{S}^{\hat{d}_i}\}_{i=1}^{N}$, which is unique up to trival translation. Precisely, if $\{\tilde{U}_i^{\varepsilon} \in \mathcal{S}^{\hat{d}_i}\}_{i=1}^{N}$ is another maximizer, then $\tilde{U}_i^{\varepsilon} - U_i^{\varepsilon} = \alpha_i \in \mathbb{R}$ with $\sum_i \alpha_i = 0$.

(iii) There exists a unique $\Gamma^{\varepsilon} \in \mathfrak{P}^{\boldsymbol{d}}$ with $\Gamma^{\varepsilon} \mapsto \boldsymbol{\gamma}$ which minimizes the functional $\mathfrak{F}^{\varepsilon}(\boldsymbol{\gamma})$. Moreover, Γ^{ε} and $\{U_i^{\varepsilon}\}$ are related via the formula

$$\Gamma^{\varepsilon} = \exp\left(\frac{\bigoplus_{i=1}^{N} U_i^{\varepsilon} - \mathrm{H}_{\mathcal{O}}}{\varepsilon}\right) \quad \text{on } \mathcal{O} \qquad \text{(A.2.3)}$$

and $\Gamma^{\varepsilon} = 0$ on $\mathcal{O}^{\perp}$.

The proof of the existence of maximizers for the dual problem follows the direct method of Calculus of Variations. Inspired by [28, 29], we introduce a non-commutative $(\mathrm{H}, \varepsilon)$−transform (see Section A.3.1) which allows to obtain a priori estimates on U and infer compactness of the maximizing sequences of Kantorovich potentials. Although this approach is not strictly necessary in our finite dimensional setting, we believe these estimates to have independent interests and, in particular, they are fundamental to prove the convergence of the so-called non-commutative Sinkhorn algorithm, the second contribution of this work.

As a byproduct of the a priori estimates obtained in Section A.3.1, it is possible to prove a stability result (with respect to the marginals) for the Kantorovich potentials and compute the Frechét derivative of $\mathfrak{F}^{\varepsilon}(\cdot)$. This is the content of the following proposition, which is proved in Section A.4. For simplicity, we here assume that the marginals have trivial kernel. With a bit more effort, and arguing as in Theorem A.2.1 (see also Remark A.3.3), one can obtain a similar result in the general setting as well.

Proposition A.2.1 (Stability and differentiability of $\mathfrak{F}^{\varepsilon}(\cdot)$)**.** *Fix $\varepsilon > 0$ and assume $\ker(\gamma_i) = \{0\}$.*

(i) Stability*: if $\boldsymbol{\gamma}^n = (\gamma_i^n)_{n\in\mathbb{N}}$, $\gamma_i^n \subset \mathfrak{P}^{d_i}$ is a sequence of density matrices converging to $\boldsymbol{\gamma} = (\gamma_i)_{n\in\mathbb{N}}$ as $n \to \infty$, then any sequence of Kantorovich potentials $\boldsymbol{U}^{\varepsilon,n}$ converges, up to subsequences and renormalisation, to a Kantorovich potential $\boldsymbol{U}^{\varepsilon}$ for $\mathfrak{F}^{\varepsilon}(\boldsymbol{\gamma})$. Therefore, the functional $\mathfrak{F}^{\varepsilon}(\cdot)$ is continuous.*

(ii) Frechét differential*: $\mathfrak{F}^\varepsilon(\cdot)$ is Fréchet differentiable and for every $i \in [N]$ it holds*

$$\left(\frac{d\mathfrak{F}^\varepsilon}{d\gamma_i}\right)_{\gamma}(\sigma) = \mathrm{Tr}\left(\boldsymbol{U}_i^\varepsilon \sigma\right), \quad \forall \sigma \in \mathcal{S}^{d_i},\ \mathrm{Tr}(\sigma) = 0\,, \tag{A.2.4}$$

where $\boldsymbol{U}^\varepsilon$ is a Kantorovich potential for $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma})$.

As derived in [55] and explained, for instance, in [96], the relevance of the functional derivative in the 1RDM-FT case is to find an eigenvalue equation to find an efficient optimization for the one-particle eigenvalue equations.

A.2.2 Non-Commutative Sinkhorn Algorithm

The second contribution of this work is to introduce and prove the convergence of a non-commutative Sinkhorn algorithm (see Section A.5), aimed at computing numerically the optimal density matrix Γ^ε and the corresponding Kantorovich potentials $\{U_i^\varepsilon\}_i$.
For this purpose, we define non-commutative (H,ε)-transform operators, which extend the notion of $(c,\varepsilon)-$transforms as introduced in [28] (see also Section A.5 for a detailed explanation). Note that the (H,ε)-transform also depends on $\boldsymbol{\gamma}$, but we omit this dependence as $\boldsymbol{\gamma}$ is a fixed parameter of the problem.

For $i \in [N]$ and $\varepsilon > 0$, we consider the operators $\mathcal{T}_i^\varepsilon : \times_{j=1}^N \mathcal{S}^{\hat{d}_j} \to \times_{j=1}^N \mathcal{S}^{\hat{d}_j}$ of the form

$$\boldsymbol{U} := (U_1, \dots, U_N), \quad \left(\mathcal{T}_i^\varepsilon(\boldsymbol{U})\right)_j = \begin{cases} U_j & \text{if } j \neq i, \\ \mathfrak{T}_i^\varepsilon(U_1, \dots, U_{i-1}, U_{i+1}, \dots U_N) & \text{if } j = i \end{cases}$$

where $\mathfrak{T}_i^\varepsilon$ is defined implicitly via

$$\mathrm{P}_i\left[\exp\left(\frac{\bigoplus_{j=1}^N \left(\mathcal{T}_i^\varepsilon(\boldsymbol{U})\right)_j - \mathrm{H}_{\mathcal{O}}}{\varepsilon}\right)\right] = \gamma_i \tag{A.2.5}$$

and P_i denotes the i-th marginal operator, obtained by tracing out all but the i-th coordinate, see (A.3.2). In Section A.5, we show that the maps $\mathcal{T}_i^\varepsilon$ are well-defined, i.e. the equation (A.2.5) admits a unique solution $\mathcal{T}_i^\varepsilon(\boldsymbol{U})$.

Note that, by construction, the matrix $\exp\left(\bigoplus_{i=1}^N \left((\mathcal{T}_i^\varepsilon(\boldsymbol{U}))_j - \mathrm{H}_{\mathcal{O}}\right)/\varepsilon\right) \in \mathfrak{P}^{\hat{\mathbf{d}}}$ and it has the i-th marginal equal to γ_i. The non-commutative Sinkhorn algorithm is then defined by iterating this procedure for every $i \in [N]$. We define the one-step Sinkhorn map as

$$\tau : \bigtimes_{j=1}^N \mathcal{S}^{\hat{d}_j} \to \bigtimes_{j=1}^N \mathcal{S}^{\hat{d}_j},$$
$$\tau(\boldsymbol{U}) := (\mathcal{T}_N^\varepsilon \circ \dots \circ \mathcal{T}_1^\varepsilon)(\boldsymbol{U}).$$

The Sinkhorn algorithm is obtained by iteration of the map τ and this is sufficient to guarantee that the limit point of the resulting sequence is an optimizer for the dual problem (A.2.2), as stated in the following Theorem.

Theorem A.2.2 (Convergence of the non-commutative Sinkhorn algorithm)**.** *Fix $\varepsilon > 0$. The definition* (A.2.5) *for the operators $\mathcal{T}_i^\varepsilon$ is well-posed. Additionally, for any initial matrix $\boldsymbol{U}^{(0)} = (U_1, \dots, U_N) \in \times_{j=1}^N \mathcal{S}^{\hat{d}_j}$, there exist $\boldsymbol{\alpha}^k \in \mathbb{R}^N$ with $\sum_{i=1}^N \boldsymbol{\alpha}_i^k = 0$ such that*

$$\boldsymbol{U}^{(k)} := \tau^k(\boldsymbol{U}^{(0)}) + \boldsymbol{\alpha}^k \to \boldsymbol{U}^\varepsilon \quad \text{as } k \to +\infty, \tag{A.2.6}$$

where $\boldsymbol{U}^\varepsilon = (U_1^\varepsilon, \dots, U_N^\varepsilon)$ is optimal for the dual problem. Consequently, if one defines for $k \in \mathbb{N}$

$$\Gamma^{(k)} := \exp\left(\frac{\bigoplus_{i=1}^N (\boldsymbol{U}^{(k)})_i - \mathrm{H}_{\mathcal{O}}}{\varepsilon}\right) \quad \text{on } \mathcal{O}, \tag{A.2.7}$$

and 0 *on* $\mathcal{O}^\perp$*, then* $\Gamma^{(k)} \to \Gamma^\varepsilon$ *as* $k \to +\infty$ *where* Γ^ε*,* $\boldsymbol{U}^\varepsilon$ *satisfy* (A.2.3)*. In particular,* Γ^ε *is optimal for* $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma})$*.*

Remark A.2.1 (Renormalisation)**.** *In the previous theorem, a renormalisation procedure is needed in order to obtain compactness for the dual potentials* $\boldsymbol{U}^k$*. Nonetheless, due to the fact that* $\sum_{i=1}^N (\boldsymbol{\alpha}^k)_i = 0$ *and by the properties of the operator* $\bigoplus$*, we observe that for* $k \in \mathbb{N}$*, the equality*

$$\Gamma^{(k)} = \exp\left(\frac{\bigoplus_{i=1}^N \tau^k(\boldsymbol{U})_i - \mathrm{H}_{\mathcal{O}}}{\varepsilon}\right) \quad \text{on } \mathcal{O}$$

is also satisfied. In fact, this shows that no renormalisation procedure is needed at the level of the primal problem, i.e. for the density matrices $\Gamma^{(k)}$*.*

Remark A.2.2. *(Umegaki Relative entropies) Similar results can be obtained if instead of the Von Neumann entropy one uses the quantum Umegaki relative entropy with respect to a reference density matrix with trivial kernel. Specifically, suppose that* $m_i \in \mathcal{S}^{d_i}$ *with* $\ker m_i = \{0\}$*. Then one can consider the minimisation problem*

$$\mathfrak{F}^\varepsilon_{\boldsymbol{m}}(\boldsymbol{\gamma}) = \inf\left\{\mathrm{Tr}(\mathrm{H}\,\Gamma) + \varepsilon S(\Gamma|\boldsymbol{m}) \ : \ \Gamma \in \mathfrak{P}^{\boldsymbol{d}} \text{ and } \Gamma \mapsto \boldsymbol{\gamma}\right\},$$

where we set $\boldsymbol{m} := \bigotimes_{i=1}^N m_i$ *and* $S(\Gamma|\boldsymbol{m}) := \mathrm{Tr}(\Gamma(\log\Gamma - \log\boldsymbol{m}))$ *denotes the relative entropy of* Γ *with respect to* $\boldsymbol{m}$*. The functional* $\mathfrak{F}^\varepsilon$ *defined in* (A.2.1) *corresponds to the case* $\boldsymbol{m}$ *equals the identity matrix. The corresponding dual functional* $\mathfrak{D}^\varepsilon$ *as defined in* (A.2.2) *is replaced by*

$$\mathfrak{D}^\varepsilon_{\boldsymbol{m}}(\boldsymbol{\gamma}) = \sup\left\{\sum_{i=1}^N \mathrm{Tr}(U_i\gamma_i) - \varepsilon\,\mathrm{Tr}\left(\exp\left[\frac{\bigoplus_{i=1}^N U_i - \mathrm{H}^\varepsilon_{\boldsymbol{m}}}{\varepsilon}\right]\right) \ : \ U_i \in \mathcal{S}^{d_i}\right\} + \varepsilon,$$

for a modified matrix $\mathrm{H}^\varepsilon_{\boldsymbol{m}} := \mathrm{H} - \varepsilon\log\boldsymbol{m}$ *(restricted to* $\mathcal{O}$ *in the case of non-trival kernels). It is easy to see that our approach can also be used in this case. In particular, performing a change of variables in the dual potentials of the form* $\tilde{\boldsymbol{U}} = \boldsymbol{U} + \varepsilon\log\boldsymbol{m}$ *and using that* $S(\Gamma|Id) = S(\Gamma|\boldsymbol{m}) + \sum_{i=1}^N [S(\gamma_i) - S(\gamma_i|m_i)]$*, one readily derives the validity of the same results obtained in Theorem A.2.1 and Theorem A.2.2, with the substitution of* H *with* $\mathrm{H}^\varepsilon_{\boldsymbol{m}}$*.*

A.2.3 The symmetric case: one-reduced density matrix functional theory

We are able to obtain the duality results stated above also in the symmetric cases (either bosonic or fermionic). For given $d, N \in \mathbb{N}$, we set $\boldsymbol{d} = d^N$. We consider the bosonic (resp. fermionic) projection operator Π_+ (resp. Π_-)

$$\Pi_+ : \bigotimes_{i=1}^N \mathbb{C}^d \to \bigodot_{i=1}^N \mathbb{C}^d, \qquad \Pi_- : \bigotimes_{i=1}^N \mathbb{C}^d \to \bigwedge_{i=1}^N \mathbb{C}^d, \tag{A.2.8}$$

where $\odot$ (resp. $\wedge$) denotes the symmetric (resp. antisymmetric) tensor product. Note that the cardinality of $\bigwedge_{i=1}^N \mathbb{C}^d$ is $\binom{d}{N}$, therefore $\bigwedge_{i=1}^N \mathbb{C}^d \neq \{0\}$ if and only if $N \leq d$. We denote by

$$\mathfrak{P}_+^{\boldsymbol{d}} := \mathfrak{P}\left(\bigodot_{i=1}^N \mathbb{C}^d\right), \quad \mathfrak{P}_-^{\boldsymbol{d}} := \mathfrak{P}\left(\bigwedge_{i=1}^N \mathbb{C}^d\right), \tag{A.2.9}$$

the set of bosonic and fermionic density matrices. We fix $\mathrm{H} \in \mathcal{S}^{\boldsymbol{d}}$ such that

$$\mathrm{S}_i \circ \mathrm{H} \circ \mathrm{S}_i = \mathrm{H}, \quad \forall i = 1, \ldots, N, \tag{A.2.10}$$

where the S_i are the permutation operators in Definition A.3.2. It is well-known that there exists $\Gamma \in \mathfrak{P}_-^d$ such that $\Gamma \mapsto \gamma$ (where $\Gamma \mapsto \gamma$ means that Γ has all one-reduced density matrices equal to γ) if and only if γ satisfies the *Pauli exclusion principle*, i.e. if and only if $\gamma \in \mathfrak{P}^d$ and $\gamma \leq 1/N$ (see for example [79, Theorem 3.2]).

Definition A.2.1 (Bosonic and fermionic primal problems). *For any $\gamma \in \mathfrak{P}^d$, we define the bosonic primal problem as*

$$\mathfrak{F}_+^\varepsilon(\gamma) := \inf\left\{\mathrm{Tr}(\mathrm{H}\,\Gamma) + \varepsilon\,\mathrm{Tr}(\Gamma\log\Gamma) \ : \ \Gamma \in \mathfrak{P}_+^{\boldsymbol{d}} \text{ and } \Gamma \mapsto \gamma\right\}. \tag{A.2.11}$$

For any $\gamma \in \mathfrak{P}^d$ such that $\gamma \leq 1/N$, we define the fermionic primal problem as

$$\mathfrak{F}_-^\varepsilon(\gamma) := \inf\left\{\mathrm{Tr}(\mathrm{H}\,\Gamma) + \varepsilon\,\mathrm{Tr}(\Gamma\log\Gamma) \ : \ \Gamma \in \mathfrak{P}_-^{\boldsymbol{d}} \text{ and } \Gamma \mapsto \gamma\right\}. \tag{A.2.12}$$

An analysis of the extremal points and the existence of the minimizer in (A.2.11) and (A.2.12) have been carried out in [22] for the zero temperature case, and in [54] in the positive temperature case. As in the non-symmetric case, we consider the associated bosonic and fermionic dual problems. For any given operator $A \in \mathcal{S}^{\boldsymbol{d}}$, we denote by $A_\pm$ the corresponding projection onto the symmetric space, obtained as $A_\pm := \Pi_\pm \circ A \circ \Pi_\pm$.

Definition A.2.2 (Bosonic and fermionic dual problems). *For any $\gamma \in \mathfrak{P}^d$, we define the bosonic dual functional $D_\gamma^{+,\varepsilon}$ and the fermionic dual functional $D_\gamma^{-,\varepsilon}$ as*

$$D_\gamma^{\pm,\varepsilon} : \mathcal{S}^d \to \mathbb{R}, \quad D_\gamma^{\pm,\varepsilon}(U) := \mathrm{Tr}(U\gamma) - \varepsilon\,\mathrm{Tr}\left(\exp\left[\frac{1}{\varepsilon}\left(\frac{1}{N}\bigoplus_{i=1}^N U - \mathrm{H}\right)_\pm\right]\right) + \varepsilon\,. \tag{A.2.13}$$

The corresponding dual problems are given by

$$\mathfrak{D}_\pm^\varepsilon(\gamma) := \sup\left\{D_\gamma^{\pm,\varepsilon}(U) \ : \ U \in \mathcal{S}^d\right\}. \tag{A.2.14}$$

We note that a priori $\mathfrak{D}_\varepsilon^-(\gamma)$ can be defined for any $\gamma \in \mathfrak{P}^d$, whereas $\mathfrak{F}_-^\varepsilon(\gamma)$ is only well defined for $\gamma \in \mathfrak{P}^d$ such that $\gamma \leq 1/N$. This constraint on the primal problem naturally translates to an admissibility condition in order to have $\mathfrak{D}_\varepsilon^-(\gamma) < \infty$. To ensure the existence of a maximizer for $\mathrm{D}_\gamma^{-,\varepsilon}$ we further need to impose $\gamma < 1/N$. The following proposition gives an interesting and variational point of view of the Pauli principle, and it is proved in Section A.6.1.

Proposition A.2.2 (Pauli's principle and duality). *We have the following equivalences:*

1. *$\mathfrak{D}_\varepsilon^-(\gamma) < \infty$ if and only if $\gamma \in \mathfrak{P}^d$ and $\gamma \leq \frac{1}{N}$,*

2. *There exists a maximiser $U_0 \in \mathcal{S}^d$ of $D_\gamma^{-,\varepsilon}$ if and only if $\gamma \in \mathfrak{P}^d$ and $0 < \gamma < \frac{1}{N}$.*

Finally we state the duality result in the fermionic and bosonic setting.

Theorem A.2.3 (Fermionic and bosonic duality)**.** *Let $\mathrm{H} \in \mathcal{S}^{\boldsymbol{d}}$ satisfying* (A.2.10).

(i) For any given $\gamma \in \mathfrak{P}^d$, such that $\gamma \leq \frac{1}{N}$, the fermionic primal and dual problems coincide, thus $\mathfrak{F}_-^\varepsilon(\gamma) = \mathfrak{D}_\varepsilon^-(\gamma)$. Moreover, if $0 < \gamma < \frac{1}{N}$ then $D_\gamma^{-,\varepsilon}$ admits a unique maximizer U_-^ε such that

$$\Gamma_-^\varepsilon = \exp\left(\frac{1}{\varepsilon}\left[\frac{1}{N}\bigoplus_{i=1}^N U_-^\varepsilon - \mathrm{H}\right]_-\right) \tag{A.2.15}$$

is the unique optimal fermionic solution to the primal problem $\mathfrak{F}_-^\varepsilon(\gamma)$.

(ii) For any given $\gamma \in \mathfrak{P}^d$, the bosonic primal and dual problems coincide, thus $\mathfrak{F}_+^\varepsilon(\gamma) = \mathfrak{D}_\varepsilon^+(\gamma)$. Moreover, if $\gamma > 0$, $D_\gamma^{+,\varepsilon}$ admits a unique maximizer U_+^ε such that

$$\Gamma_+^\varepsilon = \exp\left(\frac{1}{\varepsilon}\left[\frac{1}{N}\bigoplus_{i=1}^N U_+^\varepsilon - \mathrm{H}\right]_+\right) \tag{A.2.16}$$

is the unique optimal bosonic solution to the primal problem $\mathfrak{F}_+^\varepsilon(\gamma)$.

A.3 Preliminaries and a Priori Estimates

We start this section by recalling the setting and the notation. For $d \in \mathbb{N}$, we denote by $\mathcal{M}^d = \mathcal{M}^d(\mathbb{C})$ the set of all $d \times d$ complex matrices, by $\mathcal{S}^d$ the hermitian elements of $\mathcal{M}^d$, and by $\mathcal{S}^d_\geq$ (respectively $\mathcal{S}^d_>$) the set of all the positive semidefinite (positive definite) elements of $\mathcal{S}^d$. With a slight abuse of notation, we denote by Tr the trace operator on $\mathcal{M}_d$ for any dimension d. Furthemore, we denote by $\mathfrak{P}^d$ the set of $d \times d$ *density matrices*, namely the matrices in $\mathcal{S}^d_\geq$ with trace one. For the sake of notation, for every $N \in N$ we denote by $[N] := \{1, ..., N\}$.

For a given $N \in \mathbb{N}$ and $(d_i)_{i=1}^N \subset \mathbb{N}$, we consider for any $i \in [N]$ the injective maps

$$\begin{aligned} Q_i : \mathcal{M}^{d_i} \to \mathcal{M}^{\boldsymbol{d}} = \bigotimes_{j=1}^N \mathcal{M}^{d_j}, \quad \boldsymbol{d} := \prod_{j=1}^N d_j, \\ \forall A \in \mathcal{M}^{d_i}, \quad \mathrm{Q}_i(A) := \bigotimes_{j=1}^N A_j, \quad A_j = \begin{cases} A & \text{if } j = i, \\ \mathbb{1} & \text{if } j \neq i. \end{cases} \end{aligned} \tag{A.3.1}$$

We shall use the same notation also for subsets of $\mathbb{C}^d$. I.e., we also denote by Q_i the map $\mathrm{Q}_i : \mathbb{C}^{d_i} \to \mathbb{C}^{\boldsymbol{d}}$ defined as

$$\forall K \subset \mathbb{C}^{d_i}, \quad \mathrm{Q}_i(K) := \bigotimes_{j=1}^N K_j \subset \mathbb{C}^{\boldsymbol{d}}, \quad K_j = \begin{cases} K & \text{if } j = i, \\ \mathbb{C}^{d_j} & \text{if } j \neq i. \end{cases}$$

The *marginal* operators are the left-inverse of the Q_i, namely $\mathrm{P}_i : \mathcal{M}^{\boldsymbol{d}} \to \mathcal{M}^{d_i}$, where for every $\Gamma \in \mathcal{M}^{\boldsymbol{d}}$, $\mathrm{P}_i(\Gamma) \in \mathcal{M}^{d_i}$ is defined by duality as

$$\mathrm{Tr}(\mathrm{P}_i(\Gamma)A) = \mathrm{Tr}\Big(\Gamma\, \mathrm{Q}_i(A)\Big), \quad \forall A \in \mathcal{M}^{d_i}. \tag{A.3.2}$$

Remark A.3.1. *Observe that* $\mathrm{Tr}(\mathrm{P}_i(A)) = \mathrm{Tr}(A)$ *for every* $i = 1, \dots, N$ *and* $A \in \mathcal{M}^{\boldsymbol{d}}$. *Furthermore, if* $A = \bigotimes_{i=1}^N A_i$ *with* $\mathrm{Tr}(A_i) = 1$*, then* $\mathrm{P}_i(A) = A_i$.

For a given family of density matrices $\gamma_i \in \mathfrak{P}^{d_i}$, we use the notation $\boldsymbol{\gamma} := (\gamma_i)_{i\in[N]}$ and we write $\Gamma \mapsto \boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_N)$ whenever $\Gamma \in \mathfrak{P}^{\boldsymbol{d}}$ and $\mathrm{P}_i(\Gamma) = \gamma_i$ for every $i = [N]$. With the next definitions, we introduce the Kronecker sum and Permutation operators.

Definition A.3.1 (Kronecker sum)**.** *For* $A_i \in \mathcal{M}^{d_i}$*, we call their Kronecker sum the matrix*

$$\bigoplus_{i=1}^N A_i := \sum_{i=1}^N \mathrm{Q}_i(A_i) \in \mathcal{M}^{\boldsymbol{d}} \tag{A.3.3}$$

where Q_i *is defined in* (A.3.1).

Definition A.3.2 (Permutation operators)**.** *For any* $i \in [N]$*, we introduce the permutation operator* $\mathrm{S}_i : \mathcal{M}^{\boldsymbol{d}} \approx \bigotimes_{j=1}^N \mathcal{M}^{d_j} \to \mathcal{M}^{\boldsymbol{d}}$ *as the map defined by*

$$\mathrm{S}_i\left(\bigotimes_{j=1}^N A_j\right) = A_1 \otimes \cdots \otimes A_{i-1} \otimes A_{i+1} \otimes \cdots \otimes A_N \otimes A_i,$$

for any $A_i \in \mathcal{M}^{d_i}$ *and extended to the whole* $\mathcal{M}^{\boldsymbol{d}}$ *by linearity.*

Remark A.3.2. *The permutation operators preserve the spectral properties of any operator. Precisely,* $\sigma(\mathrm{S}_i(A)) = \sigma(A)$ *for every* $i \in [N]$, $A \in \mathcal{S}^{\boldsymbol{d}}$*, where* $\sigma(A)$ *denotes the spectrum of* A.

In particular, for every continuous function $f : \mathbb{R} \to \mathbb{R}$*, we have that* $\mathrm{Tr}(f(\mathrm{S}_i(A))) = \mathrm{Tr}(f(A))$*, for every* $A \in \mathcal{S}^{\boldsymbol{d}}$.

A.3.1 Non-Commutative $(\mathrm{H}, \varepsilon)$-transforms

For this section, we specify to the simply case of a two-fold tensor product and introduce the notion of non-commutative $(\mathrm{H}, \varepsilon)$-transform, which is a central object in our discussion. We shall see in Section A.3.2 how it is then easy to extend this notion to a general N-fold tensor product. We fix $d, d' \in \mathbb{N}$, $0 < \alpha \in \mathfrak{P}^{d'}$, $\mathrm{H} \in \mathcal{S}^{dd'}$ and $\varepsilon > 0$ and define the map $\mathrm{T}^\varepsilon_{\alpha,\mathrm{H}} : \mathcal{S}^d \times \mathcal{S}^{d'} \to \mathbb{R}$ as

$$\mathrm{T}^\varepsilon_{\alpha,\mathrm{H}}(U, V) := \mathrm{Tr}(V\alpha) - \varepsilon\,\mathrm{Tr}\left(\exp\left[\frac{U \oplus V - \mathrm{H}}{\varepsilon}\right]\right). \tag{A.3.4}$$

The $(\mathrm{H}, \varepsilon)$-transform of any $U \in \mathcal{S}^d$ is obtained as the maximiser of the map $\mathrm{T}^\varepsilon_{\alpha,\mathrm{H}}(U, \cdot)$.

Definition A.3.3 ($(\mathrm{H}, \varepsilon)$-transform)**.** *We call the unique maximizer of* $\mathrm{T}^\varepsilon_{\alpha,\mathrm{H}}(U, \cdot)$ *the* $(\mathrm{H}, \varepsilon)$*-transform of* $U \in \mathcal{S}^d$. *We use the notation*

$$\mathfrak{T}^\varepsilon_{\alpha,\mathrm{H}} : \mathcal{S}^d \to \mathcal{S}^{d'}, \quad \mathfrak{T}^\varepsilon_{\alpha,\mathrm{H}}(U) = \textit{arg max}\{\mathrm{T}^\varepsilon_{\alpha,\mathrm{H}}(U, V) \ : \ V \in \mathcal{S}^{d'}\}. \tag{A.3.5}$$

The following lemma shows that the definition of $(\mathrm{H}, \varepsilon)$-transform is indeed well-posed.

Lemma A.3.1. *Let* $U \in \mathcal{S}^d$. *Then there exists a unique maximizer* $\bar{V} \in \mathcal{S}^{d'}$ *of* $\mathrm{T}^\varepsilon_{\alpha,\mathrm{H}}(U, \cdot)$.

Proof. Fix $U \in \mathcal{S}^d$. For every $V \in \mathcal{S}^{d'}$, we write $V = V_+ - V_-$ where $V_+, V_- \in \mathcal{S}^{d'}$ denote respectively the positive and the negative part of V (with respect to its spectrum). We begin by observing that

$$\operatorname{Tr}\left(\exp\left[\frac{U \oplus V - \mathrm{H}}{\varepsilon}\right]\right) \geq \operatorname{Tr}\left(\exp\left[\frac{U \oplus V - \|\,\mathrm{H}\,\|_\infty}{\varepsilon}\right]\right)$$
$$= \operatorname{Tr}\left(\exp\left(\frac{V}{\varepsilon}\right)\right)\operatorname{Tr}\left(\exp\left(\frac{U}{\varepsilon}\right)\right)\exp\left[\frac{-\|\,\mathrm{H}\,\|_\infty}{\varepsilon}\right] =: \kappa \operatorname{Tr}\left(\exp\left(\frac{V}{\varepsilon}\right)\right) \geq \kappa e^{\varepsilon^{-1}\|V_+\|_\infty}, \tag{A.3.6}$$

where in the second step we used that $\exp(U \oplus V) = \exp(U) \otimes \exp(V)$ and $\kappa = \kappa(U, \varepsilon, \mathrm{H})$ is a *finite* constant depending on U, ε, and H. On the other hand, it clearly holds $\operatorname{Tr}(V\alpha) \leq \|V_+\|_\infty$ which combined with (A.3.6) yields for every $V \in \mathcal{S}^{d'}$

$$\mathrm{T}^\varepsilon_{\alpha,\mathrm{H}}(U, V) \leq \|V_+\|_\infty - \kappa e^{\varepsilon^{-1}\|V_+\|_\infty}. \tag{A.3.7}$$

Moreover, it is immediate to obtain that

$$\mathrm{T}^\varepsilon_{\alpha,\mathrm{H}}(U, V) \leq \operatorname{Tr}(V\alpha) = \operatorname{Tr}(V_+\alpha) - \operatorname{Tr}(V_-\alpha) \leq \|V_+\|_\infty - \sigma_{\min}(\alpha)\|V_-\|_\infty, \tag{A.3.8}$$

where $\sigma_{\min}(\alpha)$ is the spectral gap of α, which is strictly positive by assumption. Let V_n be a maximizing sequence for $\mathrm{T}^\varepsilon_{\alpha,\mathrm{H}}(U, \cdot)$, then the bounds (A.3.7) and (A.3.8) imply that $(V_n)_+$, $(V_n)_-$ (and hence V_n) are uniformly bounded. Therefore, we can obtain a subsequence (which we do not relabel) such that $V_n \to \bar{V} \in \mathcal{S}^{d'}$. The optimality of $\bar{V}$ follows from the fact that $\mathrm{T}^\varepsilon_{\alpha,\mathrm{H}}(U, \cdot)$ is continuous and strictly concave (see for example [15]), which also implies uniqueness. □

In the following lemma we use the fact that the $(\mathrm{H}, \varepsilon)$-transform is obtained through a maximization to show that it can be characterized as the solution of the associated Euler–Lagrange equation. This property is crucial for the proof of our main results.

Lemma A.3.2 (Optimality conditions for the $(\mathrm{H}, \varepsilon)$-transforms)**.** *Given $d, d' \in \mathbb{N}$, $0 < \alpha \in \mathfrak{P}^{d'}$, $\mathrm{H} \in \mathcal{S}^{dd'}$, $\varepsilon > 0$, the operator $\mathfrak{T}^\varepsilon_{\alpha,\mathrm{H}}$ can be characterized implicitly by the fact that, for any $U \in \mathcal{S}^d$, $\mathfrak{T}^\varepsilon_{\alpha,\mathrm{H}}(U)$ is the unique solution of*

$$\alpha = \mathrm{P}_2\left(\exp\left[\frac{U \oplus \mathfrak{T}^\varepsilon_{\alpha,\mathrm{H}}(U) - \mathrm{H}}{\varepsilon}\right]\right). \tag{A.3.9}$$

Proof. Let us pick any $\Lambda \in \mathcal{S}^d$ and define $V_s := \mathfrak{T}^\varepsilon_{\alpha,\mathrm{H}}(U) + s\Lambda$. By construction, due to the optimality of $\mathfrak{T}^\varepsilon_{\alpha,\mathrm{H}}(U)$, the map

$$s \mapsto g(s) := \operatorname{Tr}(V_s\alpha) - \varepsilon \operatorname{Tr}\left(\exp\left[\frac{U \oplus V_s - \mathrm{H}}{\varepsilon}\right]\right)$$

must have vanishing derivative at $s = 0$. This can be computed [15, Section 2.2] as

$$g'(0) = \operatorname{Tr}(\Lambda\alpha) - \varepsilon \operatorname{Tr}\left((I \otimes \Lambda)\exp\left[\frac{U \oplus \mathfrak{T}^\varepsilon_{\alpha,\mathrm{H}}(U) - \mathrm{H}}{\varepsilon}\right]\right). \tag{A.3.10}$$

Using the definition of partial trace and the previous formula, we infer

$$\mathrm{Tr}\left(\Lambda\Big(\alpha - \mathrm{P}_1\left(\exp\left[\frac{U \oplus \mathfrak{T}^{\varepsilon}_{\alpha,\mathrm{H}}(U) - \mathrm{H}}{\varepsilon}\right]\right)\Big)\right) = 0 \tag{A.3.11}$$

for every $\Lambda \in \mathcal{S}^d$. Note that $\alpha, U, V_s, \mathrm{H}$ being self-adjoint, it follows that the operator

$$\alpha - \mathrm{P}_1\left(\exp\left[\frac{U \oplus \mathfrak{T}^{\varepsilon}_{\alpha,\mathrm{H}}(U) - \mathrm{H}}{\varepsilon}\right]\right)$$

is self-adjoint as well. Together with (A.3.11), this shows (A.3.9). On the other hand, since (A.3.11) is the Euler Lagrange equation associated to the maximization of the strictly concave functional $\mathrm{T}^{\varepsilon}_{\alpha,\mathrm{H}}(U,\cdot)$, any solution of (A.3.11) is necessarily a maximizer and hence coincides with $\mathfrak{T}^{\varepsilon}_{\alpha,\mathrm{H}}(U)$, by uniqueness (see Lemma A.3.1).

□

The next step is to obtain some regularity estimates on $\mathfrak{T}^{\varepsilon}_{\alpha,\mathrm{H}}(U)$. To do so, we extrapolate information from the optimality conditions proved in Lemma A.3.2.

Proposition A.3.1 (Regularity of the (H,ε)-transform)**.** *Given $d, d' \in \mathbb{N}$, $0 < \alpha \in \mathfrak{P}^{d'}$, $\mathrm{H} \in \mathcal{S}^{dd'}$, $\varepsilon > 0$, we define for all $A \in \mathcal{S}^d$ (or $A \in \mathcal{S}^{d'}$)*

$$\lambda_\varepsilon(A) := \varepsilon \log\left(\mathrm{Tr}\left[\exp\left(\frac{A}{\varepsilon}\right)\right]\right). \tag{A.3.12}$$

Then for every $U \in \mathcal{S}^d$ it holds

$$\left|\mathfrak{T}^{\varepsilon}_{\alpha,\mathrm{H}}(U) - \varepsilon \log \alpha + \lambda_\varepsilon(U)\mathbb{1}\right| \leq \|\mathrm{H}\|_\infty \mathbb{1}, \tag{A.3.13}$$

$$\left|\lambda_\varepsilon(U) + \lambda_\varepsilon\Big(\mathfrak{T}^{\varepsilon}_{\alpha,\mathrm{H}}(U)\Big)\right| \leq \|\mathrm{H}\|_\infty, \tag{A.3.14}$$

$$\left|\mathfrak{T}^{\varepsilon}_{\alpha,\mathrm{H}}(U) - \varepsilon \log \alpha - \lambda_\varepsilon(\mathfrak{T}^{\varepsilon}_{\alpha,\mathrm{H}}(U))\mathbb{1}\right| \leq 2\|\mathrm{H}\|_\infty \mathbb{1}. \tag{A.3.15}$$

where the inequalities are understood as two-sided quadratic forms bounds.

Proof. Note that (A.3.15) is an immediate consequence of (A.3.13) and (A.3.14) and we shall therefore only prove the latter two. Let us start with the proof of (A.3.13). We know from Lemma A.3.2 that for every $U \in \mathcal{S}^d$, $\mathfrak{T}^{\varepsilon}_{\alpha,\mathrm{H}}(U)$ satisfies equation (A.3.9). By the properties of the partial trace (Remark A.3.1) and $\mathrm{H} \leq \|\mathrm{H}\|_\infty \mathbb{1}$, it follows that

$$\begin{aligned}
\alpha &\leq e^{\frac{\|\mathrm{H}\|_\infty}{\varepsilon}} \mathrm{P}_1\left(\exp\left[\frac{U \oplus \mathfrak{T}^{\varepsilon}_{\alpha,\mathrm{H}}(U)}{\varepsilon}\right]\right) \\
&= e^{\frac{\|\mathrm{H}\|_\infty}{\varepsilon}} \mathrm{P}_1\left(\exp\left(\frac{U}{\varepsilon}\right) \otimes \exp\left(\frac{\mathfrak{T}^{\varepsilon}_{\alpha,\mathrm{H}}(U)}{\varepsilon}\right)\right) \\
&= e^{\frac{\|\mathrm{H}\|_\infty}{\varepsilon}} \mathrm{Tr}\left(\exp\left(\frac{U}{\varepsilon}\right)\right) \exp\left(\frac{\mathfrak{T}^{\varepsilon}_{\alpha,\mathrm{H}}(U)}{\varepsilon}\right),
\end{aligned} \tag{A.3.16}$$

where in the first inequality we used that $\exp(A \oplus B) = \exp A \otimes \exp B$.

Similarly, using instead the lower bound $\mathrm{H} \geq -\|\mathrm{H}\|_\infty \mathbb{1}$, from (A.3.9) we can also obtain

$$\alpha \geq e^{\frac{-\|\mathrm{H}\|_\infty}{\varepsilon}} \operatorname{Tr}\left(\exp\left(\frac{U}{\varepsilon}\right)\right) \exp\left(\frac{\mathfrak{T}^\varepsilon_{\alpha,\mathrm{H}}(U)}{\varepsilon}\right). \tag{A.3.17}$$

We can put together the two bounds in (A.3.16), (A.3.17) to obtain

$$\alpha e^{\frac{-\|\mathrm{H}\|_\infty}{\varepsilon}} \leq \operatorname{Tr}\left(\exp\left(\frac{U}{\varepsilon}\right)\right) \exp\left(\frac{\mathfrak{T}^\varepsilon_{\alpha,\mathrm{H}}(U)}{\varepsilon}\right) \leq \alpha e^{\frac{\|\mathrm{H}\|_\infty}{\varepsilon}}. \tag{A.3.18}$$

Taking the log in the latter inequalities we conclude the proof of (A.3.13). If we instead take the trace of both sides in (A.3.18), we obtain

$$e^{\frac{-\|\mathrm{H}\|_\infty}{\varepsilon}} \leq \operatorname{Tr}\left(\exp\left(\frac{U}{\varepsilon}\right)\right) \operatorname{Tr}\left(\exp\left(\frac{\mathfrak{T}^\varepsilon_{\alpha,\mathrm{H}}(U)}{\varepsilon}\right)\right) \leq e^{\frac{\|\mathrm{H}\|_\infty}{\varepsilon}},$$

and then applying the log, we conclude the proof (A.3.14).

□

A.3.2 Vectorial $(\mathrm{H}, \varepsilon)$-transforms

In this section, we consider a vectorial version of the $(\mathrm{H}, \varepsilon)$-transforms introduced in the previous section. This turns out to be a key object in the proof of Theorem A.2.1 and Theorem A.2.2, necessary to deal with the multi-marginal setting.

Let us first introduce the general framework, which remains in force throughout the section.

Let $N \in \mathbb{N}$ and $[N]$ be a index set of N elements. For all $i \in [N]$, let $d_i \in \mathbb{N}$ and $\gamma_i \in \mathfrak{P}^{d_i}$ be density matrices. Set $\boldsymbol{\gamma} := (\gamma_i)_{i\in[N]}$, $\boldsymbol{d} = \prod_{j=1}^N d_i$. Finally, consider a Hamiltonian $\mathrm{H} \in \mathcal{S}^{\boldsymbol{d}}$.

Remark A.3.3. *(Kernels) Without loss of generality, we can assume* $\ker \gamma_i = \{0\}$, *for every* $i \in [N]$. *In the general case, it suffices to consider the restriction to the set* $\mathcal{O} := \bigotimes_{i=1}^N \left(\ker \gamma_i\right)^\perp$ *and consider the matrix* $\mathrm{H}_\mathcal{O} = \Pi_\mathcal{O}\, \mathrm{H}\, \Pi_\mathcal{O}$, *where* $\Pi_\mathcal{O}$ *is the projector onto* $\mathcal{O}$.

We therefore assume that $\ker \gamma_i = \{0\}$ for all $i \in [N]$. In this section we extend the notion of $(\mathrm{H}, \varepsilon)$-transform as introduced in previous section A.3.1 to the multi-marginal setting, and we apply it to our specific setting. We are interested in the maximization (A.2.2) of the dual functional, that we introduce below.

Definition A.3.4 (Dual Functional). *For any* $\boldsymbol{U} = (U_1, \ldots, U_N) \in \times_{j=1}^N \mathcal{S}^{d_j}$, *we define*

$$\mathrm{D}^\varepsilon_{\boldsymbol{\gamma}}(\boldsymbol{U}) = \sum_{i=1}^N \operatorname{Tr}(U_i \gamma_i) - \varepsilon \operatorname{Tr}\left(\exp\left[\frac{\bigoplus_{i=1}^N U_i - \mathrm{H}}{\varepsilon}\right]\right) + \varepsilon.$$

Remark A.3.4. *Note that* $\mathrm{D}^\varepsilon_{\boldsymbol{\gamma}}$ *is invariant by translation for any vector* $\boldsymbol{a} = (a_1, \ldots, a_N) \in \mathbb{R}^N$ *such that* $\sum_{k=1}^N a_k = 0$, *i.e.*

$$\mathrm{D}^\varepsilon_{\boldsymbol{\gamma}}(\boldsymbol{U} + \boldsymbol{a}) = \mathrm{D}^\varepsilon_{\boldsymbol{\gamma}}(\boldsymbol{U}).$$

As a consequence of this property, we see in Section A.5 that the set of maximizers is invariant by such transformations (Lemma A.4.1).

With the following definition, we introduce the vectorial $(\mathrm{H}, \varepsilon)$-transforms.

Definition A.3.5 (Vectorial $(\mathrm{H}, \varepsilon)$-transform)**.** *For any $i \in [N]$, we define the i-th vectorial $(\mathrm{H}, \varepsilon)$-transform $\mathfrak{T}_i^\varepsilon$ as the map*

$$\mathfrak{T}_i^\varepsilon : \bigtimes_{j=1,\, j\neq i}^N \mathcal{S}^{d_j} \to \mathcal{S}^{d_i},$$
$$\mathfrak{T}_i^\varepsilon(\hat{\boldsymbol{U}}_i) = \operatorname*{argmax}_{V \in \mathcal{S}^{d_i}} \left\{ \mathrm{Tr}(V\gamma_i) - \varepsilon \,\mathrm{Tr}\left(\exp\left[\frac{1}{\varepsilon} \left(U_1 \oplus \cdots \oplus U_{i-1} \oplus V \oplus U_{i+1} \oplus \cdots \oplus U_N - \mathrm{H} \right) \right] \right) \right\},$$

where for $\boldsymbol{U} \in \bigtimes_{j=1}^N \mathcal{S}^{d_j}$, we set $\hat{\boldsymbol{U}}_i$ to be the product of all the U_j but the i-th one, namely

$$\hat{\boldsymbol{U}}_i := \bigtimes_{j=1,\, j\neq i}^N U_j \in \bigtimes_{j=1,\, j\neq i}^N \mathcal{S}^{d_j}. \tag{A.3.19}$$

Remark A.3.5. *Observe that we can identify the i-th vectorial $(\mathrm{H}, \varepsilon)$-transforms with a particular case of the operators $\mathfrak{T}_{\varepsilon,\mathrm{H},\alpha}$ as introduced in Section A.3.1. Indeed, as a consequence of Remark A.3.2 it is straightforward to see that for $i \in [N]$*

$$\mathfrak{T}_i^\varepsilon(\hat{\boldsymbol{U}}_i) = \mathfrak{T}^\varepsilon_{\gamma_i,\mathrm{S}_i(\mathrm{H})} \left(\bigoplus_{j=1,\, j\neq i}^N U_i \right), \quad \mathfrak{T}^\varepsilon_{\gamma_i,\mathrm{S}_i(\mathrm{H})} : \bigotimes_{j=1,\, j\neq i}^N \mathcal{S}^{d_j} \approx \mathcal{S}^{\tilde{d}_i} \to \mathcal{S}^{d_i}, \tag{A.3.20}$$

where we set $\tilde{d}_i := \prod_{j\neq i} d_j$ and the S_i are the permutation operators in Definition A.3.2. This shows that the definition is well posed (i.e. that the argmax *appearing in the definition exists and is unique). Moreover it allows us to extend the validity of the properties of the $(\mathrm{H}, \varepsilon)$-transform shown in Section A.3.1 to the operators $\mathfrak{T}_i^\varepsilon$, as we shall see in Lemma A.3.3 and Proposition A.3.2 below. Note that the dependence on the specific entry i is reflected in both the use of γ_i and in the fact that the transform is performed w.r.t. $\mathrm{S}_i(\mathrm{H})$.*

A.3.3 One-step and Sinkhorn operators

We use the vectorial $(\mathrm{H}, \varepsilon)$-transforms to define what we call *one-step operators* and *Sinkhorn operators*. The first ones map a vector of N potentials into a vector of N potentials, exchanging its i-th entry with the i-th vectorial $(\mathrm{H}, \varepsilon)$-transform applied to the other $N-1$. The second is simply obtained by composing all the different N one-step operators.

Definition A.3.6 (One-step operators)**.** *For $i \in [N]$, we introduce the one-step operators $\mathcal{T}_i^\varepsilon$, which are defined by*

$$\mathcal{T}_i^\varepsilon : \bigtimes_{j=1}^N \mathcal{S}^{d_j} \to \bigtimes_{j=1}^N \mathcal{S}^{d_j}$$
$$\boldsymbol{U} := (U_1, \ldots, U_N) \longmapsto (U_1, \ldots, U_{i-1}, \mathfrak{T}_i^\varepsilon(\hat{\boldsymbol{U}}_i), U_{i+1}, \ldots, U_N) =: \mathcal{T}_i^\varepsilon(\boldsymbol{U}).$$

The Sinkhorn operator is simply the composition of the N one-step operators $\mathcal{T}_i^\varepsilon, i \in [N]$.

Definition A.3.7 (Sinkhorn Operator)**.** *We introduce the Sinkhorn operator τ, defined by*

$$\tau : \bigtimes_{j=1}^N \mathcal{S}^{d_j} \to \bigtimes_{j=1}^N \mathcal{S}^{d_j},$$
$$\tau(\boldsymbol{U}) := (\mathcal{T}_N^\varepsilon \circ \cdots \circ \mathcal{T}_1^\varepsilon)(\boldsymbol{U}).$$

Remark A.3.6. *Note that, by definition of τ, it follows immediately that, for any $\boldsymbol{U} \in \times_{j=1}^{N} \mathcal{S}^{d_j}$*

$$\mathrm{D}^{\varepsilon}_{\gamma}(\tau(\boldsymbol{U})) \geq \mathrm{D}^{\varepsilon}_{\gamma}(\boldsymbol{U}),$$

i.e. applying τ to any vector increases its energy. Moreover, any maximizer of $\mathrm{D}^{\varepsilon}_{\gamma}$ is a fixed point of τ (as a consequence of the uniqueness proved in Lemma A.3.1). The converse is also true and implies that the set of maximizers of $\mathrm{D}^{\varepsilon}_{\gamma}$ coincides with the set of fixed points of τ, see Remark A.4.1.

Remark A.3.7. *Note that for any vector $\boldsymbol{a} \in \mathbb{R}^N$ such that $\sum_{k=1}^{N} \boldsymbol{a}_k = 0$, one has*

$$\mathcal{T}^{\varepsilon}_{i}(\boldsymbol{U} + \boldsymbol{a}) = \mathcal{T}^{\varepsilon}_{i}(\boldsymbol{U}) + \boldsymbol{a},$$

i.e. $\mathcal{T}^{\varepsilon}_{i}$ commutes with translations by vectors whose coordinates sum up to zero (notice that this fact is particularly interesting in light of Remark A.3.4). This is a straightforward consequence of the fact that

$$\mathfrak{T}^{\varepsilon}_{i}\left(\widehat{(\boldsymbol{U} + \boldsymbol{a})}_i\right) = \mathfrak{T}^{\varepsilon}_{i}(\hat{\boldsymbol{U}}_i) + a_i,$$

which can be readily verified from the definitions.

Trivially, this also implies

$$\tau(\boldsymbol{U} + \boldsymbol{a}) = \tau(\boldsymbol{U}) + \boldsymbol{a}.$$

We now take advantage of the observations in Remark A.3.5 to deduce properties for the vectorial $(\mathrm{H}, \varepsilon)$-transforms, the one-step operators, and the Sinkhorn operator. First of all, as a corollary of Lemma A.3.2, we characterize the vectorial $(\mathrm{H}, \varepsilon)$-transforms as solutions of implicit equations.

Lemma A.3.3 (Optimality conditions for vectorial $(\mathrm{H}, \varepsilon)$-transforms)**.** *Let $i \in [N]$, $\varepsilon > 0$, $\gamma_i \in \mathfrak{P}^{d_i}$, $\mathrm{H} \in \mathcal{S}^d$, with $\ker \gamma_i = \{0\}$. For any $\boldsymbol{U} \in \times_{j=1}^{N} \mathcal{S}^{d_j}$, the one step-operator $\mathcal{T}^{\varepsilon}_{i}(\boldsymbol{U})$ (or equivalently the i-th vectorial $(\mathrm{H}, \varepsilon)$-transform $\mathfrak{T}^{\varepsilon}_{i}(\hat{\boldsymbol{U}}_i)$) is implicitly characterized as the unique solution of the equation*

$$\gamma_i = \mathrm{P}_i\left(\exp\left[\frac{1}{\varepsilon}\left(\bigoplus_{j=1}^{N}(\mathcal{T}^{\varepsilon}_{i}(\boldsymbol{U}))_j - \mathrm{H}\right)\right]\right). \tag{A.3.21}$$

Proof. As a consequence of (A.3.20), we can apply Lemma A.3.2 and deduce

$$\begin{aligned}\gamma_i &= \mathrm{P}_i\left(\exp\left[\frac{1}{\varepsilon}\left(\left(\bigoplus_{j=1,\, j\neq i}^{N} U_i\right) \oplus \mathfrak{T}^{\varepsilon}_{i}(\hat{\boldsymbol{U}}_i) - \mathrm{S}_i(\mathrm{H})\right)\right]\right)\\ &= \mathrm{P}_i\left(\exp\left[\frac{1}{\varepsilon}\left(\bigoplus_{j=1}^{N}(\mathcal{T}^{\varepsilon}_{i}(\boldsymbol{U}))_j - \mathrm{H}\right)\right]\right),\end{aligned}$$

where S_i is the i-th permutation operator, as defined in A.3.2, and in the last equality we used Remark A.3.2 and that

$$\left(\bigoplus_{j=1,\, j\neq i}^{N} U_i\right) \oplus \mathfrak{T}^{\varepsilon}_{i}(\hat{\boldsymbol{U}}_i) = \mathrm{S}_i\left(\bigoplus_{j=1}^{N}(\mathcal{T}^{\varepsilon}_{i}(\boldsymbol{U}))_j\right)$$

for every $i \in [N]$ and $\boldsymbol{U} \in \times_{j=1}^{N} \mathcal{S}^{d_j}$. □

The next proposition collects the regularity properties of the (H,ε)-transforms. Once again, they are direct consequence of the properties proved in the two marginals case, in particular in Proposition A.3.1.

Proposition A.3.2 (Regularity of the (H,ε)-transforms). *Let $i \in [N]$, $\varepsilon > 0$, $\gamma_i \in \mathfrak{P}^{d_i}$, $\mathrm{H} \in \mathcal{S}^d$, with $\ker \gamma_i = \{0\}$. Then for every $\boldsymbol{U} \in \times_{j=1}^N \mathcal{S}^{d_j}$, for every $i \in [N]$ it holds*

$$\left| \mathfrak{T}_i^\varepsilon(\hat{\boldsymbol{U}}_i) - \varepsilon \log \gamma_i + \sum_{j=1, j\neq i}^N \lambda_\varepsilon(U_j) \mathbb{1} \right| \leq \|\mathrm{H}\|_\infty \mathbb{1}\,, \tag{A.3.22}$$

$$\left| \sum_{j=1, j\neq i}^N \lambda_\varepsilon(U_j) + \lambda_\varepsilon\left(\mathfrak{T}_i^\varepsilon(\hat{\boldsymbol{U}}_i)\right) \right| \leq \|\mathrm{H}\|_\infty\,, \tag{A.3.23}$$

$$\left| \mathfrak{T}_i^\varepsilon(\hat{\boldsymbol{U}}_i) - \varepsilon \log \gamma_i - \lambda_\varepsilon\left(\mathfrak{T}_i^\varepsilon(\hat{\boldsymbol{U}}_i)\right) \mathbb{1} \right| \leq (2\|\mathrm{H}\|_\infty)\mathbb{1}, \tag{A.3.24}$$

where λ_ε is defined in (A.3.12).

Proof. The proof is a direct application of Proposition A.3.1 and the considerations in Remark A.3.5. Precisely, the estimate (A.3.22) follows from (A.3.13), (A.3.23) follows from (A.3.14) and (A.3.24) follows from (A.3.15), together with the fact that

$$\lambda_\varepsilon\left(\bigoplus_{j=1,\, j\neq i}^N U_j\right) = \sum_{j=1, j\neq i}^N \lambda_\varepsilon(U_j)\,, \quad \forall \boldsymbol{U} \in \bigtimes_{j=1}^N \mathcal{S}^{d_j}.$$

□

In light of Remark A.3.6, it is reasonable to check whether sequences of the form $\tau^k(\boldsymbol{U}_0)$ are maximizing for $\mathrm{D}_\gamma^\varepsilon$ and compact. On the other hand, a priori it is not clear how to obtain compactness for such sequences and Remark A.3.4 shows that there could even exist sequences 'converging' to the set of maximizers which are not compact. It is therefore natural to introduce a suitable renormalization operator, aimed at retrieving compactness. Note that any such operator should increase or leave invariant the value of $\mathrm{D}_\gamma^\varepsilon$ and therefore, by Remark A.3.4, any translation by vectors whose coordinates sum up to zero is a good candidate.

Definition A.3.8 (Renormalisation). *Let λ_ε be defined as in* (A.3.12). *We define the renormalisation map $\mathrm{Ren} : \times_{i=1}^N \mathcal{S}^{d_i} \to \times_{i=1}^N \mathcal{S}^{d_i}$ as the function*

$$\mathrm{Ren}(\boldsymbol{U})_i = \begin{cases} U_i - \lambda_\varepsilon(U_i), & \text{if } i \in \{1, \dots, N-1\} \\ U_N + \sum_{j=1}^{N-1} \lambda_\varepsilon(U_j), & \text{if } i = N. \end{cases}$$

In the following proposition we show that $\mathrm{Ren}\left(\tau\left(\times_{i=1}^N \mathcal{S}^{d_i}\right)\right)$ is bounded and therefore compact. This shows that the map Ren is indeed a reasonable renormalization operator for our purposes.

Proposition A.3.3 (Renormalisation of (H,ε)-transforms and uniform bounds). *Let $i \in [N]$, $\varepsilon > 0$, $\gamma_i \in \mathfrak{P}^{d_i}$, $\mathrm{H} \in \mathcal{S}^d$, with $\ker \gamma_i = \{0\}$. Then, for any $\boldsymbol{U} \in \mathcal{S}^{\boldsymbol{d}}$, one has that $\mathrm{D}_\gamma^\varepsilon(\mathrm{Ren}\,\tau(\boldsymbol{U})) \geq \mathrm{D}_\gamma^\varepsilon(\boldsymbol{U})$, and the following bounds hold true:*

$$\left| (\mathrm{Ren}\,\tau(\boldsymbol{U}))_i - \varepsilon \log \gamma_i \right| \leq 2\|\mathrm{H}\|_\infty \mathbb{1}, \quad \forall i \in [N]. \tag{A.3.25}$$

Proof. First of all, Remark A.3.4 and Remark A.3.6 trivially yield $\mathrm{D}^\varepsilon_\gamma(\mathrm{Ren}\,\tau(\boldsymbol{U})) \geq \mathrm{D}^\varepsilon_\gamma(\boldsymbol{U})$. To show (A.3.25), note that for any $i \in [N]$, $(\tau(\boldsymbol{U}))_i$ is obtained applying $\mathfrak{T}^\varepsilon_i$ to some element of $\bigtimes_{j=1,\, j\neq i}^N \mathcal{S}^{d_j}$. Therefore, applying (A.3.24) from Proposition A.3.2, we obtain

$$\|(\mathrm{Ren}\,\tau(\boldsymbol{U}))_i - \varepsilon \log \gamma_i\|_\infty = \|(\tau(\boldsymbol{U}))_i - \varepsilon \log \gamma_i - \lambda_\varepsilon((\tau(\boldsymbol{U}))_i)\|_\infty \leq 2\|\,\mathrm{H}\,\|_\infty$$

for every $i \in [N-1]$. Moreover, $(\tau(\boldsymbol{U}))_N = \mathfrak{T}^N_\varepsilon(\widehat{\tau(\boldsymbol{U})}_N)$ and hence, applying (A.3.22) from Proposition A.3.2, we arrive at

$$\|(\mathrm{Ren}\,\tau(\boldsymbol{U}))_N - \varepsilon \log \gamma_N\|_\infty = \left\|(\tau(\boldsymbol{U}))_N - \varepsilon \log \gamma_N + \sum_{j=1}^{N-1} \lambda_\varepsilon((\tau(\boldsymbol{U}))_j)\right\|_\infty \leq \|\,\mathrm{H}\,\|_\infty,$$

which completes the proof. □

A.4 Non-Commutative Multi-Marginal Optimal Transport

In this section we prove Theorem A.2.1, our first main result stated in Section A.2, exploiting the tools developed in Section A.3. Again, we fix the setup, which remains in force throughout the whole Section A.4 and Section A.5. Let $N \in \mathbb{N}$, and for $i \in [N]$ we consider density matrices $\gamma_i \in \mathfrak{P}^{d_i}$. Set $\boldsymbol{\gamma} := (\gamma_i)_{i\in[N]}$, $\boldsymbol{d} = \prod_{j=1}^N d_i$, and assume that $\ker \gamma_i = \{0\}$ (see Remark A.3.3). We also fix $\mathrm{H} \in \mathcal{S}^{\boldsymbol{d}}$.

In this section, we prove the Theorem A.2.1.

We begin by introducing the primal functional, which appears in the minimisation (A.2.1).

Definition A.4.1 (Primal Functional)**.** *Let $\Gamma \in \mathfrak{P}^{\boldsymbol{d}}$ the primal functional is defined by*

$$\mathrm{F}^\varepsilon(\Gamma) = \mathrm{Tr}(\mathrm{H}\,\Gamma) + \varepsilon S(\Gamma) = \mathrm{Tr}(\mathrm{H}\,\Gamma) + \varepsilon\,\mathrm{Tr}(\Gamma \log \Gamma). \tag{A.4.1}$$

We also recall the definitions of the primal and the dual problem

$$\mathfrak{F}^\varepsilon(\boldsymbol{\gamma}) = \inf\left\{\mathrm{F}^\varepsilon(\Gamma) \;:\; \Gamma \in \mathfrak{P}^{\boldsymbol{d}} \text{ and } \Gamma \mapsto (\gamma_1, \dots, \gamma_N)\right\}, \tag{A.4.2}$$

$$\mathfrak{D}^\varepsilon(\boldsymbol{\gamma}) = \sup\left\{\mathrm{D}^\varepsilon_\gamma(\boldsymbol{U}) \;:\; \boldsymbol{U} \in \bigtimes_{i=1}^N \mathcal{S}^{d_i}\right\}, \tag{A.4.3}$$

where the dual functional $\mathrm{D}^\varepsilon_\gamma$ is given in Definition A.3.4.

A.4.1 Lower bound primal-dual functionals

We begin with the proof of the lower bound for the primal functional (A.4.1), in terms of the dual functional (A.3.4).

Proposition A.4.1 (Lower bound)**.** *Fix $N \in \mathbb{N}$ and $\varepsilon > 0$. For all $i \in [N]$, let $\gamma_i \in \mathfrak{P}^{d_i}$ be density matrices, $\mathrm{H} \in \mathcal{S}^{\boldsymbol{d}}$. Then, for all $\boldsymbol{U} \in \bigtimes_{i=1}^N \mathcal{S}^{d_i}$ and every $\Gamma \in \mathfrak{P}^{\boldsymbol{d}}$, $\Gamma \mapsto \boldsymbol{\gamma}$ we have that*

$$\mathrm{F}^\varepsilon(\Gamma) \geq \mathrm{D}^\varepsilon_\gamma(\boldsymbol{U})\,.$$

Proof. For any $\boldsymbol{U} \in \times_{i=1}^N \mathcal{S}^{d_i}$ and any admissible $\Gamma \in \mathfrak{P}^{\boldsymbol{d}}$, $\Gamma \mapsto \boldsymbol{\gamma}$, we can write

$$\begin{aligned}\mathrm{F}^\varepsilon(\Gamma) &= \mathrm{F}^\varepsilon(\Gamma) + \sum_{j=1}^N \mathrm{Tr}(U_j\gamma_j) - \mathrm{Tr}\left(\left(\bigoplus_{j=1}^N U_j\right)\Gamma\right) \\ &= \sum_{j=1}^N \mathrm{Tr}(U_j\gamma_j) + \varepsilon S(\Gamma) - \mathrm{Tr}\left(\Gamma\left(\bigoplus_{j=1}^N U_j - \mathrm{H}\right)\right).\end{aligned}$$

Let us denote the Hilbert-Schmidt scalar product (on $\mathcal{M}^{\boldsymbol{d}}$) by $\langle\cdot,\cdot\rangle_{HS}$. It follows that

$$\mathrm{F}^\varepsilon(\Gamma) = \sum_{j=1}^N \mathrm{Tr}(U_j\gamma_j) + \varepsilon\left[S(\Gamma) - \langle\Gamma, \overline{Y}\rangle_{HS}\right] \geq \sum_{j=1}^N \mathrm{Tr}(U_j\gamma_j) - \varepsilon S^*(\overline{Y}), \tag{A.4.4}$$

where $\overline{Y} = \varepsilon^{-1}\left(\bigoplus_{j=1}^N U_j - \mathrm{H}\right) \in \mathcal{S}^{\boldsymbol{d}}$ and, for any $Y \in \mathcal{S}^{\boldsymbol{d}}$

$$S^*(Y) := \sup_{\Gamma\in\mathcal{S}^{\boldsymbol{d}}_{\geq}} \{\langle Y, \Gamma\rangle_{HS} - S(\Gamma)\}$$

denotes the Legendre transform of S on the subspace $\mathcal{S}^{\boldsymbol{d}}_{\geq}$. This can be explicitly computed as

$$S^*(Y) = \mathrm{Tr}\left[\exp(Y-1)\right], \quad \forall Y \in \mathcal{S}^{\boldsymbol{d}}. \tag{A.4.5}$$

For the sake of completeness, let us explain how to prove (A.4.5). First of all we show that for any $Y \in \mathcal{S}^{\boldsymbol{d}}$ the supremum appearing in the definition of $S^*(Y)$ is attained at some $\bar{\Gamma} \in \mathcal{S}^{\boldsymbol{d}}_{>}$. Indeed, for any $\Gamma \geq 0$ define σ_+ to be the maximum of its spectrum, then it holds

$$\langle Y, \Gamma\rangle_{HS} - S(\Gamma) \leq \boldsymbol{d}^2\|Y\|_\infty\sigma_+ - \sigma_+\log\sigma_+ - \min_{\mathbb{R}_+}\{x\log x\}(\boldsymbol{d}^2-1) \xrightarrow{\sigma_+\to\infty} -\infty.$$

This implies that the super-levels of $\langle y, \Gamma\rangle_{HS} - f(\Gamma)$ are bounded and hence pre-compact and allows us to conclude the existence of a maximizer $\bar{\Gamma}$. Moreover, it is straightforward to show that $\bar{\Gamma} > 0$, otherwise one would have a contradiction by perturbing $\bar{\Gamma}$ with $\Pi_{\ker\bar{\Gamma}}$ (the projector onto $\ker\bar{\Gamma}$).

Let us derive the optimality conditions for $\bar{\Gamma}$. Define $\Gamma_s := \bar{\Gamma} + s\Gamma'$ with $\Gamma' \in \mathcal{S}^{\boldsymbol{d}}$ (note that for any $\Gamma' \in \mathcal{S}^{\boldsymbol{d}}$ for s sufficiently small Γ_s is positive since $\bar{\Gamma} > 0$), then the Euler-Lagrange equation for the maximization problem reads

$$0 = \frac{d}{ds}\Big|_{s=0} (\langle Y, \Gamma_s\rangle_{HS} - S(\Gamma_s)) = \langle Y, \Gamma'\rangle_{HS} - \mathrm{Tr}\left[\Gamma'(\log\bar{\Gamma} + 1)\right].$$

This yields $\bar{\Gamma} = \exp(Y-1)$. Substituting in the expression for S^*, we arrive at (A.4.5).

Plugging this into (A.4.4) with $Y = \overline{Y}$ and recalling the definition of Y, we obtain

$$\mathrm{F}^\varepsilon(\Gamma) \geq \sum_{j=1}^N \mathrm{Tr}(U_j\gamma_j) - \varepsilon\,\mathrm{Tr}\left(\exp\left(\frac{\bigoplus_{j=1}^N U_j - \mathrm{H} - \varepsilon}{\varepsilon}\right)\right).$$

Changing the variable U_1 to $\tilde{U}_1 := U_1 + \varepsilon$, we conclude the proof. $\square$

Remark A.4.1 (The non-commutative Schrödinger problem)**.** *Suppose that* $\boldsymbol{U} \in \times_{i=1}^N \mathcal{S}^{d_i}$ *is a fixed point for* τ*, namely* $\tau(\boldsymbol{U}) = \boldsymbol{U}$*. This can be equivalently recast as* $\mathfrak{T}_i^\varepsilon(\hat{\boldsymbol{U}}_i) = U_i$*,* $\forall i \in [N]$*. Then Lemma A.3.3,* (A.3.21) *imply that the density matrix defined by*

$$\Gamma := \exp\left(\frac{\bigoplus_{i=1}^N U_i - \mathrm{H}}{\varepsilon}\right) \tag{A.4.6}$$

has the correct marginals $\Gamma \mapsto (\gamma_1, \ldots, \gamma_N)$ *and thus it is admissible for the primal problem. In particular, it has trace* 1 *and we have*

$$\mathrm{D}_\gamma^\varepsilon(U_1, \ldots, U_N) = \mathrm{D}_\gamma^\varepsilon(\boldsymbol{U}) = \sum_{i=1}^N \mathrm{Tr}(U_i \gamma_i) = \mathrm{Tr}\left(\left(\bigoplus_{i=1}^N U_i\right)\Gamma\right).$$

On the other hand, directly from formula (A.4.6)*, we compute*

$$\Gamma\,\mathrm{H} + \varepsilon\,\Gamma \log \Gamma = \Gamma\,\mathrm{H} + \Gamma\left(\bigoplus_{i=1}^N U_i - \mathrm{H}\right) = \Gamma\left(\bigoplus_{i=1}^N U_i\right)$$

and thus

$$\mathrm{F}^\varepsilon(\Gamma) = \mathrm{Tr}\left(\left(\bigoplus_{i=1}^N U_i\right)\Gamma\right) = \mathrm{D}_\gamma^\varepsilon(U_1, \ldots, U_N). \tag{A.4.7}$$

In light of Proposition A.4.1, this shows that if we are able to find a fixed point of τ*, then this must be optimal for the dual problem (note that any maximizer is also a fixed point for* τ *as discussed in Remark A.3.6) and the corresponding* Γ *as obtained in* (A.4.6) *must be optimal for the primal problem.*

Another consequence of the above observations is that the set of maximizers for the dual problem is invariant under translations.

Lemma A.4.1 (Structure of the maximizers)**.** *Let* $\boldsymbol{U}$ *and* $\boldsymbol{V}$ *be two maximizers of* $\mathrm{D}_\gamma^\varepsilon$*, then there exists* $\boldsymbol{\alpha} \in \mathbb{R}^N$ *such that* $\sum_{i=1}^N \boldsymbol{\alpha}_i = 0$ *and* $\boldsymbol{U} = \boldsymbol{V} + \boldsymbol{\alpha}$*.*

Proof. Thanks to Remark A.4.1 and using that the primal functional admits an unique minimizer by strict convexity, we find

$$\exp\left(\frac{\bigoplus_{i=1}^N (\boldsymbol{U})_i - \mathrm{H}}{\varepsilon}\right) = \exp\left(\frac{\bigoplus_{i=1}^N (\boldsymbol{V})_i - \mathrm{H}}{\varepsilon}\right) \implies \bigoplus_{i=1}^N (\boldsymbol{U})_i = \bigoplus_{i=1}^N (\boldsymbol{V})_i\ . \tag{A.4.8}$$

Applying the partial traces to the latter equality, we obtain

$$(\boldsymbol{U})_i = (\boldsymbol{V})_i + \sum_{j=1, j\neq i}^N \mathrm{Tr}(\boldsymbol{V})_j - \mathrm{Tr}(\boldsymbol{U})_j =: (\boldsymbol{V})_i + \boldsymbol{\alpha}_i.$$

Using (A.4.8) once again, one sees that

$$\sum_{i=1}^N \boldsymbol{\alpha}_i = (N-1)\left(\mathrm{Tr}\left(\bigoplus_{i=1}^N (\boldsymbol{U})_i\right) - \mathrm{Tr}\left(\bigoplus_{i=1}^N (\boldsymbol{V})_i\right)\right) = 0,$$

which concludes the proof. □

A.4.2 Proof of Theorem A.2.1

We are finally ready to prove the equivalence between dual and primal problem, and to characterise the optimisers of the two problems. For the sake of clarity, recall that

$$\mathrm{Ren}(\boldsymbol{U})_i = \begin{cases} U_i - \lambda_\varepsilon(U_i), & \text{if } i \in \{1, \dots, N-1\} \\ U_N + \sum_{j=1}^{N-1} \lambda_\varepsilon(U_i), & \text{if } i = N, \end{cases}$$

as in Definition A.3.8 and λ_ε is defined in (A.3.12) as $\lambda_\varepsilon(A) := \varepsilon \log\left(\mathrm{Tr}\left[\exp\left(\frac{A}{\varepsilon}\right)\right]\right)$, for every $A \in \mathcal{S}^d$, $d \in \mathbb{N}$.

Proof of Theorem A.2.1. (ii). Take a maximizing sequence $\boldsymbol{U}_n$ for the dual problem and consider $\tilde{\boldsymbol{U}}_n := \mathrm{Ren}\, \tau(\boldsymbol{U}_n)$, where $\tau = \mathcal{T}_N^\varepsilon \circ \cdots \circ \mathcal{T}_1^\varepsilon$ is the Sinkhorn operator as introduced in Definition A.3.7. Thanks to Proposition A.3.3, $\tilde{\boldsymbol{U}}_n$ is again a maximizing sequence that satisfies

$$\left\|\tilde{\boldsymbol{U}}_n\right\|_\infty \leq 2\| \mathrm{H} \|_\infty + \varepsilon \sup_{i\in[N]} \| \log \gamma_i \|_\infty < \infty, \quad \forall n \in \mathbb{N},$$

and it is therefore compact. Pick any $\boldsymbol{U}^\varepsilon \in \times_{i=1}^N \mathcal{S}^{d_i}$ limit point of $\tilde{\boldsymbol{U}}_n$. By continuity of the dual functional we infer

$$\mathfrak{D}^\varepsilon(\boldsymbol{\gamma}) = \lim_{N\to\infty} \mathrm{D}^\varepsilon_{\boldsymbol{\gamma}}(\tilde{\boldsymbol{U}}_n) = \mathrm{D}^\varepsilon_{\boldsymbol{\gamma}}(\boldsymbol{U}^\varepsilon)$$

which shows that $\boldsymbol{U}^\varepsilon$ is a maximizer for $\mathfrak{D}^\varepsilon(\boldsymbol{\gamma})$. The fact that any other maximizer must coincide with $\boldsymbol{U}^\varepsilon$ follows from Lemma A.4.1.

$(i)\&(iii)$ Proposition A.4.1 proves one of the inequalities. To show the other inequality, we take any maximizer $\boldsymbol{U}^\varepsilon$ (which exists by the previous proof of (ii)). By construction of the Sinkhorn map, $\boldsymbol{U}^\varepsilon$ must be a fixed point of τ. Thanks to Remark A.4.1, we conclude that

$$\Gamma^\varepsilon = \exp\left(\frac{\bigoplus_{i=1}^N \boldsymbol{U}_i^\varepsilon - \mathrm{H}}{\varepsilon}\right)$$

satisfies $\mathrm{D}^\varepsilon_{\boldsymbol{\gamma}}(\boldsymbol{U}^\varepsilon) = \mathrm{F}^\varepsilon(\Gamma^\varepsilon) \geq \mathfrak{F}^\varepsilon(\boldsymbol{\gamma})$. Hence Γ^ε is optimal for F^ε and $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma}) = \mathfrak{D}^\varepsilon(\boldsymbol{\gamma})$. □

A.4.3 Stability and the functional derivative of $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma})$

In this last section, we show stability of the Kantorovich potentials with respect to the marginals $\boldsymbol{\gamma}$ and compute the Fréchet differential of $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma})$ (or simply the differential in our finite dimensional setting). A similar result was first obtained by Pernal in [96] at zero temperature and in [54] in the positive temperature 1RDMFT case, i.e. considering also the fermionic and bosonic symmetry constraints. In [96], the result follows by a direct computation via chain rule, by taking the partial derivatives with respect to the eigenvalues and eigenvectors of a density matrix Γ. On the other hand, [54] uses tools from convex analysis and exploits the regularity of $\mathfrak{F}^\varepsilon$.

Our strategy is based on the Kantorovich formulation of (A.2.1) and follows ideas contained in [29].

Proof of Proposition A.2.1. The proof follows the same ideas of [29]. We adapt it here for the sake of completeness.

Consider $\boldsymbol{\gamma}^n \xrightarrow{n\to\infty} \boldsymbol{\gamma}$ and pick any sequence of Kantorovich potentials $\boldsymbol{U}^{\varepsilon,n}$ for $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma}^n)$. By optimality, they must be a fixed point for τ and hence, thanks to Proposition A.3.3, $\mathrm{Ren}(\boldsymbol{U}^{\varepsilon,n})$ is uniformly bounded. Note that $\mathrm{Ren}(\boldsymbol{U}^{\varepsilon,n})$ are also maximizers for $\mathfrak{D}^\varepsilon(\boldsymbol{\gamma}^n)$. This implies that any limit point of $\mathrm{Ren}(\boldsymbol{U}^{\varepsilon,n})$ must be a maximizer for $\mathfrak{D}^\varepsilon(\boldsymbol{\gamma})$. The continuity of $\mathfrak{F}^\varepsilon(\cdot)$ directly follows from this stability property.

Let us prove the differentiability. Fix $\sigma \in \mathcal{S}^{d_i}$, with $\mathrm{Tr}(\sigma) = 0$, and denote by $\boldsymbol{\gamma}^h$ the pertubation of $\boldsymbol{\gamma}$ with $+h\sigma$ in the ith entry. Denote by $\boldsymbol{U}^\varepsilon$ any Kantorovich potential for $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma})$. From duality (Theorem A.2.1) we can estimate

$$\frac{1}{h}\left(\mathfrak{F}^\varepsilon(\boldsymbol{\gamma}^h) - \mathfrak{F}^\varepsilon(\boldsymbol{\gamma})\right) \geq \frac{1}{h}\left(\sum_{i=1}^N \mathrm{Tr}\left(\boldsymbol{U}_i^\varepsilon \gamma_i^h - \boldsymbol{U}_i^\varepsilon \gamma_i\right)\right) = \mathrm{Tr}(\boldsymbol{U}_i^\varepsilon \sigma) \tag{A.4.9}$$

for every $h \in \mathbb{R}$. Reversely, denote by $\boldsymbol{U}^{\varepsilon,h}$ any sequence of Kantorovich potentials for $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma}^h)$. Then for every $h > 0$ we obtain

$$\frac{1}{h}\left(\mathfrak{F}^\varepsilon(\boldsymbol{\gamma}^h) - \mathfrak{F}^\varepsilon(\boldsymbol{\gamma})\right) \leq \frac{1}{h}\left(\sum_{i=1}^N \mathrm{Tr}\left(\boldsymbol{U}_i^{\varepsilon,h} \gamma_i^h - \boldsymbol{U}_i^{\varepsilon,h} \gamma_i\right)\right) = \mathrm{Tr}\Big(\boldsymbol{U}_i^{\varepsilon,h} \sigma\Big). \tag{A.4.10}$$

From the first part of the proof, we know that any limit point of $\mathrm{Ren}(\boldsymbol{U}_i^{\varepsilon,h})$ is a Kantorovich potential, which up to translation (Lemma A.4.1) must coincide with $\boldsymbol{U}_i^\varepsilon$. Therefore, passing to the limit in (A.4.9) and (A.4.10), we obtain (A.2.4). □

A.5 Non-Commutative Sinkhorn Algorithm

In this section we introduce and prove convergences guarantees (Theorem A.2.2) of the non-commutative version of the Sinkhorn algorithm, allowing us to compute numerically the minimiser (A.2.3) of the non-commutative multi-marginal optimal transport problem (A.4.1).

The idea of the Sinkhorn algorithm is to fix the shape of an ansatz

$$\Gamma^{(k)} = \exp\left(\frac{\bigoplus_{i=1}^N U_i^{(k)} - \mathrm{H}}{\varepsilon}\right),$$

since it is the actual shape of the minimizer in (A.2.3), and alternately project the Kantorovich potentials $U_i^{(k)}$ via the $(\mathrm{H}, \varepsilon)$-transforms (Definition A.3.5) to approximately reach the constraints $\Gamma^{(k)} \mapsto (\gamma_1, \dots, \gamma_N)$. Recall that for $i \in [N]$, the one-step operators $\mathcal{T}_i^\varepsilon : \times_{i=1}^N \mathcal{S}^{d_j} \to \times_{i=1}^N \mathcal{S}^{d_j}$ are given by

$$\boldsymbol{U} := (U_1, \dots, U_N), \quad \Big(\mathcal{T}_i^\varepsilon(\boldsymbol{U})\Big)_j = \begin{cases} U_j & \text{if } j \neq i, \\ \mathfrak{T}_i^\varepsilon(U_1, \dots, U_{i-1}, U_{i+1}, \dots U_N) & \text{if } j = i \end{cases}$$

where $\mathfrak{T}_i^\varepsilon$ can be implicitly defined (Lemma A.3.3) solving the equation

$$\mathrm{P}_i\left[\exp\left(\frac{\bigoplus_{i=1}^N \left(\mathcal{T}_i^\varepsilon(\boldsymbol{U})\right)_j - \mathrm{H}}{\varepsilon}\right)\right] = \gamma. \tag{A.5.1}$$

Connection with the multi-marginal Sinkhorn algorithm: let us shortly describe what is the corresponding picture in the commutative setting [28],[29]. For every $i \in [N]$, let X_i be Polish Spaces, $\rho_i \mathfrak{m}_i \in \mathcal{P}(X_i)$ be probability measures with reference measures $\mathfrak{m}_i$. The Hamiltonian H corresponds to a bounded cost function $c : X_1 \times \cdots \times X_N \to \mathbb{R}$.

The Sinkhorn iterates define recursively the sequences $(a_j^n)_{n\in\mathbb{N}}, j \in [N]$ by

$$\begin{aligned} a_j^0(x_j) &= \rho_j(x_j), \quad j \in \{2, \dots, N\}, \\ a_j^n(x_j) &= \frac{\rho_j(x_j)}{\int \otimes_{i<j}^N a_i^n(x_i) \otimes_{i>j}^N a_i^{n-1}(x_i) e^{-c(x_1,\dots,x_N)/\varepsilon} d(\otimes_{i\neq j}^N \mathfrak{m}_i)}, \ \forall n \in \mathbb{N} \text{ and } j \in [N]. \end{aligned} \tag{A.5.2}$$

Via the new variables $u_j^n = \varepsilon \ln\left(a_j^n\right)$, $j \in [N]$, one can rewrite the Sinkhorn sequences (A.5.2) as

$$\begin{aligned} u_j^n(x_j) &= -\varepsilon \log\left(\int_{\Pi_{i\neq j} X_i} \exp\left(\frac{\sum_{i\neq j} u_i^n(x_i) - c(x_1, \dots, x_N)}{\varepsilon}\right) d\left(\otimes_{i\neq j}^N \mathfrak{m}_i\right)\right) + \varepsilon \log(\rho_j) \\ &= (\hat{u_j^n})^{(N,c,\varepsilon)}(x_j). \end{aligned}$$

Or, more generally, for every $j \in [N]$, $u_j^n(x_j)$ corresponds to the solution of the maximisation

$$\underset{u_i \in L^\infty(X_i)}{\operatorname{argmax}} \left\{ \sum_{i=1}^N \int_{X_j} u_i \rho_j d\mathfrak{m}_j - \varepsilon \int_{\Pi_{i\neq j}^N X_i} \exp\left(\frac{\sum_{i\neq j} u_i^n + u - c}{\varepsilon}\right) d\left(\otimes_{i\neq j}^N \mathfrak{m}_i\right) \right\} + \varepsilon \log(\rho_j)$$

which corresponds to the commutative counterpart of the i-th vectorial $(\mathrm{H}, \varepsilon)$-transform in Definition A.3.5.

A.5.1 Definition of the algorithm

The non-commutative Sinkhorn algorithm is then defined iterating the $(\mathrm{H}, \varepsilon)$-transforms as in (A.5.1) for every $i \in [N]$. Note that, by construction, the matrix $\exp\left(\bigoplus_{i=1}^N \left((\mathcal{T}_i^\varepsilon(\boldsymbol{U}))_j - \mathrm{H}\right)/\varepsilon\right) \in \mathfrak{P}^{\boldsymbol{d}}$ and its i-th marginal coincide with γ_i. We define the one-step Sinkhorn map as

$$\begin{aligned} \tau : \bigtimes_{j=1}^N \mathcal{S}^{d_j} &\to \bigtimes_{j=1}^N \mathcal{S}^{d_j}, \\ \tau(\boldsymbol{U}) &:= (\mathcal{T}_N^\varepsilon \circ \cdots \circ \mathcal{T}_1^\varepsilon)(\boldsymbol{U}). \end{aligned}$$

Note that this is the non-commutative counterpart of the iteration defined in (A.5.2). The Sinkhorn algorithm is obtained iterating the map τ in the following way.

Step 0. We fix $\boldsymbol{U}^{(0)} \in \times_{i=1}^N \mathcal{S}^{d_i}$ an initial vector of potentials and define the density matrix

$$\Gamma^{(0)} := \exp\left(\frac{\bigoplus_{i=1}^N \boldsymbol{U}_i^{(0)} - \mathrm{H}}{\varepsilon}\right) \in \mathfrak{P}^{\boldsymbol{d}}.$$

Step k. For every $k \in \mathbb{N}$, we define the k-th density matrix via the formula

$$\Gamma^{(k)} := \exp\left(\frac{\bigoplus_{i=1}^N \tau^k(\boldsymbol{U}^{(0)})_i - \mathrm{H}}{\varepsilon}\right) \in \mathfrak{P}^{\boldsymbol{d}}, \tag{A.5.3}$$

where we write $\tau^k := \tau \circ \cdots \circ \tau$ the composition of τ for k-times.

Our goal is to prove the convergence $\Gamma^{(k)} \to \Gamma^\varepsilon$ where Γ^ε is optimal for $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma})$. To do so, our plan is to obtain compactness at the level of the corresponding dual potentials. Nonetheless, the vectors $\tau^k(\boldsymbol{U}^{(0)})$ do not enjoy good a priori estimates and a renormalisation procedure is needed. For any given sequence $(\boldsymbol{\alpha}^k)_{k\in\mathbb{N}} \subset \mathbb{R}^N$ such that $\sum_{i=1}^N \boldsymbol{\alpha}_i^k = 0$, we define

$$\boldsymbol{U}^{(k)} := \tau^k(\boldsymbol{U}^{(0)}) + \boldsymbol{\alpha}^k, \quad k \in \mathbb{N}, \tag{A.5.4}$$

and observe that, by the properties of $\bigoplus$, the correspond density matrix does not change, thus

$$\Gamma^{(k)} = \exp\left(\frac{\bigoplus_{i=1}^N \boldsymbol{U}_i^{(k)} - \mathrm{H}}{\varepsilon}\right) \in \mathfrak{P}^{\boldsymbol{d}}, \quad \forall k \in \mathbb{N}. \tag{A.5.5}$$

Thanks to the good property of the renormalisation map and the Sinkhorn operator, we claim we can find a sequence $\boldsymbol{\alpha}^k$ such that the corresponding potentials $\boldsymbol{U}^{(k)}$ as defined in (A.5.4) do enjoy good a priori estimates and they can be used to prove the convergence of the algorithm, as we see in the next section.

A.5.2 Convergence guarantees: proof of Theorem A.2.2

We are ready to prove our main result Theorem A.2.2, which follows from the next Proposition.

Proposition A.5.1 (Convergence of non-commutative Sinkhorn algorithm)**.** *Fix* $N \in \mathbb{N}$ *and* $\varepsilon > 0$. *For all* $i \in [N]$, *let* $\gamma_i \in \mathfrak{P}^{d_i}$ *be density matrices,* $\mathrm{H} \in \mathcal{S}^{\boldsymbol{d}}$, *with* $\ker \gamma_i = \{0\}$. *For any initial potential* $\boldsymbol{U}^{(0)} \in \bigtimes_{i=1}^N \mathcal{S}^d$, *we consider the sequence* $\Gamma^{(k)} \in \mathfrak{P}^{\boldsymbol{d}}$ *as defined in* (A.5.3).

1. *There exist* $\boldsymbol{\alpha}^k \in \mathbb{R}^N$ *with* $\sum_{i=1}^N \alpha_i^k = 0$ *such that*
$$\boldsymbol{U}^{(k)} = \tau^k(\boldsymbol{U}) + \boldsymbol{\alpha}^k \to \boldsymbol{U}^\varepsilon \quad \text{as } k \to +\infty. \tag{A.5.6}$$
2. $\boldsymbol{U}^\varepsilon = (\boldsymbol{U}_1^\varepsilon, \ldots, \boldsymbol{U}_N^\varepsilon)$ *is optimal for the dual problem* $\mathfrak{D}^\varepsilon(\gamma)$, *as defined in* (A.4.3).
3. $\Gamma^{(k)}$ *converges as* $k \to \infty$ *to some* $\Gamma^\varepsilon \in \mathfrak{P}^{\boldsymbol{d}}$ *which is optimal for the primal problem* $\mathfrak{F}^\varepsilon(\boldsymbol{\gamma})$, *as defined in* (A.4.2). *In particular, it holds*
$$\Gamma^\varepsilon = \exp\left(\frac{\bigoplus_{i=1}^N \boldsymbol{U}_i^\varepsilon - \mathrm{H}}{\varepsilon}\right). \tag{A.5.7}$$

Proof. For any $\boldsymbol{U}^{(0)} \in \bigtimes_{i=1}^N \mathcal{S}^{d_i}$, we define the sequence $\boldsymbol{U}_k := \operatorname{Ren} \tau^k(\boldsymbol{U}^{(0)})$. Note that $\boldsymbol{U}_k$ is of the form (A.5.4), for some $\boldsymbol{\alpha}^k$. Thanks to Proposition A.3.3, we infer that $\boldsymbol{U}_k$ is uniformly bounded and hence compact. Therefore, there exists a subsequence $\boldsymbol{U}_{k_j} \to \boldsymbol{U}^\varepsilon$. We first show that $\boldsymbol{U}^\varepsilon$ is a maximizer for the dual problem. Indeed, using the properties of Ren and τ, it holds

$$\mathrm{D}_\gamma^\varepsilon(\tau(\boldsymbol{U}_{k_j})) = \mathrm{D}_\gamma^\varepsilon(\tau^{k_j+1}(\boldsymbol{U}^{(0)})) \leq \mathrm{D}_\gamma^\varepsilon(\tau^{k_{j+1}}(\boldsymbol{U}^{(0)})) = \mathrm{D}_\gamma^\varepsilon(\boldsymbol{U}_{k_{j+1}}).$$

Passing to the limit the previous inequality, using the continuity of $\mathrm{D}_\gamma^\varepsilon$ and τ and recalling that for any $\boldsymbol{U}$ we have $\mathrm{D}_\gamma^\varepsilon(\tau(\boldsymbol{U})) \geq \mathrm{D}_\gamma^\varepsilon(\boldsymbol{U})$, we obtain

$$\mathrm{D}_\gamma^\varepsilon(\tau(\boldsymbol{U}^\varepsilon)) = \mathrm{D}_\gamma^\varepsilon(\boldsymbol{U}^\varepsilon).$$

By definition, this means that $\boldsymbol{U}^\varepsilon$ is a fixed point for τ and therefore a maximizer (Remark A.4.1).

In order to prove (1), we show there exists a choice $\boldsymbol{\alpha}^k$ such that $\boldsymbol{U}_k + \boldsymbol{\alpha}^k \to \boldsymbol{U}^\varepsilon$. For $k = k_j$ for some j, we pick $\boldsymbol{\alpha}^k = 0$, for all the others k, we instead pick $\boldsymbol{\alpha}^k$ defined by

$$\boldsymbol{\alpha}^k = \operatorname{argmin}_{\boldsymbol{\alpha}} \left\{ \|\boldsymbol{U}_k + \boldsymbol{\alpha} - \boldsymbol{U}^\varepsilon\|_\infty \ : \ \sum_{i=1}^N \boldsymbol{\alpha}_i = 0 \right\}.$$

Note that, by Lemma A.4.1, this is equivalent to picking $\boldsymbol{\alpha}^k$ such that $\boldsymbol{U}^\varepsilon$ is the closest maximizer to $\boldsymbol{U}_k + \boldsymbol{\alpha}^k$. We claim this is the right choice. Suppose indeed by contradiction that there exists a subsequence $\boldsymbol{U}_{k'_j}$ such that $\|\boldsymbol{U}_{k'_j} + \boldsymbol{\alpha}_{k_j} - \boldsymbol{U}^\varepsilon\|_\infty \geq \delta > 0$, then by construction $\|\boldsymbol{U}_{k'_j} + \boldsymbol{\alpha}_{k_j} - \boldsymbol{U}'\|_\infty \geq \delta$ for any other maximizer $\boldsymbol{U}'$. By compactness, this is a contradiction, since there exists a further subsequence $\boldsymbol{U}_{k''_j}$ of $\boldsymbol{U}_{k'_j}$ converging to a maximizer $\boldsymbol{U}'$ (by the same reasoning carried out above). This proves (1) and by optimality of $\boldsymbol{U}^\varepsilon$, (2) as well. The convergence of $\Gamma^{(k)}$ follows from the compactness of $\boldsymbol{U}^{(k)}$ and (A.5.5), whereas the optimality of the limit point Γ^ε and (A.5.7) are consequence of the optimality of $\boldsymbol{U}^\varepsilon$ and Remark A.4.1. □

A.6 One-body Reduced Density Matrix Functional Theory

In this last section, we prove Proposition A.2.2 and consequently Theorem A.2.3.

For given $d, N \in \mathbb{N}$, we set $\boldsymbol{d} = d^N$ and consider the space of bosonic (resp. fermionic) density matrices $\mathfrak{P}^d_+$ (resp. $\mathfrak{P}^d_-$) as introduced in (A.2.9). Recall as well that for any given operator $A \in \mathcal{S}^{\boldsymbol{d}}$, we denote by $A_\pm$ the corresponding projection onto the symmetric space, obtained as $A_\pm := \Pi_\pm \circ A \circ \Pi_\pm$, where $\Pi_\pm$ are defined in (A.2.8).

The universal functional in the bosonic and in the fermionic case is then given as in Definition A.2.1, which we recall here for simplicity is given by

$$\mathfrak{F}^\varepsilon_\pm(\gamma) := \inf \left\{ \operatorname{Tr}(\mathrm{H}\,\Gamma) + \varepsilon \operatorname{Tr}(\Gamma \log \Gamma) \ : \ \Gamma \in \mathfrak{P}^{\boldsymbol{d}}_\pm \text{ and } \Gamma \mapsto \gamma \right\},$$

whereas the corresponding dual functional and problem (see Definition A.2.2) are given by

$$\mathsf{D}^{\pm,\varepsilon}_\gamma(U) := \operatorname{Tr}(U\gamma) - \varepsilon \operatorname{Tr}\left(\exp\left[\frac{1}{\varepsilon} \left(\frac{1}{N} \bigotimes_{i=1}^N U - \mathrm{H} \right)_\pm \right] \right) + \varepsilon\,,$$
$$\mathfrak{D}^\varepsilon_\pm(\gamma) := \sup \left\{ \mathsf{D}^{\pm,\varepsilon}_\gamma(U) \ : \ U \in \mathcal{S}^d \right\}.$$

We are interested in fully characterizing the existence of the optimizers in the primal and the dual problems, for both bosonic and fermionic cases. Proceeding in a similar way as in the proof of Lemma A.3.2, one can prove that every maximizer $U^\varepsilon_\pm$ of the dual functional $\mathsf{D}^{\pm,\varepsilon}_\gamma(\cdot)$ must satisfy the corresponding Euler-Lagrange equation given by

$$\gamma = \mathrm{P}_1 \left(\exp\left[\frac{1}{\varepsilon} \left(\frac{1}{N} \bigoplus_{i=1}^N U^\varepsilon_\pm - \mathrm{H} \right)_\pm \right] \right). \tag{A.6.1}$$

A.6.1 Fermionic dual problem and Pauli's exclusion principle

The aim of this section is to prove Proposition A.2.2. For simplicity we assume, with no loss of generality, that $\varepsilon = 1$ and set $\mathrm{D}_\gamma^- := \mathrm{D}_\gamma^{-,1}$.

For any $U \in \mathcal{S}^d$, we fix a basis of normalized eigenvectors of U, denoted by $\{\psi_j\}_j$, and consider the decomposition

$$U = \sum_{j=1}^{d} u_j |\psi_j\rangle\langle\psi_j|, \quad u_j \in \mathbb{R} \quad \text{(eigenvalues)}\,. \tag{A.6.2}$$

We also denote by $\gamma_j := \langle\psi_j|\gamma|\psi_j\rangle$. In particular, the linear terms read

$$\mathrm{Tr}(U\gamma) = \sum_{j=1}^{d} \gamma_j u_j\,.$$

For any such basis $\{\psi_i\}_i$, we obtain a basis of the fermionic tensor product

$$\psi_{\boldsymbol{j}}^{as} := \bigwedge_{i=1}^{N} \psi_{j_i}\,, \quad \boldsymbol{j} = (j_i)_{i=1}^N \in \Theta_-\,,$$
$$\Theta_- := \Big\{(j_1, \dots, j_N) \;:\; j_i \in \{1, \dots, d\},\ j_i \neq j_k, \text{ if } i \neq k\Big\}/\S_N\,,$$

where $\S_N$ denotes the set of permutations of N elements. With respect to this basis, we can write

$$\frac{1}{N}\left(\bigoplus_{i=1}^{N} U\right)_- = \sum_{\boldsymbol{j}\in\Theta_-}\left(\frac{1}{N}\sum_{i=1}^{N} u_{j_i}\right)|\psi_{\boldsymbol{j}}^{as}\rangle\langle\psi_{\boldsymbol{j}}^{as}|\,. \tag{A.6.3}$$

Using the monotonicity of the exponential and the trace, we obtain the following result.

Lemma A.6.1 (Bounds for $\mathrm{D}_\gamma^-(U)$)**.** *Fix $U \in \mathcal{S}^d$ with eigenvalues u_j and eigenvectors $\{\psi_j\}_j$. For $\gamma \in \mathfrak{P}(d)$, set $\gamma_j := \langle\psi_j|\gamma|\psi_j\rangle$. Then one has*

$$\begin{aligned} \sum_{j=1}^{d}\gamma_j u_j - C\sum_{\boldsymbol{j}\in\Theta_-}\exp\left(\frac{1}{N}\sum_{i=1}^{N} u_{j_i}\right) &\leq D_\gamma^-(U) - 1 \\ &\leq \sum_{j=1}^{d}\gamma_j u_j - \frac{1}{C}\sum_{\boldsymbol{j}\in\Theta_-}\exp\left(\frac{1}{N}\sum_{i=1}^{N} u_{j_i}\right), \end{aligned} \tag{A.6.4}$$

where $C = \exp\Big(\|\,\mathrm{H}\,\|_\infty\Big) \in (0, +\infty)$.

Before moving to the proof of Proposition A.2.2, we need the following technical lemma.

Lemma A.6.2 (Linear term estimates)**.** *Consider $\{u_j\}_{j=1}^d \subset \mathbb{R}$ and $\{\gamma_j\}_{j=1}^d$ such that*

$$\gamma_j \in \left(\delta, \frac{1}{N} - \delta\right), \quad \sum_{j=1}^{d}\gamma_j = 1\,, \tag{A.6.5}$$

for some $\delta \in \left[0, \frac{1}{2N}\right)$. Suppose that $u_j \leq u_k$ if $j \leq k$. Then we have

$$\sum_{j=1}^{d}\gamma_j u_j \leq \frac{1}{N}\sum_{i=1}^{N} u_j - \delta(u_1 - u_d)\,. \tag{A.6.6}$$

Proof. Thanks to the fact the u_j are ordered, we have the inequality

$$\sum_{j=1}^{d} \bar{\gamma}_j u_j \le \frac{1}{N} \sum_{i=1}^{N} u_j, \quad \forall\, 0 \le \bar{\gamma}_j \le \frac{1}{N}, \quad \sum_{j=1}^{d} \bar{\gamma}_j = 1\,.$$

Then (A.6.6) follows applying the above inequality to

$$\bar{\gamma}_1 := \gamma_1 + \delta \in \Big(0, \frac{1}{N}\Big), \quad \bar{\gamma}_j := \gamma_j, \quad \bar{\gamma}_d := \gamma_d - \delta \in \Big(0, \frac{1}{N}\Big),$$

for every $j \in \{2, \dots, d-1\}$. □

We are ready to prove Proposition A.2.2.

Proof. ($\gamma \le 1/N \Rightarrow \sup \mathsf{D}^-_\gamma < \infty$). This is consequence of Proposition A.6.2 with $\delta = 0$. More precisely, pick $U \in \mathcal{S}^d$ and consider a decomposition in eigenfunctions as in (A.6.2). Assume that $\{u_j\}_j$ are non increasing in j (with no loss of generality). We can then apply Proposition A.6.2 with $\delta = 0$ and from (A.6.6) and (A.6.4) we deduce

$$\mathsf{D}^-_\gamma(U) - 1 \le \frac{1}{N} \sum_{i=1}^{N} u_j - \frac{1}{C} \sum_{j \in \Theta_-} \exp\left(\frac{1}{N} \sum_{i=1}^{N} u_{j_i}\right) \le \frac{1}{N} \sum_{i=1}^{N} u_j - \frac{1}{C} \exp\left(\frac{1}{N} \sum_{i=1}^{N} u_j\right),$$

where in the last inequality we used the positivity of the exponential. Therefore

$$\sup_{U \in \mathcal{S}^d} \mathsf{D}^-_\gamma(U) \le \sup_{x \in \mathbb{R}} (x - \frac{1}{C} e^x) + 1 = \log C < \infty\,.$$

($\sup \mathsf{D}^-_\gamma < \infty \Rightarrow \gamma \le 1/N$). Suppose by contradiction that the Pauli's principle is not satisfied. With no loss of generality, we can assume that

$$\gamma = \sum_{i=1}^{d} \gamma_i |\psi_i\rangle\langle\psi_i|, \quad \gamma_1 > \frac{1}{N}\,.$$

We build the sequence of bounded operators $U^n \in \mathcal{S}^d$ given by

$$U^n := \sum_{i=1}^{d} u_i^n |\psi_i\rangle\langle\psi_i|, \quad u_1^n := n\,, \quad u_j^n := -\frac{n}{N-1}, \quad \forall j \ge 2\,. \tag{A.6.7}$$

Observe that by construction, we can estimate the non-linear part of $\mathsf{D}^-_\gamma(U)$ as

$$\forall \boldsymbol{j} \in \Theta_-, \quad \exp\left(\frac{1}{N} \sum_{i=1}^{N} u_{j_i}\right) \begin{cases} = 1 & \text{if } j_i = 1 \text{ for some } i\,, \\ \le 1 & \text{otherwise}\,. \end{cases}$$

It follows that we can bound from below $\mathsf{D}^-_\gamma(U^n)$ as

$$\mathsf{D}^-_\gamma(U^n) \ge \sum_{j=1}^{d} \gamma_j u_j^n - C\binom{d}{N}\,. \tag{A.6.8}$$

We claim that the linear contribution goes to $+\infty$ as $n \to +\infty$. To see that, note that

$$\sum_{j=1}^{d} \gamma_j u_j^n = n\Big(\gamma_1 - \frac{1}{N-1}\sum_{i=2}^{d}\gamma_2\Big) = \frac{n}{N-1}\Big(N\gamma_1 - 1\Big), \tag{A.6.9}$$

where we used that $\sum_i \gamma_i = 1$. From this, using $\gamma_1 > \frac{1}{N}$ and (A.6.8) we deduce $\mathsf{D}_\gamma^-(U^n) \to +\infty$ as $n \to +\infty$, thus a contradiction.

(*Equation for the maximizer and uniqueness*). If a maximizer exists, then it solves the equation (A.6.1). Thanks to the Peierls inequality, we also know that D_γ^- is strictly concave (because the exponential is strictly convex), hence the uniqueness of the maximizer.

(*Existence of* $\operatorname{argmax}\mathsf{D}_\gamma^- \Rightarrow 0 < \gamma < 1/N$). We proceed as in the latter proof. By contradiction, assume that

$$\gamma = \sum_{j=1}^{d} \gamma_j |\psi_j\rangle\langle\psi_j|, \quad \gamma_1 = \frac{1}{N}, \quad \gamma_j \in \Big(0, \frac{1}{N}\Big), \quad \forall j \geq 2\,.$$

The case $\gamma_j = 0$ can be directly ruled out from the Euler-Lagrange equation for a maximizer (A.6.1). We can then consider the very same sequence U^n as defined in (A.6.7). From (A.6.8), (A.6.9), and the first part of Theorem A.2.2, on one hand we deduce

$$-C\binom{d}{N} \leq \mathsf{D}_\gamma^-(U^n) \leq \log C\,, \quad \forall n \in \mathbb{N}\,.$$

On the other hand, $\|U^n\|_\infty \to +\infty$ as $n \to \infty$, which means that D_γ^- is not coercive. Thanks to Peierls inequality, we also know that D_γ^- is strictly concave, which implies that D_γ^- can not attain its maximum.

($0 < \gamma < 1/N \Rightarrow$ *existence of* $\operatorname{argmax}\mathsf{D}_\gamma^-$). Let $U \in \mathcal{S}^d$ and consider a decomposition in eigenfunctions as in (A.6.2). Assume that $\{u_j\}_j$ are non increasing in j (with no loss of generality) and denote by $\gamma_j := \langle\psi_j|\gamma|\psi_j\rangle$. By assumption, there exists $\delta \in \Big(0, \frac{1}{N}\Big)$ such that

$$\sum_{j=1}^{d} \gamma_j = 1, \quad \gamma_j \in \Big(\delta, \frac{1}{N} - \delta\Big), \quad \forall j \in \{1, \ldots, d\}\,. \tag{A.6.10}$$

We can then apply Proposition A.6.2 and (A.6.4) to obtain

$$\mathsf{D}_\gamma^-(U) - 1 \leq \frac{1}{N}\sum_{i=1}^{N} u_j - \frac{1}{C}\sum_{j\in\Theta_-}\exp\left(\frac{1}{N}\sum_{i=1}^{N} u_{j_i}\right) - \delta(u_1 - u_d) \tag{A.6.11}$$

$$\leq \frac{1}{N}\sum_{i=1}^{N} u_j - \frac{1}{C}\exp\left(\frac{1}{N}\sum_{i=1}^{N} u_j\right) - \delta(u_1 - u_d), \tag{A.6.12}$$

where we used the positivity of the exponential. Set $S := \sup_x(x - \frac{e^x}{C}) + 1 < \infty$, and infer

$$\mathsf{D}_\gamma^-(U) \leq S - \delta(u_{max} - u_{min}), \quad \forall U \in \mathcal{S}^d, \quad U = \sum_{j=1}^{d} u_j |\psi_j\rangle\langle\psi_j|\,, \tag{A.6.13}$$

where u_{max} and u_{min} denotes respectively the maximum/minimum eigenvalue of U. Let us use this estimate to prove to existence of a maximizer for D_γ^-. Consider a maximizing sequence U^n of bounded operators. In particular, we can assume that $-I := \inf_n \mathsf{D}_\gamma^-(U^n) \geq -\infty$. If the sequence $\{U^n\}_n$ is bounded in $\mathcal{S}^d$, then any limit point is a maximum for D_γ^-, by concavity and continuity of D_γ^-, and the proof is complete. Suppose by contradiction that $\|U^n\|_\infty \to +\infty$ as $n \to +\infty$. Note that from (A.6.13) we deduce

$$\sup_{n\in\mathbb{N}} \left(u^n_{max} - u^n_{min}\right) \leq \frac{S+I}{\delta} < \infty \,, \tag{A.6.14}$$

therefore we deduce that either $u^n_j \to -\infty$ or $u^n_j \to +\infty$ for every $j \in \{1, \dots, d\}$. In the first case, we would have a contradiction, because

$$-I \leq \mathsf{D}_\gamma^-(U^n) \leq \sum_{j=1}^d \gamma_j u^n_j + 1 \to -\infty \quad \text{as } n \to +\infty \,.$$

In the second case, we can use (A.6.11) to find a contradiction, because

$$-I \leq \mathsf{D}_\gamma^-(U^n) \leq \frac{1}{N}\sum_{i=1}^N u^n_j - \frac{1}{C}\exp\left(\frac{1}{N}\sum_{i=1}^N u^n_j\right) + 1 \to -\infty \,,$$

where we used that $\lim_{x\to+\infty}(x - C^{-1}e^x) = -\infty$. The proof is complete. □

A.6.2 Duality theorem for fermionic and bosonic systems

In this section we prove Theorem A.2.3. The proof relies on the use of Theorem A.2.1 and the existence of maximizers for $\mathsf{D}_\gamma^{-,\varepsilon}$, proved in Proposition A.2.2, and $\mathsf{D}_\gamma^{+,\varepsilon}$. The latter can be proven easily by noting that the spectrum of $\left(\bigoplus_{j=1}^N U_j\right)_+$ contains the spectrum of U and, applying similar computations to the ones used in the case of $\mathsf{D}_\gamma^{-,\varepsilon}$, deducing the coercivity of $\mathsf{D}_\gamma^{+,\varepsilon}$. We also need the following observation.

Remark A.6.1. *If* H *satisfies* (A.2.10) *and* $\boldsymbol{\gamma} = (\gamma_i)_i$, $\gamma_i = \gamma$, *then the minimizers of* $\mathrm{D}^\varepsilon_{\boldsymbol{\gamma}}$ *(the dual functional without symmetry constraints) can be taken to satisfy* $U_i \equiv U$, *for some* $U \in \mathcal{S}^d$. *In particular*

$$\mathfrak{D}^\varepsilon(\boldsymbol{\gamma}) = \sup_{\boldsymbol{U}\in(\mathcal{S}^{\boldsymbol{d}})^N} \mathrm{D}^\varepsilon_{\boldsymbol{\gamma}}(\boldsymbol{U}) = \sup_{U\in\mathcal{S}^d}\left\{\mathrm{Tr}(U\gamma) - \varepsilon\,\mathrm{Tr}\left(\exp\left[\frac{1}{\varepsilon}\left(\frac{1}{N}\bigotimes_{i=1}^N U - \mathrm{H}\right)\right]\right)\right\} + \varepsilon \,.$$

This follows from the observation that if $\boldsymbol{U} \in (\mathcal{S}^{\boldsymbol{d}})^N$, *then we obtain a symmetric competitor* $\tilde{\boldsymbol{U}}$

$$(\tilde{\boldsymbol{U}})_i = \frac{1}{N}\sum_{j=1}^N U_j \,, \quad \textit{such that} \quad \mathrm{D}^\varepsilon_{\boldsymbol{\gamma}}(\tilde{\boldsymbol{U}}) = \mathrm{D}^\varepsilon_{\boldsymbol{\gamma}}(\boldsymbol{U}) \,.$$

Proof of Theorem A.2.3. Let us assume that $\gamma > 0$ in the bosonic case ($0 < \gamma < \frac{1}{N}$ in the fermionic case). The general duality result (including the case γ in which does not satisfy the above strict inequalities) can be handled by decomposition of the space, in the same way as in Remark A.3.3.

Under these assumptions, thanks to Proposition A.2.2, we know that a maximizer $U^\varepsilon_\pm$ exists and satisfies (A.6.1).

We then define the N-particle density matrix

$$\tilde{\Gamma}^{\varepsilon}_{\pm} := \exp\left[\frac{1}{\varepsilon}\left(\frac{1}{N}\bigoplus_{i=1}^{N} U^{\varepsilon}_{\pm} - \mathrm{H}\right)_{\pm}\right] \in \mathcal{S}^{\boldsymbol{d}},$$

and thanks to Remark A.4.1, we know that $\tilde{\Gamma}^{\varepsilon}_{\pm}$ is optimal for the problem $\mathfrak{F}^{\varepsilon}\Big(\mathrm{P}_1(\tilde{\Gamma}^{\varepsilon}_{\pm})\Big)$ without symmetry contraints. Observing that $(\tilde{\Gamma}^{\varepsilon}_{\pm})_{\pm} = \Gamma^{\varepsilon}_{\pm}$ (defined in (A.2.15),(A.2.16)), we deduce that $\Gamma^{\varepsilon}_{\pm}$ must be optimal for the primal problem $\mathfrak{F}^{\varepsilon}_{\pm}(\gamma)$ with symmetry constraints. This also proves the equality between primal and dual problems and concludes the proof. □