Polarons in Bose gases and polar crystals

Some rigorous energy estimates

by

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Abstract

The polaron model is a basic model of quantum field theory describing a single particle interacting with a bosonic field. It arises in many physical contexts. We are mostly concerned with models applicable in the context of an impurity atom in a Bose-Einstein condensate as well as the problem of electrons moving in polar crystals.

The model has a simple structure in which the interaction of the particle with the field is given by a term linear in the field's creation and annihilation operators. In this work, we investigate the properties of this model by providing rigorous estimates on various energies relevant to the problem. The estimates are obtained, for the most part, by suitable operator techniques which constitute the principal mathematical substance of the thesis.

The first application of these techniques is to derive the polaron model rigorously from first principles, i.e., from a full microscopic quantum-mechanical many-body problem involving an impurity in an otherwise homogeneous system. We accomplish this for the $N + 1$ Bose gas in the mean-field regime by showing that a suitable polaron-type Hamiltonian arises at weak interactions as a low-energy effective theory for this problem.

In the second part, we investigate rigorously the ground state of the model at fixed momentum and for large values of the coupling constant. Qualitatively, the system is expected to display a transition from the quasi-particle behavior at small momenta, where the dispersion relation is parabolic and the particle moves through the medium dragging along a cloud of phonons, to the radiative behavior at larger momenta where the polaron decelerates and emits free phonons. At the same time, in the strong coupling regime, the bosonic field is expected to behave purely classically. Accordingly, the effective mass of the polaron at strong coupling is conjectured to be asymptotically equal to the one obtained from the semiclassical counterpart of the problem, first studied by Landau and Pekar in the 1940s. For polaron models with regularized form factors and phonon dispersion relations of superfluid type, i.e., bounded below by a linear function of the wavenumbers for all phonon momenta as in the interacting Bose gas, we prove that for a large window of momenta below the radiation threshold, the energy-momentum relation at strong coupling is indeed essentially a parabola with semi-latus rectum equal to the Landau–Pekar effective mass, as expected.

For the Fröhlich polaron describing electrons in polar crystals where the dispersion relation is of the optical type and the form factor is formally UV–singular due to the nature of the point charge-dipole interaction, we are able to give the corresponding upper bound. In contrast to the regular case, this requires the inclusion of the quantum fluctuations of the phonon field, which makes the problem considerably more difficult.

The results are supplemented by studies on the absolute ground-state energy at strong coupling, a proof of the divergence of the effective mass with the coupling constant for a wide class of polaron models, as well as the discussion of the apparent UV singularity of the Fröhlich model and the application of the techniques used for its removal for the energy estimates.

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I would like to thank my supervisor Robert Seiringer for his invaluable guidance, his help concerning the reconciliation of work and personal life, and his opennes to offer a research project to somebody without the canonical background typically required in the field.

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I would like to dedicate this work - not necessarily the present work, being just a document, but all the sweat and doubts of the last four years - to my family: my wife, sons, mother, and parents-in-law, as well as the memory of my father.

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About the Author

Krzysztof Myśliwy was born and raised in Toruń, northern Poland, and studied at the of University of Warsaw, from which he graduated in 2018 with a M.Sc. in Theoretical Physics obtained within the interdisciplinary MISMaP programme. In 2019, he joined the mathematical physics group of Robert Seiringer at the ISTA in Klosterneuburg, Austria, where he worked on his PhD research project centered on a rigorous analysis of the polaron problem. His scientific interests concern various theoretical aspects of interacting atomic many-body systems, especially with impurities or inhomogeneities.

List of Collaborators and Publications

This thesis contains the following published papers:

- K. Myśliwy and R. Seiringer, *Microscopic derivation of the Fröhlich Hamiltonian for the Bose polaron in the mean-field limit*, Ann. Henri Poincaré **21**, 4003-4025 (2020).
- K. Myśliwy and R. Seiringer, *Polaron models with regular interactions at strong coupling*, J. Stat. Phys. **186**, 5 (2022)

as well as the submitted paper

- D. Mitrouskas, K. Myśliwy and R. Seiringer, *Optimal parabolic upped bound for the energy-momentum relation of a strongly-coupled polaron*, arXiv:2203.02454.

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CHAPTER 1

Introduction

1.1 The polaron

1.1.1 Wider context

An important goal of XXI century physics is to understand the emergent properties, i.e., properties that are not inherent to individual constitutents of a large system, but arise due to mutual interactions between them. For this reason it is important to investigate the interactions between basic constituents of ordinary materials on a very fundamental level, including the methods of mathematical physics.

Interesting effects due to complex interactions arise already when the chemical composition of the system is entirely uniform, but a siginificant degree of complexity is added if one considers inhomogeneous systems. The simplest case corresponds to a single object - an atom, molecule, or even an elementary particle - immersed in a large, excitable medium. The model we shall be considering here, the polaron model, is arguably one of the most basic examples. It concerns the motion of a quantum particle interacting with a large medium modelled by a bosonic field. The basic nature of the model makes it perfectly fit for a rigorous analysis. In fact, it is relatively simple and many aspects of it are tractable with the use of the mathematical methods at hand, while at the same time it is complicated enough to pose several hard problems, the solution of which might both increase our understanding of the underlying physics and lead to new, interesting developments in mathematics.

1.1.2 The Fröhlich Hamiltonian

The Hamiltonian that we are going to analyze has been first introduced by Fröhlich [67]. It has the form

$$\mathbb{H} = \frac{-\Delta_x}{2m} + \int_{\mathbb{R}^3} \epsilon(k) a_k^\dagger a_k dk + \sqrt{\alpha} \int_{\mathbb{R}^d} \left(v(k) a_k e^{ik\cdot x} + \overline{v(k)} a_k^\dagger e^{-ik\cdot x} \right) dk \tag{1.1}$$

and acts on the Hilbert space $L^2(\mathbb{R}^d) \otimes \mathcal{F}$, with

$$\mathcal{F} := \bigoplus_{n=0}^{\infty} \bigotimes_{\text{sym}}^{n} L^2(\mathbb{R}^d) \tag{1.2}$$

denoting the bosonic Fock space, where $\bigotimes_{\text{sym}}^{n} L^2(\mathbb{R}^d)$ is the space of symmetric square intergable functions of n variables. By definition $\bigotimes_{\text{sym}}^{0} L^2(\mathbb{R}^d) = \mathbb{C}$, and this case is referred to as the *vacuum*. Furthermore, $a_k^\dagger, a_k$ are the *bosonic creation and annihilation operators*, actually operator-valued distributions, satisfying the commutation relation

$$[a_k, a_q^\dagger] = \delta(k - q) \tag{1.3}$$

with $\delta(\cdot)$ denoting the delta distribution. At this level, these operators are introduced formally, but their proper definition poses no difficulty once the usual annihilation operators are introduced. For a function $f \in L^2(\mathbb{R}^d)$, we have

$$a(f) : \bigotimes_{\text{sym}}^{n} L^2(\mathbb{R}^d) \to \bigotimes_{\text{sym}}^{n-1} L^2(\mathbb{R}^d), \tag{1.4}$$

$$(a(f)\Psi)(x_1, \cdot, x_{n-1}) = \sqrt{n} \int dx \overline{f(x)} \Psi(x_1, \cdots, x_{n-1}, x). \tag{1.5}$$

It is a simple exercise to compute the adjoint $a^\dagger(f)$

$$(a^\dagger(f)\Psi)(x_1, \cdots, x_n) = \frac{1}{\sqrt{n}} \sum_{i=0}^{n} f(x_i) \Psi(x_1, \cdots, x_{i-1}, x_i, \cdots, x_n) \tag{1.6}$$

and to verify that the *canonical commutation relations* hold true:

$$[a(g), a^\dagger(f)] = \langle g | f \rangle \tag{1.7}$$

where we employed the Dirac bra-ket notation for the inner product in L^2.

(1.1) thus models a quantum particle of mass $m > 0$ and position $x \in \mathbb{R}^d$ interacting with a scalar bosonic field. Its main ingredients are as follows:

- $-\Delta_x$ is the Laplacian in the particle variable, and $\frac{-\Delta_x}{2m}$ describes the particle's kinetic energy;
- $\epsilon(\cdot)$ is the *dispersion relation*, and the term involving this quantity in (1.1) is called the *field energy*;
- the term involving the function $v(\cdot)$ is the interaction term, and $v(\cdot)$ is called the *form factor*;
- $\alpha > 0$ is a coupling constant traditionally appearing in (1.1) under the square root.

It is to be noted that the interaction is linear in the creation and annihilation operators, which is the most distinctive feature of the model. One typically assumes that $\epsilon(k) > 0$ for all $k \in \mathbb{R}^d$ and that $v \in L^2(\mathbb{R}^d)$, in which case (1.1) is well defined on the intersection of the domains of the particle's Laplacian and the field energy, although one physically important model discussed here has $v(k) \sim |k|^{-1}$ in $d = 3$, and the UV divergence in this case constitutes one of the most mathematically involved aspects of this and various preceding works. Let us finally remark that the k modes of the field are called *phonons*, a term well-known from elementary physics.

(1.1) arises in many physical contexts, and our analysis shall be focused on the case of an electron in a polar crystal, hereafter referred to as the *Fröhlich (large) polaron*, and an impurity atom immersed in a cold atomic gas comprising of bosonic atoms, called *the Bose polaron*. Our two principal goals are

1. the derivation of (1.1) as an effective theory from first principles, i.e., from a microscopic quantum-mechanical many-body problem;

2. the analysis of the properties of (1.1) at strong coupling, especially in the context of the energy-momentum relation and the emergence of the polaron quasi-particle, and the verification of the semiclassical approximation in this case.

Let us discuss these points in some detail, including the basic physics background, and present our results.

1.1.3 Derivation of the Fröhlich Hamiltonian as an effective theory

The Fröhlich case: a physics derivation

(1.1) has first appeared in the physics literature in the context of the problem of electronic motion in polar crystals [67, 68]. This corresponds to the choice

$$\epsilon(k) = 1, \quad v(k) = \frac{1}{(2\pi)^3|k|}, \quad d = 3 \quad \text{(Fröhlich case).} \tag{1.8}$$

Of course, $|k|^{-1}$ is not an $L^2(\mathbb{R}^3)$ function, but using the methods recalled in Chapter 4 one can show that if one introduces a cutoff K in the form factor, i.e. sets $v(k) = (2\pi)^{-3}|k|^{-1}$ for $|k| \leq K$ and zero otherwise, then the resulting Hamiltonian is bounded from below uniformly in K, and thus one can define the corresponding Hamiltonian for $K = \infty$ via a suitable quadratic form. For a thorough discussion concerning the definition and domain of the Hamiltonian with the choice (1.8), we refer to [74].

For the sake of this introductory section, we are first interested in physical arguments leading to the Fröhlich model (1.8). The situation is the following: consider an electron moving through a ionic lattice, i.e, a lattice whose sites are occupied by ions. For simplicity, imagine the case of the lattice being simply $\mathbb{Z}^3$, and the situation in which each site is occupied by an ion surrounded by oppositely charged ions occupying the nearest neighbor sites. The ions are not entirely immobile and can perform small oscillations around their equilibrium positions. The moving electron distorts the lattice by attracting the positive ions and repelling the negative ones, which, in turn, leads to the formation of local dipole moments spreading through the lattice in the form of optical phonons. The origin of the Fröhlich model is then best seen once the Hamiltonian is rewritten in position space for the phonons. It reads

$$\mathbb{H} = -\Delta_x + \int_{\mathbb{R}^3} a_y^\dagger a_y \, dy + \sqrt{\alpha} \int_{\mathbb{R}^3} \frac{a_y^\dagger + a_y}{2\pi^2|x-y|^2} dy. \tag{1.9}$$

In order to arrive at (1.9) as a model for the electron-ionic lattice system, one argues as follows:

1. The first thing to note is the choice of units, in which the Planck's constant $\hbar$ and the phonon frequency is set to unity, as well as $m = 1/2$ for the mass of the electron. In fact, this mass is not the *bare* mass of the electron in vacuum, but the *band mass*. The origin of this lies in band theory of solids, for our purposes it is enough to point out that the band mass is an effective way of taking the interaction of the electron with the *immobile* ions into account. The actual value of the band mass depends on the material (i.e., the chemical composition and the geometric structure of the crystal).

2. One essential ingredient here is the continuum approximation, in which the discrete lattice is replaced by a continuous polarizable medium. The physical argument behind this is that when considering this problem, the electron is supposed to be a relatively slow one, thus having a low kinetic energy and consequently a wave function with small gradients, which is then presumably spread over many lattice sites.

3. Related to this is the choice $\epsilon(k) = 1$, corresponding to optical phonons. These are quantized oscillations in which the adjacent ions oscillate out of phase which leads to a dipole moment. Their dispersion relation tends to a positive constant at $k = 0$, is essentially flat for small k and the deviations from a constant dispersion relation reveal themselves for k of the order of the inverse lattice spacing, and can therefore be neglected in the continuum approximation, which justifies the choice $\epsilon(k) = 1$ for all k.

4. The term $\frac{1}{2\pi^2|x-y|^2}$ is the interaction potential of a charge located at x and a dipole located at y. This corresponds to the form factor $v(k) = \frac{1}{(2\pi)^3}\frac{1}{|k|}$ (and the exponential factors e^{ikx}) via Fourier transform.

5. In the units chosen, the coupling constant is

$$\alpha = \frac{1}{2}\left(\frac{1}{\varepsilon(\infty)} - \frac{1}{\varepsilon}\right) \tag{1.10}$$

   where $\varepsilon(\infty)$ is the *high-frequency* dielectric permittivity of the material in question, and ε is its static permittivity. This particular combination arises here due to the fact that the ε contains contributions also from the high-frequency polarization effects happening at the level of the electronic structure of the ions themselves, which are neglected here and thus the number $\varepsilon(\infty)$ describing them needs to be subtracted from the equations. A detailed analysis of the underlying electrodynamics leads to this particular form of α.

For more details, we refer the interested reader to the review [87]. Although the above physical arguments are well-founded and plausible, a rigorous derivation of (1.9) from the underlying microscopic model of an electron in a polar crystal would be a formidable task (note, however, the work [25], in which the Pekar functional, a model related to the Hamiltonian (1.1), is derived from a simplified model of a crystal in the Hartree-Fock setting). Our first contribution in this work is a rigorous derivation of (1.1) from a microscopic model of another instance of the polaron problem, the $N+1$ Bose gas. Its microscopic structure is much simpler, but the $N+1$ Bose gas, or the Bose polaron problem, lies at the forefront of modern cold atomic physics, and hence the problem is of great interest of its own.

The Bose polaron

The Bose polaron problem, that is, the problem of an impurity atom immersed in an interacting Bose gas, has been investigated both theoretically and experimentally in the recent years, and has an extensive physics literature. One of the most prominent models in these investigations is via a suitable Fröhlich Hamitonian [1]. Our goal is to derive this effective model rigorously from first principles, on a simple example. We hence start with a specific model of an impurity in a Bose gas, in which the constituents are confined to a finite-size box modelled by the unit torus in d dimensions, and show how the Fröhlich model arises from it in a natural way.

We thus consider a system of N bosons of mass $1/2$ and one additional particle (of an unspecified type of statistics) of mass M. We assume that the particles confined to move on the unit torus in d dimensions, $\mathbb{T}^d$. Moreover we assume that the bosons interact among themselves via a positive two-body potential $v : \mathbb{T}^d \to \mathbb{R}$ and that the additional impurity particle interacts with the bosons via a positive real-valued two-body potential $w : \mathbb{T}^d \to \mathbb{R}$. The positions of the bosons are labeled by $\{x_i\}_{i=1}^N, x_i \in \mathbb{T}^d$ and the position of the impurity by $R \in \mathbb{T}^d$. The Hamiltonian of this system reads

$$H_{N,1} = \frac{-\triangle_R}{2M} - \sum_{i=1}^N \triangle_{x_i} + \lambda \sum_{1\le i<j\le N} v(\eta(x_i - x_j)) + \mu \sum_{i=1}^N w(\nu(x_i - R)) \tag{1.11}$$

and acts on the Hilbert space $L^2(\mathbb{T}^d) \otimes \left(\otimes_{\mathsf{sym}}^N L^2(\mathbb{T}^d)\right)$. The pairs of real numbers (λ, η) and (μ, ν) are scaling parameters describing the strength and the ranges of the potentials v, w respectively. (1.11) is our starting point as a microscopic many-body theory from which we are going to derive a version of the Fröhlich Hamiltonian (1.1) as an effective *low-energy* theory in an appropriate limiting scaling. In order to introduce the main strategy, it is instructive to view $H_{N,1}$ as an operator on $L^2(\mathbb{T}^d) \otimes \mathcal{F}$ (here, in the definition of $\mathcal{F}$, we simply replace $\mathbb{R}^d$ with $\mathbb{T}^d$ in (1.2)) and express it via the creation and annihilation operators corresponding to the functions $x \to e^{ipx}, p \in (2\pi\mathbb{Z})^d$, forming an orthonormal basis of $L^2(\mathbb{T}^d)$. In this way, we arrive at the *second-quantized version of* (1.11):

$$\begin{aligned} H_{N,1} =& \frac{-\triangle_y}{2M} + E_{\mathrm{H}}(N) + \sum_{p\neq 0} p^2 a_p^\dagger a_p + \sum_{p\neq 0} v_{p/\eta} \sum_{q,k} a_{p+k}^\dagger a_{q-p}^\dagger a_q a_k + \\ &+ \mu \sum_{p\neq 0} w_{p/\nu} e^{-i\nu^{-1}py} \sum_k a_{p+k}^\dagger a_k. \end{aligned} \tag{1.12}$$

Here $w.$ $v.$ are the Fourier coefficients of the potentials w, v, and $E_{\mathrm{H}}(N)$ is the *Hartree energy* $\frac{\lambda}{2}N(N-1)v_0 + N\mu w_0$. Note that in order to arrive at (1.12), translation invariance is crucial (we also assume parity invariance so that the Fourier coefficients are real, and hence even functions of p).

We are interested in a low-energy effective theory of $H_{N,1}$, and predict that it should lead to a version of the Fröhlich Hamiltonian if one follows the appropriately adjusted approach laid down by Bogoliubov [33]. First of all, it is to be expected that for low energies most of the bosons have very low momenta, in fact, that most of the processes that occur at low energy involve bosons having zero momentum. Accordingly, we expect that at low energies, one can replace the operators $a_0, a_0^\dagger$ by *numbers* $\sqrt{N}$. The heuristic reason for this is that most of the bosons are predicted to have momentum zero and thus $a_0^\dagger a_0 \sim N$, and therefore also $a_0 a_0^\dagger = 1 + a_0^\dagger a_0 \sim N$ and $a_0, a_0^\dagger$ are effectively commuting. After this replacement, one retains only terms which are at most *quadratic* in the creation and annihilation operators (which, after the above replacement, depend only on the non-zero momenta). In the boson-impurity interaction, one goes even further and retains only the *linear terms* in the creation and annihilation operators, neglecting all the *scattering terms*. At this stage, we take the simplest choice of (λ, η) and (μ, ν) so as to meet two conditions. First, we wish that the $v-$ dependent term in E^{H} is extensive, i.e., linear in N. Moreover, we want the boson-boson and the impurity-boson interactions beyond E^{H} to lead to an $N-$ independent $O(1)$ contribution to the energy. This leads to the *mean-field scaling* $\lambda = \frac{1}{N-1}, \mu = \frac{1}{\sqrt{N}}$ for the strengths and $\eta = \nu = 1$ for the ranges. This corresponds to the case of weak long-ranged potentials. This is physically expected to be accurate at high boson densities, or for large N in our approach, as the volume of the torus is set to unity in our setting. It has to be noted that since actual gases used in experiments are typically *dilute*, the mean-field scaling serves mainly as a toy model, against which various other approaches are tested. In this sense, it is a bit artificial, but has an important theoretical value. We shall henceforth take this limit in our considerations on the derivation of the Bose polaron model. For a discussion of other scalings, see Chapter 2.

With the mean-field scaling and the Bogoliubov approximation, we arrive at the Hamiltonian

$$\begin{aligned} H^{\mathrm{pre-F}} =& \frac{N}{2}v_0 + \sqrt{N}w_0 + \frac{-\Delta_R}{2M} + \sum_{p\neq 0}\left((p^2+v_p)a_p^\dagger a_p + \frac{v_p}{2}(a_p^\dagger a_{-p}^\dagger + a_p a_{-p})\right) \\ &+ \sum_{p\neq 0} w_p e^{-ipR}(a_p^\dagger + a_{-p}). \end{aligned}$$

Note that this one does not leave the $L^2(\mathbb{T}^d)\otimes\left(\otimes_{\mathsf{sym}}^N L^2(\mathbb{T}^d)\right)$ subspace invariant, in contrast to (1.12). We see that once the aforementioned approximation is made, we arrive at our goal, since $H^{\mathrm{pre-F}} - \frac{N}{2}v_0 - \sqrt{N}w_0$ is unitarily equivalent to the Fröhlich Hamiltonian

$$\mathbb{H}^{\mathrm{F}} = -\frac{\Delta_R}{2M} + \sum_{p\neq 0}\epsilon_p b_p^\dagger b_p + \sum_{p\neq 0}\tilde{w}_p\left(e^{-ipR}b_p^\dagger + e^{ipR}b_p\right) + E^{\mathrm{B}} \tag{1.13}$$

where E^{B} is an explicit constant, the dispersion equals

$$\epsilon_p = \sqrt{p^4 + 2v_p p^2} \tag{1.14}$$

and the form factors turns out to be

$$\tilde{w}_p = \frac{|p|w_p}{\sqrt{e_p}} \tag{1.15}$$

The operators $b_p, b_p^\dagger$ are also bosonic, and given by $b_p^\dagger = \alpha_p a_p^\dagger + \beta_p a_{-p}$ where α_p, β_p are appropriate constants chosen such that $[b_p, b_q^\dagger] = \delta_{p,q}$. Explicitly, $\alpha_p = (1-\gamma_p)^{-1/2}$ with $\gamma_p = 1 + \frac{p^2 - e_p}{v_p}$ and $\beta_p = \gamma_p\alpha_p$. An important thing to note is that

$$\epsilon_p \geq c|p| \tag{1.16}$$

for all p, for some $c > 0$ (since v is positive, $v_0 > 0$). This fact is related to the onset of superfluidity in the interacting Bose gas at low temperatures [33]. Accordingly, a dispersion relation satisfying $\inf_k |k|^{-1}\epsilon(k) > 0$ will be said to be *of superfluid type*, and this will play an important role also below.

Contributions of the author

In Chapter 2 we perform a rigorous derivation of the Fröhlich Hamiltonian (1.13) as an effective low-energy theory of the *excitations* of $H_{N,1}$ in the mean-field limit. More precisely, we compare the low-lying parts of the spectra of $H_{N,1}$ and $E^{\mathrm{H}}(N) + \mathbb{H}^{\mathrm{F}}$ and show that they agree for N large, provided that the eigenvalues lie in an energy window which grows not too fast with N. This is the content of the following Theorem.

Theorem 1.1.1 (M-Seiringer 2020). *Let $H_{N,1}$ and $\mathbb{H}^{\mathrm{F}}$ be defined by Eqs.* (1.12) *and* (1.13)*, respectively, and let $E_{\mathrm{H}}(N) := \frac{N}{2}v_0 + \sqrt{N}w_0$. Assume that v and w are positive and bounded, and that v is positive definite. Then for all eigenvalues $e_i(H_{N,1})$ such that $e_i(H_{N,1}) - e_0(H_{N,1}) \leq \xi$ for some $\xi \geq 1$ we have*

$$|e_i(H_{N,1}) - E_{\mathrm{H}}(N) - e_i(\mathbb{H}^F)| \leq C_{v,w}\xi\left(\frac{\xi}{N}\right)^{1/2} \tag{1.17}$$

for some constant $C_{v,w} > 0$ independent of the parameters ξ and N.

This result on the lower part of the spectrum is supplemented by a statement on the eigenvectors, see Theorem 2 in Chapter 2.

The method of proof uses techniques developed for the justification of the Bogoliubov approximation for interacting Bose gases developed in the mathematical physics literature in the past few years. The main tool are suitable operator inequalities that compare $H_{N,1}-E^{\mathrm{H}}(N)$ with $\mathbb{H}^{\mathrm{F}}$. From these inequalites, one can draw two important conclusions: first, it holds that the difference of the two operators is essentially of the order $N^{-1/2}N_+$, where N_+ is the excitation number operator $N_+ = \sum_{p\neq 0} a_p^\dagger a_p$. The second conclusion is that this operator is uniformly bounded in N on states with sufficiently small energy. This allows us to conclude the desired statement by the min-max principle. Of course, there is a certain number of technical issues that need to be taken into account, most of them stemming from the fact that $H_{N,1}$ and $\mathbb{H}^{\mathrm{F}}$ act on different Hilber spaces and cannot be directly compared. This is handled by a unitary transformation introduced by Nam, Lewin, Serfaty and Solovej in 2016 [28] as well as Fock space localization techniques utilized in [48], whose application turns out to be quite effective in our mean-field case due to the operator inequalities obtained.

1.1.4 The energy-momentum relation at strong-coupling

The next topic is focused on one of the central points of polaron theory. The origin of the term *polaron* lies in the physical picture of a quasi-particle emerging in the system composed of an impurity and a boson field as described by the Fröhlich Hamiltonian. The impurity is imagined to excite and drag along a cloud of phonons as it moves, and this composite structure - the particle plus the cloud of phonons attached to it - is viewed as a separate entity, a quasi-particle termed the polaron. As we shall see, this picture can be translated to the level of equations and theorems. To this end, let us first note that due to translation invariance, the Hamiltonian (1.1) commutes with the total momentum operator

$$P_{\text{tot}} = -i\nabla_x + P_f, \quad P_f = \int dk\ k\ a_k^\dagger a_k. \tag{1.18}$$

It therefore makes sense to consider the infimum of the spectrum of $\mathbb{H}$ as defined in (1.1) on the subspace where the total momentum equals $P \in \mathbb{R}^d$. Thanks to the unitary transformation introduced by Lee, Low and Pines [10], one can introduce another definition of this quanity, which involves explicit objects and is hence much easier to manipulate. The Lee-Low-Pines unitary operator has the form $e^{iP_f x}$ and satisfies

$$e^{iP_f x} a_k^\dagger e^{-iP_f x} = e^{ikx} a_k^\dagger.$$

A computation thus shows that $\mathbb{H}$ unitarily equivalent to $\int^\oplus dP\ \mathbb{H}_P$ with

$$\mathbb{H}_P = \frac{1}{2m}(P-P_f)^2 + \int_{\mathbb{R}^d} \epsilon(k) a_k^\dagger a_k dk + \sqrt{\alpha}\int_{\mathbb{R}^d}\left(v(k)a_k + \overline{v(k)}a_k^\dagger\right) dk.$$

Note that this operator acts on $\mathcal{F}$ only. The energy-momentum relation is then defined as

$$E(P) = \inf \operatorname{spec} \mathbb{H}_P$$

which is the ground-state energy at fixed total momentum P. This quantity shall be our main object of interest.

In order to motivate our further analysis, let us start with the simplest case $\alpha = 0$. Assume for simplicity that the dispersion relation is strictly positive and subadditive, i.e., $\epsilon(k_1 + k_2) \leq \epsilon(k_1) + \epsilon(k_2)$ for all $k_1, k_2 \in \mathbb{R}^d$. Then

$$E(P) = \min \left\{ \frac{P^2}{2m}, \inf_{Q \in \mathbb{R}^d} \left(\frac{(P-Q)^2}{2m} + \epsilon(Q) \right) \right\}. \tag{1.19}$$

In other words, either the free particle carries the entire momentum and no phonons are produced, or, once the momentum is too large, the energy is distributed among the particle and the phonons and partially released in the form of radiation. Note that in the particular case of optical phonons, the infimum over Q in (1.19) equals unity, and thus the particle decelerates completely and transfers the entire momentum to the phonon field. For $\alpha > 0$, we expect a similar picture and a *smoothed out* version of (1.19), in the sense that $E(P)$ should continuously interpolate between the *quasi-particle* and the *radiation regime*, see Fig. 1.1. The quasi-particle regime corresponds precisely to the polaron picture and is determined by a parabolic behavior of $E(P)$, but with the bare mass of the particle m replaced by an α dependent effective mass. In fact, it is known [71]that $E(P)$ has at least a local minimum at $P = 0$ and is analytic in its vicinity, and hence that the limit

$$\lim_{P \to 0} \frac{P^2}{2(E(P) - E(0))} =: M_{\text{eff}} \tag{1.20}$$

exists. The number M_{eff} is the *effective mass*. It can be shown that $M_{\text{eff}} > m$ for $\alpha > 0$. Thus the energy-momentum relation at sufficiently small P is approximately parabolic with semi-latus rectum M_{eff} , which corresponds to the dispersion relation of a free non-relativistic particle having the effective mass M_{eff}. This is precisely the polaron as envisaged physically. On the other hand, for P large, it is known under certain natural assumptions that [90]

$$\lim_{P \to \infty} (E(P) - E_{\text{ess}}(P)) = 0 \tag{1.21}$$

where $E_{\text{ess}}(P)$ is the *bottom of the essential spectrum*

$$E_{\text{ess}}(P) := \inf_{Q \in \mathbb{R}^d} (E(P-Q) + \epsilon(Q)) \tag{1.22}$$

(comp. Eq. (1.19)). This corresponds to the *radiative regime*, where the part of the momentum is transferred to the phonons, just as in the non-interacting case discussed above.

In this work, we are interested in the opposite extreme of the non-interacting case (1.19), the strong coupling limit $\alpha \gg 1$. We wish to confirm the quasi-particle transition picture as depicted in 1.1 and use this picture to confirm validity of the semiclassical analysis applied to the energy-momentum relation. More precisely, define first the transition momentum as the absolute value of momenta satisfying the equation

$$\frac{P_t^2}{2M_{\text{eff}}} = \inf_{Q \in \mathbb{R}^d} \left(\frac{(P-Q)^2}{2M_{\text{eff}}} + \epsilon(Q) \right) \bigg|_{P = P_t}. \tag{1.23}$$

We shall consider dispersion relations that are strictly positive, radial and non-decreasing in $|P|$. We expect that

1. $E(P) - E(0)$ remains essentially a parabolic curve for momenta $|P| \ll |P_t|$ and approaches $E_{\text{ess}}(P)$ for $|P| \gg |P|_t$, and undergoes a swift transition between the two cases for momenta around $P \sim P_t$.

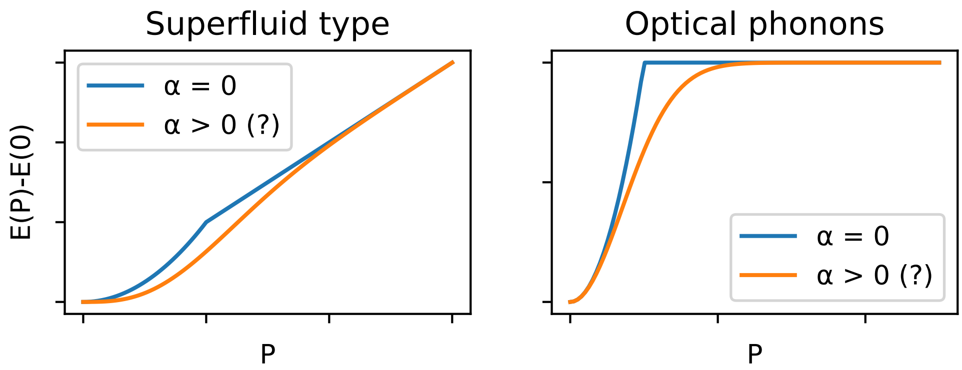

Figure 1.1: A schematic plot of the expected behaviour of $E(P)$ at non-zero coupling: the non-interacting case is added for comparison.

2. At large coupling, the parabola approximating $E(P) - E(0)$ in the quasi-particle regime should be determined by the effective mass coefficient as obtained from the semiclassical theory of Landau and Pekar.

In order to motivate the second point in more detail, we need to explain the connection between the strong coupling and semiclassical limits of the polaron problem, which we shall do next. This connection has been subject to an extensive investigation in the mathematics literature [2, 85, 60].

1.1.5 Semiclassical theory of the polaron and the strong-coupling limit

Ground-state energy

The semiclassical approximation boils down to the replacement of the creation and annihilation operators in (1.1) by complex-valued functions, and taking the expectation value in the electron variable. This leads to the *Pekar functional*

$$\begin{aligned}\mathcal{G}(\psi,\varphi) =& \frac{1}{2m}\int |\nabla\psi(x)|^2 dx + 2\sqrt{\alpha}\,\mathfrak{Re}\int v(k)\varphi(k)\rho_\psi(k)dk \\ &+ \int \epsilon(k)|\varphi(k)|^2 dk\end{aligned} \tag{1.24}$$

with

$$\rho_\psi(k) = \frac{1}{(2\pi)^d}\int dx |\psi(x)|^2 e^{-ikx}. \tag{1.25}$$

For a given ψ, the minimizing field is $\varphi_0(k) = -\sqrt{\alpha}\overline{\frac{v(k)\rho_\psi(k)}{\epsilon(k)}}$, and the electronic Pekar functional is

$$\mathcal{E}_\alpha^{\text{Pek}}(\psi) = \frac{1}{2m}\int |\nabla\psi(x)|^2 - \alpha \iint |\psi(x)|^2 g(x-y)|\psi(y)|^2 dxdy \tag{1.26}$$

with $g(x) = \int \frac{|v(k)|^2}{\epsilon(k)} e^{ik\cdot x} dk$. In particular, in the Fröhlich case $g(x) = \frac{1}{4\pi|x|}$.
We define the Pekar energy:

$$E^{\text{Pek}}(\alpha) = \inf_{\psi\in L^2(\mathbb{R}^d), \|\psi\|_2=1} \mathcal{E}_\alpha^{\text{Pek}}(\psi).$$

The validity of the semiclassical approximation is, among other things, expected to manifest itself in the fact that for the ground state of $\mathbb{H}$, we should have

$$\inf \operatorname{spec} \mathbb{H} =: E_0(\alpha) = \inf_P E(P) \approx E^{\mathrm{Pek}}(\alpha) \tag{1.27}$$

for α large. In fact, one can verify that the Pekar energy is an upper bound for $E_0(\alpha)$ for all α by taking a suitable product state on $L^2(\mathbb{R}^d) \otimes \mathcal{F}$, and thus one way to proceed in proving the above asymptotics is to provide a suitable lower bound. We shall now distinguish between two cases:

1. the Fröhlich case, correspondng to the choice $\epsilon(k) = 1$ and $v(k) = \frac{1}{(2\pi)^3} \frac{1}{|k|}$ in $d = 3$ as discussed above;

2. the regular case, corresponding to $\epsilon(k)$ continuous, radial and positive, and with $v(k)$ satisfying $(1 + k^2)v(k) \in L^2(\mathbb{R}^d)$.

In the Fröhlich case, one has by scaling that

$$E^{\mathrm{Pek}}(\alpha) = \alpha^2 E^{\mathrm{Pek}}(1), \quad \text{Fröhlich case.} \tag{1.28}$$

In particular, the kinetic energy of the electron $\|\nabla\psi\|_2^2$ is of the order α^2 and contributes to the Pekar energy at leading order - the electron maintains its quantum nature. In contrast, in the regular case, one can verify by dominated convergence that

$$\lim_{\alpha \to \infty} \frac{E^{\mathrm{Pek}}(\alpha)}{\alpha} = -g(0) = -\int \frac{|v(k)|^2}{\epsilon(k)} dk, \quad \text{regular case.} \tag{1.29}$$

Here, the kinetic energy of the electron is negligible at leading order for large α, and the electron behaves at large coupling as a classical particle sitting at the bottom of the potential well determined by the function g. This conclusion is also valid for the quantum problem, since $-\alpha g(0)$ is a simple lower bound in the regular case, obtained simply by neglecting the kinetic energy of the electron and completing the square. The non-trivial problem here is to establish whether the semiclassical approximation is still valid beyond the extremely large coupling limit, i.e., at the order of the energy where the kinetic energy of the electron contributes to the total energy. By expanding the exponential factor in the definition of g, it is not difficult to predict that the next order correction corresponds to quantum harmonic oscillations in the well determined by g, with frequency

$$\omega = \sqrt{\frac{2\alpha}{dm}} \sqrt{\int dk \frac{k^2 |v(k)|^2}{\epsilon(k)}}$$

The validity of this prediction is our first result, which is the starting point for further considerations concerning the validity of the semiclassical approximation for the energy-momentum relation in the regular case.

Contributions by the author

For the Fröhlich case, the lower bound was obtained by Lieb and Thomas [2], and in Chapter 4 where we discuss its slight improvement based on [66] and present one of the methods of handling the UV divergence of the form factor. For the regular case, we provide the lower bound in Chapter 3. Its slightly simplified statement is as follows.

Theorem 1.1.2 (M-Seiringer 2021). *In the regular case, for α sufficiently large,*

$$E_0(\alpha) \geq -\alpha \int \frac{|v(k)|^2}{\epsilon(k)} dk + \frac{d\omega}{2} - O(1)$$

Both the Lieb–Thomas bound with our extension and the bound in the regular case are obtained with the use of suitable operator techniques, but there is an important distinction between them: the bound of Lieb and Thomas is provided on the Hamiltonian (1.1) in the Fröhlich setting and hence is performed on $L^2(\mathbb{R}^3) \otimes \mathcal{F}$, while our bound in the regular case we prove a lower bound on $E(P)$ which is uniform in P. The ideas used resemble the ones of Lieb and Yamazaki [3], which were devised for the Fröhlich case, but there they do not result in a sharp lower bound.

1.1.6 Effective mass in the semiclassical approximation

The semiclassical approximation is thus shown to be valid as far as the ground state energy is concerned (there are also results about the dynamics, see, e.g., [64, 13, 81]). Our next goal is to discuss its validity in the effective mass problem, or on the level of $E(P)$ for non-zero P. To this end, we shall introduce the result by Landau and Pekar [8] concerning the effective mass of the polaron in the semiclassical approximation. One way to derive this result in a formal way is to consider the infimum of the Pekar functional (1.24) restricted to the set of functions (ψ, φ) having total momentum P, i.e., satisfying the condition

$$\int \overline{\psi(x)}(-i\nabla_x)\psi(x)dx + \int p|\varphi(p)|^2 dp = P. \tag{1.30}$$

A heuristic analysis (see Sec. 3.1.3) leads to the prediction that the when we restrict the minimization to states satisfying (1.30), the Pekar energy gets increased by a factor $\frac{P^2}{2M_\alpha^{\mathrm{Pek}}}$, with the Landau–Pekar mass

$$M_\alpha^{\mathrm{Pek}} = \frac{2\alpha}{d} \int \frac{k^2|v(k)^2}{\epsilon(k)^3} |\rho^{\mathrm{Pek}}(k)|^2 dk \tag{1.31}$$

where $\rho^{\mathrm{Pek}}(k)$ equals (1.25) evaluated at the minimizer of (1.26), $\psi_\alpha^{\mathrm{Pek}}$ (for the sake of the present discussion, we dispense with questions related to their existence, uniqueness, etc.). In the Fröhlich case, due to scaling, we arrive after a formal computation at

$$M_\alpha^{\mathrm{Pek}} = \frac{2\alpha^4}{3} \|\psi_1^{\mathrm{Pek}}\|_4^4 =: \alpha^4 M^{\mathrm{LP}} \tag{1.32}$$

while in the regular case, since the electron wave function tends to a delta function as suggested by Theorem 1.1.2, we expect that

$$\lim_{\alpha\to\infty} \frac{M_\alpha^{\mathrm{Pek}}}{\alpha} = \frac{2}{d} \int \frac{k^2|v(k)|^2}{\epsilon(k)^3} dk =: M^{\mathrm{Pek}} \tag{1.33}$$

The Landau–Pekar conjecture is

Conjecture. *For all polaron models described by Hamiltonians of the type* (1.1)*, we have*

$$\lim_{\alpha\to\infty} \frac{M_{\mathrm{eff}}}{M_\alpha^{\mathrm{Pek}}} = 1. \tag{1.34}$$

In particular, M_{eff} should diverge with α as $\alpha \to \infty$; in the Fröhlich case, the growth should be proportional to the fourth power of α, and in the regular case we expect a linear divergence. The Landau–Pekar conjecture is still open. In our work, we are prepared to prove two related results in the regular case, and provide the first upper bound on $E(P)$ in the Fröhlich case that is compatible with (1.34).

Contributions by the author

The first result concerns strictly the effective mass in the regular case.

Theorem 1.1.3 (M-Seiringer 2021)**.** *For polaron models satisfying the assumptions of Theorem 1.1.2 we have that for all α sufficiently large there exists a constant $C > 0$ such that*

$$M_{\text{eff}} \geq C\alpha^{1/4}. \tag{1.35}$$

The lower bound is far from the expected $\sim \alpha$ behaviour; nevertheless, we can conclude that the effective mass is in fact divergent *in all spatial dimensions* for a wide class of polaron models. The first result on the divergence of the effective mass was given by Lieb and Seiringer [85] for the Fröhlich case. Recently, this result has been supplemented by a bound on the rate of that divergence [53].

The above divergence result is in line with the conclusion that can be drawn from the Landau–Pekar conjecture, but the actual value of the Pekar mass does not appear in the proof. In order to give the Landau–Pekar semiclassical calculation a qualitiative evidence for its validity from a different angle, we turn our attention to the behaviour of $E(P)$ away from zero but *below the transition momentum* P_t as defined by the condition (1.23). The effective mass is related to the curvature and analyticity of $E(P)$ at zero, as expressed by

$$E(P) = E(0) + \frac{P^2}{2M_{\text{eff}}} + O(P^4), \quad \text{close to } P = 0. \tag{1.36}$$

If the transition picture mentioned above is valid, we expect that another expansion is true at strong coupling, namely

$$E(P) = E^{\text{Pek}}(\alpha) + \frac{P^2}{2M_\alpha^{\text{Pek}}}\left(1 + O\left(\frac{|P|}{|P_t|}\right)^2\right) + E^{\text{Pek}}o(1) \quad \alpha \gg 1 \tag{1.37}$$

which can be viewed as a combination of (1.36) and (1.27). The exact value of P_t depends on the form of ϵ. Here, we restrict our discussion to two cases: the optical phonons $\epsilon(k) = 1$ and a superfluid-type dispersion relation satifying

$$\inf_k \frac{\epsilon(k)}{|k|} = c > 0. \tag{1.38}$$

As we have seen, optical phonons are found in the ionic crystal (Fröhlich) problem, and a superfluid-type dispersion relation naturally appears in the Bose polaron. Assuming the Landau–Pekar asymptotics of the effective mass at strong coupling, from (1.23) we arrive at the conclusion that $P_t \sim \alpha$ for ϵ of superfluid type in the regular case and $P_t \sim \alpha^2$ for optical phonons in the Fröhlich case, so that P_t grows with α at large coupling, suggesting that terms of the order $(|P|/|P_t|)^2$ can be in fact expected to be much smaller than unity for a range of P. The last term on the right-hand side of (1.37) describes the order of magnitude of corrections to the semiclassical approximation for the ground state energy, and can be expected to be of order unity in all cases, as we shall explain below. For the regular case with a superfluid-type dispersion relation, the parabolic Landau–Pekar term is thus much larger than these corrections if $|P| \gg \alpha^{1/2}$. Thus, there is a window of momenta $\alpha^{1/2} \ll |P| \ll \alpha$ where (1.37) makes sense as an approximation for $E(P)$ at large coupling, where the leading order quanties are calculated entirely using the semiclassical analysis. The proof of this fact is one of the central results of this thesis.

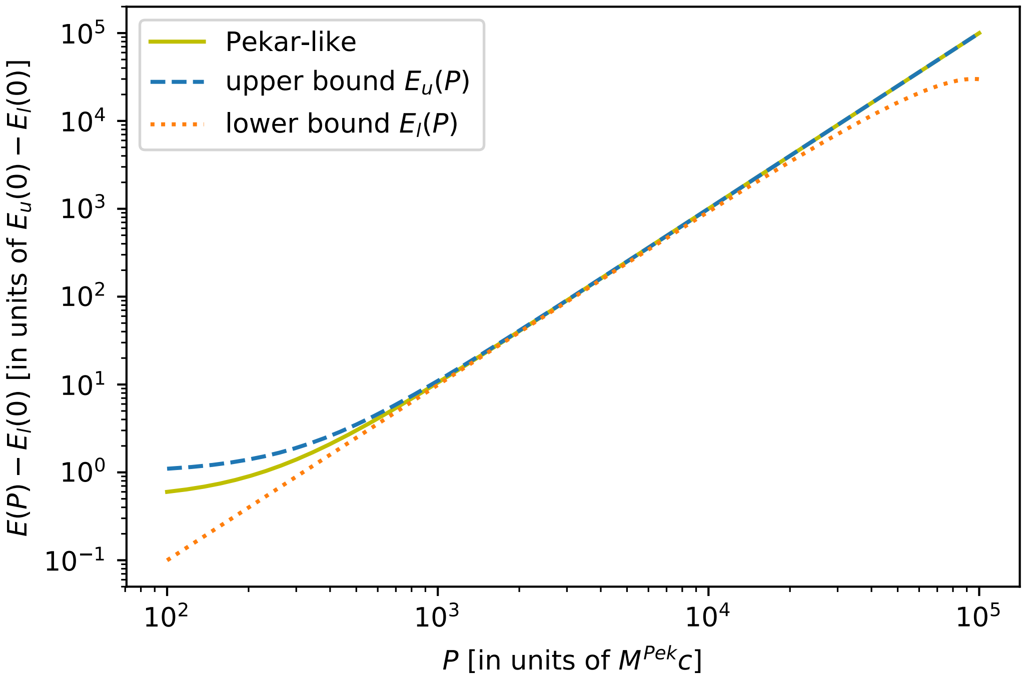

Figure 1.2: Plot of the lower and upper bounds from Theorem 1.1.3, on a log-log scale. In a window of momenta beyond the transition momentum, the curves are well-approximated by the prediction from the Pekar conjecture.

Theorem 1.1.4 (M-Seiringer 2021)**.** *Assume that v satisfies the regularity assumptions in 1.1.1 and that ϵ is strictly positive and of superfluid type. Then*

$$\lim_{\substack{\alpha\to\infty \\ \alpha^{1/2}\ll|P|\ll\alpha}} \alpha^{-1}\frac{P^2}{2(E(P)-E(0))} = M^{\mathrm{Pek}}. \tag{1.39}$$

In fact, we have for $\mathbb{H}$ regular, for all P with $|P| \leq C\alpha$ for some $C > 0$, independent of P and α,

$$E(P) \leq -\alpha g(0) + \frac{d\omega}{2} + \frac{P^2}{2\alpha M^{\mathrm{Pek}}} + O(\frac{|P|}{\alpha}).$$

If in addition the dispersion relation is assumed to be massive (i.e., strictly positive) and of superfluid type, we have for all P such that $|P| \leq C'\alpha$ with $C' > 0$ small enough,

$$E(P) \geq -\alpha g(0) + \frac{d\omega}{2} + \frac{P^2}{2\alpha M^{\mathrm{Pek}}} - O(1) - O(P^2\alpha^{-3/2}).$$

This proves that in the window of momenta where (1.37) is valid, $E(P) - E(0)$ is, at large coupling, approximately parabolic with semi-latus rectum determined by the Landau–Pekar approximation, see Fig. 1.2. It also shows that if the transition picture is correct, then the effective mass equals the Landau–Pekar mass at leading order in α.

The proof of the lower bound is performed using the operator techniques from the proof of Theorem 1.1.1, while for the upper bound, we propose a novel trial state for $\mathbb{H}_P$ see Chapter 3.

1.1.7 The energy-momentum relation in the Fröhlich case

In contrast to the regular case with a superfluid-type dispersion relation, in the Fröhlich case the expansion (1.37) is not meaningful as it stands, and one has to incorporate the explicit form of the leading order correction to $E^{\mathrm{Pek}}(\alpha)$. The reason is that for the Landau–Pekar term $\frac{P^2}{2\alpha^4 M^{\mathrm{LP}}}$ to be larger than this correction, one needs $P \gg \alpha^2$, in particular $P \gg P_t$. Thus, in order to proceed, we need to know what to expect from the subleading correction to $E_\alpha(0)$ beyond the Pekar energy.

The theory of quantum fluctuations in the strong coupling limit appears to have been first considered decades ago by various authors [98, 51]. Although it works the same way for a general choice of the dispersion relation and form factor, here we restrict ourselves to the Fröhlich case. In short, just as the Pekar theory arises if one takes the trial state for (1.1) in the form of a pure tensor product $\psi \otimes \Phi$ where $\psi \in L^2(\mathbb{R}^d)$ and $\Phi \in \mathcal{F}$, the quantum corrections arise if one takes a trial state of the form

$$\psi(x, \{a^\dagger, a\})\Phi', \tag{1.40}$$

where $\Phi' \in \mathcal{F}$ and ψ can be thought to be a function on $L^2(\mathbb{R}^d)$ that depends *parametrically* on a specific combination of the creation and annihilation operators. This structure is analogous to the Born-Oppenheimer theory of electronic motion in molecules. Since the semiclassical theory corresponds to a pure product of a suitable Φ with the Pekar minimizer $\psi_\alpha^{\mathrm{Pek}}$ one can further suspect that in order to arrive at the next order term using the structure (1.40), it suffices to take

$$\psi(x, \{a^\dagger, a\}) = \psi_\alpha^{\mathrm{Pek}}(x) + a(r_x) + a^\dagger(r_x) \tag{1.41}$$

for an appropriately chosen phonon function r_x depending parametrically on x. In order to motivate a specific choice of r_x, assume that the field undergoes a fluctuation changing the value $\varphi_\alpha^{\mathrm{Pek}}$ to $\varphi_\alpha^{\mathrm{Pek}} + \hat{\eta}$, where $\varphi_\alpha^{\mathrm{Pek}}$ is the field minimizer of (1.26) The function η can be viewed as a perturbation on the level of the Pekar functional (1.26), and thus, by first-order perturbation theory, the electron wave function changes into

$$\psi_\eta(x) = \psi_\alpha^{\mathrm{Pek}}(x) + \frac{\sqrt{\alpha}}{2\pi^2}\left(R\,\eta * \frac{1}{|\cdot|^2}\psi_\alpha^{\mathrm{Pek}}\right)(x) \tag{1.42}$$

where R is the resolvent of

$$-\Delta_x + 2\frac{\sqrt{\alpha}}{(2\pi)^3}\int \frac{\varphi_\alpha^{\mathrm{Pek}}(k)}{|k|}e^{ikx}dk + E^{\mathrm{Pek}}(\alpha) - \int |\varphi_\alpha^{\mathrm{Pek}}(k)|^2 dk. \tag{1.43}$$

$r_x(y)$ is then chosen to be the functional derivative of ψ_η with respect to $\eta(y)$, i.e.,

$$r_x(y) = \sqrt{\frac{\alpha}{(2\pi^2)^2}}\left(R\frac{1}{|\cdot - y|^2}\psi_\alpha^{\mathrm{Pek}}\right)(x) \tag{1.44}$$

so that (1.41) can be formally viewed as an expansion of a general $\psi(x, \{a^\dagger, a\})$ around the case where the creation and annihilation operators are replaced by the function $\varphi_\alpha^{\mathrm{Pek}}$. Note that the eigenvalues of (1.43) are of order α^2, so that $r_x(y)$ is in fact formally small with respect to the Pekar minimizer $\psi_\alpha^{\mathrm{Pek}}(x)$. Taking the expectation value of the Fröhlich Hamiltonian (1.9) on $\psi(x, \{a^\dagger, a\})\Phi'$ and retaining only terms linear in r_x leads to a quadratic operator in the phonon creation and annihilation operators, which can be further diagonalized using a suitable Bogoliubov transformation. We shall not perform the details of this computation here, referring to [89]; it leads to the prediction that

$$E_\alpha(0) = E^{\mathrm{Pek}}(\alpha) + \frac{1}{2}\mathrm{Tr}(\sqrt{H^{\mathrm{Pek}}} - 1) + o(1) \tag{1.45}$$

where H^{Pek} is an integral operator on $L^2(\mathbb{R}^3)$ with the kernel

$$H^{\mathrm{Pek}}(x,y) = \delta(x-y) - 4\frac{\alpha}{(2\pi^2)^2}\langle\psi_\alpha^{\mathrm{Pek}}|\frac{1}{|\cdot - y|^2}R\frac{1}{|\cdot - x|^2}\psi_\alpha^{\mathrm{Pek}}\rangle \tag{1.46}$$

By scaling, the term involving the resolvent R in (1.46) does not depend on α, and the correction term in (1.45) is indeed of order unity. One can show that the trace term is, in fact, finite. Thus, we expect that the following expansion is valid in the Fröhlich case:

$$E(P) = E^{\mathrm{Pek}}(\alpha) + \frac{1}{2}\mathrm{Tr}(\sqrt{H^{\mathrm{Pek}}} - 1) + o(1) + \frac{P^2}{2\alpha^4 M^{\mathrm{LP}}}\left(1 + O\left(\frac{P}{|P_t|}\right)^2\right). \tag{1.47}$$

In fact, the expectation is that the subleading correction to the quantum fluctuation term is of order α^{-2}, so that there is a momentum window $\alpha \ll |P| \ll P_t \sim \alpha^2$ for the Landau–Pekar term to be *visible* on the energy scale related to the expansion (1.47). In this work, we are able to prove an upper bound on $E(P)$ in line with the expansion (1.47).

Theorem 1.1.5 (Mitrouskas-M-Seiringer 2022)**.** *Consider the Fröhlich polaron problem. Then for every $c, \varepsilon > 0$ there exists a constant $C_{c,\varepsilon}$ such that*

$$E(P) \;\leq\; E^{\mathrm{Pek}}(\alpha) + \frac{\mathrm{Tr}(\sqrt{H^{\mathrm{Pek}}} - 1)}{2} + \frac{P^2}{2\alpha^4 M^{\mathrm{LP}}} + C_{c,\varepsilon}\alpha^{-\frac{1}{2}+\varepsilon}$$

holds for all $|P|/\alpha^2 \leq c$ and all α large enough.

In particular,in (1.47), the corrections to the parabolic quasi-particle behaviour should always be negative. On the other hand, since $E(0) \leq E(P)$, our result also gives an upper bound on the ground state energy compatible with (1.45).

Since the quantum fluctuation term has to be included in the analysis, this is arguably the most challenging part of the thesis, despite the fact that it is only the upper bound, and that the trial state used has its roots in the one used for the proof of Theorem 1.1.2. The structure of the trial state is, in our view, the main mathematical novelty of this part of the thesis. We also believe that it might be useful in other translation-invariant models of quantum field theory. We refer to Chapter 5 for details: the trial state we use is discussed in Sec. 5.2.2, and the heuristic idea behind the proof is expounded in Sec. 5.3.2.

Remark about different choices of units in the Fröhlich model. In the present Section, we use the units with the coupling contant under the squre root in front of the interaction term in order to make it explicitly connected to (1.1). In Chapter 4 and 5 we use the *strong coupling units* and rescale all lengths by α so as to extract the leadding order α^2 dependence. More precisely, we use the unitary transformation U_α on $L^2(\mathbb{R}^3) \otimes \left(\otimes^n_{\mathrm{sym}} L^2(\mathbb{R}^3)\right)$

$$U_\alpha\psi(x, y_1, \cdots, y_n) = \alpha^{\frac{3}{2}(n+1)}\psi(\alpha x, \alpha y_1, \cdots, \alpha y_n) \tag{1.48}$$

which can be easily extended to $L^2(\mathbb{R}^3) \otimes \mathcal{F}$. A computation using the homogeneity of the function $|x-y|^{-2}$ shows that

$$\alpha^{-2} U_\alpha^\dagger \mathbb{H} U_\alpha = \tilde{\mathbb{H}} = -\Delta_x + \frac{1}{\alpha^2} \int dy\, a_y^\dagger a_y + \frac{1}{\alpha} \int dy \frac{1}{2\pi^2 |x-y|^2} \left(a_y^\dagger + a_y \right). \tag{1.49}$$

In Chapter 4 we further redefine $\alpha^{-1} a_y \to a_y$ so that the new operators commute to

$$[a(f), a^\dagger(g)] = \frac{1}{\alpha^2} \langle f | g \rangle. \tag{1.50}$$

In these units, $\tilde{\mathbb{H}}$ is at first sight independent on α and the α dependence is transferred to the commutation relations, highlighting the connection between the strong coupling and semiclassical limits. To our knowledge, these units were first introduced in [64]. This is the choice we adopt in Chapter 4, while in Chapter 5 we keep the standard creation and annihilation operators.

1.2 Structure of the thesis

The individual chapters that now follow contain the original research papers on the topics discussed in their entirety. In particular, they start with extensive introductory sections which discuss the background, motivation and methods of the proofs in much more detail than presented here, and can also be consulted by readers who are interested in the basic aspects of the subject of this thesis and not necessarily the proofs, which are, of course, included in the subsequent chapters.

The thesis starts with the rigorous microscopic derivation of the Fröhlich Hamiltonian as an effective theory of the Bose polaron in the mean-field limit in Chapter 2, which contains the paper

- K. Myśliwy and R. Seiringer, *Microscopic derivation of the Fröhlich Hamiltonian for the Bose polaron in the mean-field limit*, Ann. Henri Poincaré **21**, 4003-4025 (2020).

devoted to the precise statement and proof of Theorem 1.1.1 along with the supplementary result on the projections onto the respective eigenspaces.

Chapter 3 takes up the problem of the energy-momentum relation of the polaron at strong-coupling, which is discussed in the regular setting mentioned above. It contains the paper

- K. Myśliwy and R. Seiringer, *Polaron models with regular interactions at strong coupling*, J. Stat. Phys. **186**, 5 (2022)

together the detailed statements and proofs of Theorems 1.1.2 and 1.1.3. Since the case of a superfluid-type dispersion relation plays a central role in this analysis, this Chapter has largely the Bose polaron as its physical background. In this sense, it is a continuation of the previous one containing the derivation result, and thus Chapters 2 and 3 can be seen as the first part of the thesis devoted mainly to the Bose polaron.

The second part of the thesis, comprised of Chapters 4 and 5, is concerned with the Fröhlich polaron in a ionic crystal, and the main, and most voluminous part of it, extends the ideas utilized in the proof of the upper bound on the energy-momentum relation in Chapter 3 to this case. In this sense Chapter 3 provides a smooth transition between the first part of the thesis, where mostly the Bose polaron is discussed, to the second one which is focused on the Fröhlich polaron.

As already pointed out, the analysis of the Fröhlich polaron is more complicated, and this is so for two reasons. The first one is technical and is related to the UV singularity of the form factor $\sim |k|^{-1}$ encountered in the Fröhlich case. For the most part, this can be handled by the commutator method of Lieb and Yamazaki [86] and its various extensions. For this reason, before giving the proof of the upper bound on $E(P)$ in the Fröhlich case in Chapter 5, in the preceding Chapter 4, which contains the unpublished note

- K. Myśliwy, *Ground state energy of the strongly-coupled polaron in free space - lower bound, revisited* (2019)

we apply a version of the commutator method and combine it with several ideas developed for the confined Fröhlich polaron [66] in order to provide a slightly improved lower bound on the absolute ground-state energy of the Fröhlich polaron at strong coupling. In this way, we are able to introduce, on a working example, the ideas behind the UV regularization of the model, which are then used extensively in the upper bound in Chapter 5.

The second aspect responsible for the increased level of difficulty in the case of the Fröhlich polaron is more subtle, and is related to the fact that we need to incorporate the quantum corrections to the semiclassical asymptotics of the polaron problem into account as explained above. This requires a fair amount of work, which is summarized in Chapter 5, which contains the submitted paper

- D. Mitrouskas, K. Myśliwy and R. Seiringer, *Optimal parabolic upped bound for the energy-momentum relation of a strongly-coupled polaron*, arXiv:2203.02454.

Its subject is the proof of Theorem 1.1.5. It is arguably the most technically involved and certainly the longest paper constituting this thesis. For this reason, this Chapter includes an exhaustive heuristic section explaining the principal idea behind the proof, as well as a discussion of the trial state used. The general idea behind the construction of this trial state is applied already in Chapter 4, and we believe it might be of relevance also to other translationally invariant models, placing the result in Chapter 5 in a broader context beyond the polaron model.

CHAPTER 2

Microscopic derivation of the Fröhlich Hamiltonian for the Bose polaron in the mean-field limit

This Chapter contains the work

- K. Myśliwy and R. Seiringer, *Microscopic derivation of the Fröhlich Hamiltonian for the Bose polaron in the mean-field limit*, Ann. Henri Poincare **21**, 4003-4025 (2020)

Abstract
We consider the quantum mechanical many-body problem of a single impurity particle immersed in a weakly interacting Bose gas. The impurity interacts with the bosons via a two-body potential. We study the Hamiltonian of this system in the mean-field limit and rigorously show that, at low energies, the problem is well described by the Fröhlich polaron model.

2.1 Introduction and main results

2.1.1 The polaron

The behavior of impurity particles interacting with a large background constitutes an important class of problems within condensed matter physics [50, 21]. Among these, one of the most prominent is the polaron problem, where one considers a quantum particle of mass M linearly coupled to a scalar boson field. For a translation invariant system, this corresponds to the formal Hamiltonian

$$H = \frac{P^2}{2M} + \sum_k e_k a_k^\dagger a_k + \sum_k \left(g_k a_k e^{ikR} + g_k^* a_k^\dagger e^{-ikR} \right), \tag{2.1}$$

where R denotes the position of the impurity particle, and k labels the momentum modes of the field. Moreover, $P = -\mathrm{i}\nabla_R$ is the particle's momentum operator in the canonical representation, and $a_k^\dagger, a_k$ are the usual field mode creation and annihilation operators. They satisfy the canonical commutation relations $[a_k, a_{k'}^\dagger] = \delta_{k,k'}, [a_k, a_{k'}] = 0$. The g_k are coefficients quantifying the coupling of the particle to the field, with * denoting the complex conjugate, and e_k is the free field dispersion relation. The natural domain of this Hamiltonian lies in the Hilbert space $\mathcal{H} \otimes \mathcal{F}(\mathcal{K})$, where $\mathcal{H}$ is the Hilbert space of the particle and $\mathcal{K}$ is the Hilbert space of a single field mode, with $\mathcal{F}(\mathcal{K})$ denoting the symmetric Fock space over $\mathcal{K}$. $\mathcal{K}$ and $\mathcal{H}$ are appropriate L^2 spaces, whose exact specification depends on the underlying physical situation; our choice thereof is discussed below.

The Hamiltonian (2.1) is commonly referred to as the Fröhlich Hamiltonian, as it was introduced by Fröhlich in 1937 [67] in order to describe electronic motion in polar crystals. The *polaron* in this context refers to the picture of an electron dressed with the emerging optical phonons dragged along as it moves. Later, this concept was extended to include other phenomena related to mobile impurities coupled to excitations of the background, giving rise to interesting effects in many materials [50, 22, 20] which are still the subject of ongoing research [23, 24].

In this work, we are interested in a rigorous justification of the use of Hamiltonians of the type (2.1) as an effective description of a full quantum mechanical many-body problem. In the case of the original Fröhlich model this task seems too ambitious due to a complicated microscopic structure of the background (see, however, [25], where the classical approximation to the original polaron problem, the Pekar functional, is rigorously derived from a specific model of an electron moving through a quantum crystal). The applicability of the polaron picture is not limited to electrons in crystal lattices, however. In fact, recent progress in experiments with ultracold atoms opened the possibility of studying impurity atoms immersed in an environment consisting of many bosonic atoms at low temperatures, displaying Bose–Einstein condensation. As discussed below, at sufficiently low energies the excitations of the bosonic bath correspond to quantized acoustic phonons, and hence the *Bose polaron* corresponds to the impurity atom dressed with these phonons. We refer to [1] for a review of recent theoretical progress concerning the application of Fröhlich Hamiltonians to these systems. As the mathematical description of cold Bose systems, and in particular the structure of their excitation spectra at low energies, have recently been studied rigorously in numerous works [29, 27, 28, 26, 30, 31], we find it natural to provide a rigorous microscopic derivation of (2.1) based on these results.

2.1.2 The $N+1$ Bose gas

We consider a system of N bosons of mass 1/2 and one additional particle (of an unspecified type of statistics) of mass M, all confined to move on the unit torus in d dimensions, $\mathbb{T}^d$.

Assumption 1 (Assumptions on the potentials)**.** *We assume that*

1. *the bosons interact among themselves via a two-body potential $v : \mathbb{T}^d \to \mathbb{R}$ which is bounded, Borel measurable, even and of positive type, i.e., all its Fourier coefficients v_p are non-negative.*
2. *the additional impurity particle interacts with the bosons via a real-valued two-body potential $w : \mathbb{T}^d \to \mathbb{R}$, which is bounded, Borel measurable and even.*

Note that no assumption is made on the Fourier coefficients w_p of w. Nevertheless w being even implies $w_p = w_{-p} \in \mathbb{R}$. Without loss of generality, we may in addition assume that v and w are non-negative, since they can be shifted by a constant otherwise.

The positions of the bosons are labeled by $\{x_i\}_{i=1}^N, x_i \in \mathbb{T}^d$ and the position of the impurity by $R \in \mathbb{T}^d$. The Hamiltonian of this system reads

$$\frac{-\triangle_R}{2M} - \sum_{i=1}^{N} \triangle_{x_i} + \lambda \sum_{1\leq i<j\leq N} v(\eta(x_i - x_j)) + \mu \sum_{i=1}^{N} w(\nu(x_i - R)) \tag{2.2}$$

where we introduced some coupling (λ,μ) and scaling (η,ν) parameters to be chosen. It acts on $L^2(\mathbb{T}^d) \otimes \mathcal{H}_N$ with $\mathcal{H}_N$ being the Hilbert space of square-integrable symmetric functions on $\mathbb{T}^{dN}$. Here, $\triangle_y$ denotes the $d-$dimensional Laplacian in the coordinate y acting on functions on the unit torus. The coupling parameters λ and μ determine the strength of the potentials v and w (for the functional forms of v and w being fixed), whereas η and ν determine the respective ranges (relative to the system size). They can be adjusted to consider various scaling regimes. The usual thermodynamic limit corresponds to the choice $\eta \sim \nu \sim N^{1/d}$ and $\lambda \sim \mu \sim N^{2/d}$. In contrast, we consider here the mean-field limit, where the interactions are weak and extend over the entire system. In particular, we choose $\lambda = (N-1)^{-1}$, $\mu = N^{-1/2}$, and $\eta = \nu = 1$. For systems without impurity, this was the scaling for which the first rigorous results on the excitation spectrum were obtained [26, 28, 31, 32], and our analysis is based on them. The choice $\mu = N^{-1/2}$ for the impurity-boson coupling turns out to be a natural in the analysis, compatible with the methods from [26, 28] we use, as explained below (see, in particular, Remark 1.1). Therefore, from now on we consider the Hamiltonian

$$H_N := \frac{-\triangle_R}{2M} - \sum_{i=1}^{N} \triangle_{x_i} + \frac{1}{N-1} \sum_{1\leq i<j\leq N} v(x_i - x_j) + \frac{1}{\sqrt{N}} \sum_{i=1}^{N} w(x_i - R) \tag{2.3}$$

on $L^2(\mathbb{T}^d) \otimes \mathcal{H}_N$, with v and w non-negative 1-periodic functions satisfying Assumption 1.

Motivation of the Fröhlich Hamiltonian

With v_p and w_p denoting the Fourier coefficients of v and w, respectively, the second-quantized version of H_N in (3.1) reads

$$\frac{-\triangle_R}{2M} + E_{\mathrm{H}}(N) + \sum_{p\neq 0} p^2 a_p^\dagger a_p + \frac{1}{2(N-1)} \sum_{\substack{p,q,k\in(2\pi\mathbb{Z})^d \\ p\neq 0}} a_{p+k}^\dagger a_{q-p}^\dagger a_q a_k + \frac{1}{\sqrt{N}} \sum_{\substack{p,k\in(2\pi\mathbb{Z})^d \\ p\neq 0}} w_p e^{-ipR} a_{p+k}^\dagger a_k. \tag{2.4}$$

We defined the *Hartree ground state energy*

$$E_{\mathrm{H}}(N) = \frac{N}{2} v_0 + \sqrt{N} w_0, \tag{2.5}$$

which captures the effect of interactions between particles in the $p = 0$ mode. The sums run over $(2\pi\mathbb{Z})^d$ with $p = 0$ excluded. Here, a_p denotes the usual annihilation operator $\mathcal{H}_N \to \mathcal{H}_{N-1}$ acting as

$$(a_p\Psi)(x_1, x_2, \cdots, x_{N-1}) = \sqrt{N} \int_{\mathbb{T}^d} \Psi(x_1, \cdots, x_{N-1}, x) e^{-ipx} dx. \tag{2.6}$$

The second-quantized Hamiltonian (2.4) acts on $L^2(\mathbb{T}^d) \otimes \mathcal{F}$, with $\mathcal{F}$ the bosonic Fock space $\mathcal{F}$ over $L^2(\mathbb{T}^d)$, i.e., $\mathcal{F} := \bigoplus_{i=0}^{\infty} \mathcal{H}_i$ (with $\mathcal{H}_0 = \mathbb{C}$). Actually, it preserves $L^2(\mathbb{T}^d) \otimes \mathcal{H}_N$. For the system without impurity, it was predicted by Bogoliubov [33] that for sufficiently low energies, the excitation spectrum of H_N should be composed of elementary excitations, which are physically interpreted as quantized (acoustic) free phonons. This serves as the basis for the microscopic explanation of the onset of superfluid behavior in low-temperature bosonic systems. From the formal perspective, it provides a specific example of the emergence of an effective quantum field theoretical description of a many-body system. The low-energy effective theory is predicted to be that of the Hamiltonian

$$\mathbb{H}^{\mathsf{B}} = \sum_{p\neq 0} e_p b_p^\dagger b_p \,. \tag{2.7}$$

Here, $b_p^\dagger = \alpha_p a_p^\dagger + \beta_p a_{-p}$ where α_p, β_p are appropriate constants chosen such that $[b_p, b_q^\dagger] = \delta_{p,q}$. Explicitly, $\alpha_p = (1-\gamma_p)^{-1/2}$ with $\gamma_p = 1 + \frac{p^2 - e_p}{v_p}$ and $\beta_p = \gamma_p \alpha_p$. These algebraic relations are realized via a suitable unitary (Bogoliubov) transformation. From (2.7) we deduce that, for low energies, the excitation spectrum is expected to be composed of free bosonic quasi-particles with dispersion relation e_p. In the mean-field scaling $\lambda = (N-1)^{-1}$ considered here, one can prove [26] that $e_p = \sqrt{p^4 + 2v_p p^2}$. Additionally, it can be shown that in this scaling the ground state energy equals $\frac{1}{2}Nv_0 + E^{\mathrm{B}} + o(1)$ with the constant E^{B} equal to

$$E^{\mathrm{B}} = -\frac{1}{2}\sum_{p\neq 0}\left(p^2 + v_p - \sqrt{p^4 + 2p^2 v_p}\right). \tag{2.8}$$

The method employed by Bogoliubov leading to $\mathbb{H}^{\mathsf{B}}$ consists of the following steps:

1. the operators $a_0, a_0^\dagger$ are replaced by the number $\sqrt{N}$
2. all the terms of higher order than quadratic in creation and annihilation operators that remain in the Hamiltonian are dropped.

This procedure is physically motivated by the expectation that for sufficiently small energies there is Bose–Einstein condensation in the system, that is, the $p = 0$ mode is occupied by an overwhelming fraction of particles. Whereas this has not been proven for a generic bosonic system with general interactions, the validity of the Bogoliubov approximation has been rigorously verified (in the case $w \equiv 0$) for a variety of assumptions on v [26, 30, 28, 31, 40]. The first such result [26] refers precisely to our conditions on v and, as already mentioned, the mean-field scaling $\lambda = (N-1)^{-1}$, which corresponds to a very weak and long-ranged potential.

If one applies the Bogoliubov approximation to the Hamiltonian (2.4) with impurity, one expects that the system is, for small energies, effectively described by the Fröhlich Hamiltonian

$$\mathbb{H}^{\mathsf{F}} := \frac{-\triangle_R}{2M} + \sum_{p\neq 0}(p^2 + v_p) a_p^\dagger a_p + \frac{1}{2}\sum_{p\neq 0} v_p (a_p^\dagger a_{-p}^\dagger + a_p a_{-p}) + \sum_{p\neq 0} w_p e^{-ipR}(a_p^\dagger + a_{-p}). \tag{2.9}$$

By expressing the a_p's in terms of the operators $b_p, b_{-p}^\dagger$, we see that it equals

$$\mathbb{H}^{\mathsf{F}} = \frac{-\triangle_R}{2M} + \sum_{p\neq 0} e_p b_p^\dagger b_p + \sum_{p\neq 0}\frac{|p| w_p}{\sqrt{e_p}} e^{-ipR}(b_p^\dagger + b_{-p}) + E^{\mathrm{B}} \tag{2.10}$$

which belongs to the class of Hamiltonians defined in (2.1). The Hamiltonian $\mathbb{H}^{\mathsf{F}}$ acts on $L^2(\mathbb{T}^d) \otimes \mathcal{F}_+$, where $\mathcal{F}_+$ is the Fock space over the complement of the normalized constant function in $L^2(\mathbb{T}^d)$, describing solely the $p \neq 0$ modes of the field. In order to obtain (2.10) via a Bogoliubov approximation, we supplemented this procedure by additionally dropping, in the impurity-boson interaction, all the terms that are of higher order than *linear* in the creation and annihilation operators (after first replacing the a_0 and its adjoint by $\sqrt{N}$), whereas we kept the quadratic terms in the boson-boson interaction. One of elements of our analysis below is the justification of this additional step while checking that the other steps, known to be rigorously justifiable in the mean-field case in the absence of an impurity, are still applicable. It is important, however, to realize that in some instances, especially when the impurity-boson interaction is strong, additional terms not present in the Fröhlich Hamiltonian (2.10) cannot be neglected [34, 35, 36].

2.1.3 Main results

The interpretation of our main results, as stated below, is that the Fröhlich Hamiltonian (2.10) may indeed be seen as an effective low-energy, large N theory for the original model described by H_N in (3.1). Our analysis consists of a rigorous justification of the extended Bogoliubov approximation, based on suitable operator inequalities. It leads to two main theorems, the first of which concerns the excitation spectrum of H_N.

Theorem 1: convergence of eigenvalues

Let us denote by $e_i(A)$ the $i-$th eigenvalue resp. the $i-$th min-max value of an operator A, starting at $i = 0$. Our first Theorem states that as long as one considers the energy levels of H_N lying in a not too large window above the ground state, their values are provided by the corresponding eigenvalues of the Fröhlich Hamiltonian if N is sufficiently large. In particular, we provide explicit bounds on the size of that window as compared with N.

Theorem 1. *Let H_N and $\mathbb{H}^{\mathrm{F}}$ be defined by Eqs.* (3.1) *and* (2.10)*, respectively, and let $E_{\mathrm{H}}(N) := \frac{N}{2}v_0 + \sqrt{N}w_0$. Assume that v and w satisfy Assumption 1. Then for all eigenvalues $e_i(H_N)$ such that $e_i(H_N) - e_0(H_N) \leq \xi$ for some $\xi \geq 1$ we have*

$$|e_i(H_N) - E_{\mathrm{H}}(N) - e_i(\mathbb{H}^{F})| \leq C_{v,w}\xi \left(\frac{\xi}{N}\right)^{1/2} \tag{2.11}$$

for some constant $C_{v,w} > 0$ independent of the parameters ξ and N.

Remark 1.1. In the special case of the ground state energy we have

$$\inf\operatorname{spec} H_N = \frac{1}{2}Nv_0 + \sqrt{N}w_0 + \inf\operatorname{spec}\mathbb{H}^{\mathrm{F}} + O(N^{-1/2}). \tag{2.12}$$

The interaction with the impurity thus gives rise to a $N^{1/2}$ contribution to the ground state energy and, more importantly, leads to an $O(1)$ contribution to the excitation spectrum via the last term in (2.9). This can be understood as follows. In the impurity-free case, the effect of the emergence of phonons is reflected as a $O(1)$ correction to the ground state and low-lying excitation energies, in the mean-field limit considered here. There are only finitely many (even for large N) phonons that emerge in the system. The Fröhlich model describes the impurity creating and annihilating excitations of the background. The number of the latter being $O(1)$, we expect that this phonon-impurity interaction should as well give rise to an $O(1)$ correction. The Bogoliubov approximation suggests that this interaction should scale as $\mu N^{1/2}$, hence we see that $\mu \sim 1/\sqrt{N}$ is consistent with these considerations.

Remark 1.2. The error bounds are of the form $\xi(\xi/N)^{1/2}$. Therefore, as long as the total excitation energy satisfies $\xi \ll N$, the error made by using the Fröhlich Hamiltonian instead of the original one when computing the energy levels is small compared to the total excitation energy. The size of this energy window is presumably optimal. In fact, if the condition $\xi \ll N$ is not fulfilled one cannot expect the onset of BEC anymore, which is an essential assumption in the Bogoliubov approximation. It is noteworthy that precisely the same error scaling was obtained in [26] for the pure bosonic system. The effects of the inclusion of the impurity thus manifest themselves only in the value of the constant $C_{v,w}$.

Remark 1.3. By a direct inspection of the proof, one sees that the result can easily be generalized to the case of multiple impurities (as long as their number is fixed, i.e., independent of N). This holds irrespectively of the statistics of the impurities, i.e. they could be fermions, bosons, or distinguishable (in particular, different) particles.

Remark 1.4. Extending the results to the case of more realistic, short-ranged potentials remains a challenge. In fact, the $w \equiv 0$ cases with either $\lambda = N^{2/d}$, $\eta = N^{1/d}$ (equivalent to the thermodynamic limit) or $\lambda = N^2$, $\eta = N$ in $d = 3$ (the *Gross-Pitaevskii* limit) were rigorously analyzed only very recently. The results for the thermodynamic limit concern the ground state energy only [27, 37, 38, 39], whereas in the Gross-Pitaevskii scaling regime the emergence of the Bogoliubov spectrum for low energies was shown as well [40].

Remark 1.5. If a contact interaction is used to model both boson-boson and boson-impurity interaction, one encounters the *Bogoliubov–Fröhlich Hamiltonian* [1, 41]

$$\mathbb{H}^{\text{B-F}} = \frac{P^2}{2M} + \sum_p \epsilon_p b_p^\dagger b_p + \sqrt{n_0} g_{IB} \sum_p \left(\frac{(\zeta p)^2}{2 + (\zeta p)^2} \right)^{1/4} (b_p^\dagger + b_{-p}) e^{-ipR}, \tag{2.13}$$

where n_0 is the condensate density and $\zeta = (2 g_{BB} n_0)^{-1/2}$ is the healing length; the parameters g_{IB} and g_{BB} are the coupling constants describing the impurity-boson and boson-boson interactions, respectively. Additionally, $\epsilon_p = \sqrt{c^2 p^2 (1 + (\zeta p)^2)}$ with $c = 1/\zeta = \sqrt{2 g_{BB} n_0}$ denoting the speed of sound in the bosonic bath. This Hamiltonian displays an evident ultraviolet divergence, recently analyzed in [41]. By naively replacing v_p and w_p in (2.10) with the respective coupling constants g_{BB} and g_{IB}, one arrives at $\mathbb{H}^{\text{B-F}}$ with unit condensate density. We conjecture that (2.13), resp. some renormalized version of it, arises in place of $\mathbb{H}^{\text{F}}$ in scaling regimes corresponding to more realistic interactions of shorter range than the mean-field limit considered here.

Remark 1.6. Our proof makes use of methods from [26] and [28]. In particular, in the case $w \equiv 0$, we reproduce the results of [26], but by utilizing techniques from [28] we are able to substantially simplify the proof.

Theorem 2: convergence of eigenvectors

In order to compare the two operators H_N and $\mathbb{H}^{\text{F}}$, which act on different Hilbert spaces, we utilize an operator introduced by Lewin, Nam, Serfaty and Solovej in [28], which maps $\mathcal{H}_N$ to (a subspace of) $\mathcal{F}_+$. We give here a quick review of their construction, as it is important to formulate our second result.

The LNSS transform

If $\{v_i\}_{i\geq 0}$ is an orthonormal basis of some Hilbert space $\mathcal{H}$, then the N-fold symmetric tensor product of $\mathcal{H}$ is spanned by N-fold tensor products

$$v_{i_1} \otimes_{\mathrm{s}} \cdots \otimes_{\mathrm{s}} v_{i_N} := \mathcal{N} \sum_{\sigma \in S_N} v_{\sigma(i_1)} \otimes \cdots \otimes v_{\sigma(i_N)}$$

for all choices of indices $i_j \in \mathbb{N} \cup \{0\}$ with $\mathcal{N}$ a normalization constant. Let us fix an element v_0 in the basis of $\mathcal{H}$. If one defines $\mathcal{H}_l^0$ to be the span of $\bigotimes_{\mathrm{s}}^l v_0 \otimes_{\mathrm{s}} v_{i_{l+1}} \otimes_{\mathrm{s}} \cdots v_{i_N}$ for all choices of the $N-l$ indices $i_j \neq 0$, it is clear that

$$\mathcal{H}_N = \bigoplus_{l=0}^{N} \mathcal{H}_l^0.$$

For convenience, we further define $\mathcal{H}_m^+$ by the relation $\mathcal{H}_{N-m}^0 = \{\otimes_{\mathrm{s}}^{N-m} v_0\} \otimes_{\mathrm{s}} \mathcal{H}_m^+$. Explicitly,

$$\mathcal{H}_m^+ = \bigotimes\nolimits_{\mathsf{s}}^{m} \mathcal{H}^+, \quad \mathcal{H}^+ := \{v_0\}^\perp.$$

For every element $\Psi \in \mathcal{H}_N$, define the linear operator

$$U : \mathcal{H}_N \to \mathcal{F}_+^{\leq N}, \quad \Psi \mapsto \phi_0 \oplus \cdots \phi_N$$

where the $\phi_i \in \mathcal{H}_i^+$, $i \in \{0, \ldots, N\}$, are uniquely determined by the above considerations. The space $\mathcal{F}_+^{\leq N}$ is naturally seen to be a proper subset of the Fock space over the orthogonal complement of $v_0 \in \mathcal{H}$. Moreover, U is unitary. Performing this construction for $\mathcal{H} = L^2(\mathbb{T}^d)$ with, for instance, the plane wave basis and with $v_0 \equiv 1$ we arrive at a unitary transformation $U : \mathcal{H}_N \to \mathcal{F}_+^{\leq N} \subset \mathcal{F}_+$ with $\mathcal{F}_+$ being the Fock space over the orthogonal complement of the unit function on $\mathbb{T}^d$. This space has a clear physical interpretation of being the space of excitations from the condensate, and the fully condensed state plays the role of the vacuum. It is due to the algebraic properties of U, however, that it becomes helpful in the analysis, as it can be seen to rigorously realize the Bogoliubov substitution of $a_0, a_0^\dagger$ by $\sqrt{N}$. More precisely, with $\mathcal{Q}$ denoting the projection onto the orthogonal complement of the unit function in $L^2(\mathbb{T}^d)$, one can check that (the annihilation operator is here understood to be the standard operator in the purely bosonic Fock space)

$$U(\Psi) = \bigoplus_{j=0}^{N} \mathcal{Q}^{\otimes_{\mathrm{s}} j} \left(\frac{a_0^{N-j}}{\sqrt{(N-j)!}} \Psi \right) \tag{2.14}$$

for all $\Psi \in \mathcal{H}_N$ and consequently that for $k, l \neq 0$

$$U^\dagger a_k^\dagger a_0 U = a_k^\dagger \sqrt{N - N_+} \tag{2.15}$$

$$U^\dagger a_k^\dagger a_l a_0^\dagger a_0 U = a_k^\dagger a_l (N - N_+) \tag{2.16}$$

$$U^\dagger a_k^\dagger a_l^\dagger a_0 a_0 U = a_k^\dagger a_l^\dagger \sqrt{(N - N_+)(N - N_+ - 1)}. \tag{2.17}$$

The last two identities follow from the first, in fact. We trivially extend this transformation to an operator $L^2(\mathbb{T}^d) \otimes \mathcal{H}_N \to L^2(\mathbb{T}^d) \otimes \mathcal{F}_+^{\leq N}$ by tensor-multiplying it by the unit operator on the impurity Hilbert space. This extended U is again unitary and satisfies (2.15) with a_0 defined by (2.6). One should keep in mind that U depends on N. Equipped with the extended operator U, we now state our second main result concerning the eigenvectors.

Theorem 2. *Let $\mathbb{P}_i$ denote the orthogonal projection onto the eigenspace of $\mathbb{H}^{\mathsf{F}}$ corresponding to energy $e_i(\mathbb{H}^{\mathsf{F}})$. Under Assumption 1, the following statements hold true.*

1. *The spectra of both H_N and $\mathbb{H}^{\mathsf{F}}$ are discrete.*

2. *For all i such that there exists an eigenstate Ψ_i of H_N corresponding to energy $e_i(H_N)$ with $e_i(H_N) - e_0(H_N) < \xi$ where $\xi > 0$ is fixed, we have*

$$\lim_{N\to\infty} (\Psi_i, U^\dagger \mathbb{P}_i U \Psi_i)_{L^2(\mathbb{T}^d)\otimes\mathcal{F}_+} = 1. \tag{2.18}$$

Remark 2.1. In contrast to the case without impurity, the eigenstates of $\mathbb{H}^{\mathrm{F}}$ are not explicit. In particular, they display non-trivial correlations among the phonons and are not quasi-free.

Remark 2.2. We have not tried to find the rate of growth of the size of the energy window in N so as provide the corresponding error for replacing eigenvectors. This rate is probably much worse than the one from Theorem 3.

Remark 2.3. Theorems 3 and 2 together imply, as $N \to \infty$, the norm resolvent convergence of $H_N - E_{\mathrm{H}}(N)$ towards $\mathbb{H}^{\mathsf{F}}$, that is, for any $z \in \mathbb{C}\backslash\mathbb{R}$,

$$\lim_{N\to\infty} ||(U_N(H_N - E_{\mathrm{H}}(N))U_N^\dagger - z)^{-1} - (\mathbb{H}^{\mathsf{F}} - z)^{-1}|| = 0 \tag{2.19}$$

in operator norm. Here U_N has to be understood as a partial isometry, i.e., $U_N^\dagger$ is extended by 0 to all of $L^2(\mathbb{T}^d) \otimes \mathcal{F}_+$.

Remark 2.4. Another interesting problem concerns the dynamics of the impurity and the use of the Fröhlich Hamiltonian as its generator. This question has been recently studied from a physics perspective [35, 42]. From a mathematical point of view, there exist results concerning the dynamics of a tracer particle immersed in a Bose gas [43, 44], which concern a different scaling limit than the one considered here and do not utilize the Fröhlich description. The convergence (2.19) can also be reformulated as convergence of the corresponding group of time evolutions, and hence can be used to determine also the dynamics of small excitations of the condensate. In the absence of an impurity, more general results are known where the condensate itself is excited and evolves according to the time-dependent Hartree equation (see, e.g., [45, 46]).

The remainder of this paper contains the proofs of Theorems 3 and 2. Throughout the text, the symbol C denotes a positive constant whose value may change at different appearances. Moreover, unless stated otherwise, all states on the relevant Hilbert spaces are normalized. Finally, all operators that are defined as acting on functions of the Bose gas coordinates or the field modes only are actually everywhere understood as their tensor products with the unit operator on $L^2(\mathbb{T}^d)$, the latter being the Hilbert space of the impurity particle.

2.2 Auxiliary considerations

In this Section we introduce four preparatory Lemmas that will be needed in the proofs of Theorems 3 and 2. For their statement, we need to introduce some notation. We shall often denote the terms on the right side of (3.1), from left to right, by $P^2/2M, T, V$ and W. Let $\mathcal{P}$

denote the projection onto the normalized constant wave function in $L^2(\mathbb{T}^d)$, and $\mathcal{Q} = 1 - \mathcal{P}$. We define the excitation number operator

$$N_+ = \sum_{i=1}^{N} \mathcal{Q}_i \tag{2.20}$$

as an operator on $\mathcal{H}_N$. The sub-index in Q_i means here that we project onto the orthogonal complement of the normalized constant wave function in the i-th variable. The second quantized form of the excitation number operator in the plane wave basis equals

$$N_+ = \sum_{p \neq 0} a_p^\dagger a_p. \tag{2.21}$$

The first Lemma explores the consequences of the mean-field structure of H_N. In particular, the ground state energy of H_N is, to leading order in N, equal to $E_{\mathrm{H}}(N)$, and the excitation number operator is uniformly bounded in N for states of fixed excitation energy.

Lemma 2.2.1. *The ground state energy of H_N, $e_0(H_N)$, satisfies the bounds*

$$\frac{Nv_0}{2} + \sqrt{N} w_0 \geq e_0(H_N) \geq \frac{Nv_0}{2} + \sqrt{N} w_0 - \delta E \tag{2.22}$$

with $\delta E = \int (2\pi^2)^{-1} w^2 + (v(0) - v_0) \geq 0$. Moreover, we have the operator inequality

$$N_+ \leq C(H_N - e_0(H_N)) + C. \tag{2.23}$$

Remark 2.5. Below, we will make use of a direct consequence of this Lemma, namely

$$(\Psi, N_+ \Psi) \leq C\xi + C \tag{2.24}$$

for any state Ψ such that $(\Psi, H_N \Psi) \leq e_0(H_N) + \xi$ with $\xi > 0$.

Proof. The upper bound on the ground state energy is obtained by taking the constant wave function in $L^2(\mathbb{T}^d) \otimes \mathcal{H}_N$ as trial function. We write $H_N = \frac{P^2}{2M} + \frac{1}{2}T + V + (\frac{1}{2}T + W)$; by a standard argument using the positivity of the Fourier coefficients of v we have

$$\begin{aligned} V &= \frac{1}{2(N-1)} \sum_{i,j \in \{1,\dots,N\}} v(x_i - x_j) - \frac{Nv(0)}{2(N-1)} \\ &= \frac{1}{2(N-1)} \sum_p v_p \left| \sum_{i=1}^{N} e^{\mathrm{i}px_i} \right|^2 - \frac{Nv(0)}{2(N-1)} \\ &\geq \frac{N}{2} v_0 - \frac{N}{2(N-1)} (v(0) - v_0) \end{aligned} \tag{2.25}$$

since $\sum_{p \neq 0} v_p \left| \sum_{i=1}^{N} e^{\mathrm{i}px_i} \right|^2 \geq 0$. Next, we use Temple's inequality, see, e.g.,[47]. Consider a Hamiltonian $H = H_0 + Z$ with non-negative self-adjoint operators Z and H_0 with ground state energy satisfying $e_0(H_0) = 0$. Denoting by e_0, e_1 the first two eigenvalues of H, we have clearly $(H - e_0)(H - e_1) \geq 0$. We evaluate this at the ground state of H_0, Ψ_0. We get

$$(\Psi_0, (H - e_0)(H - e_1)\Psi_0) = (\Psi_0, (Z - e_0)(Z - e_1)\Psi_0) \geq 0$$

and rewrite this, since $e_1 > 0$, as

$$e_0 \geq -\frac{(\Psi_0, Z^2 \Psi_0)}{e_1} + \left(1 + \frac{e_0}{e_1}\right) (\Psi_0, Z\Psi_0). \tag{2.26}$$

Using the positivity of Z and $e_1 \geq e_1(H_0)$ we finally get

$$e_0 \geq (\Psi_0, Z\Psi_0) - \frac{(\Psi_0 Z^2 \Psi_0)}{e_1(H_0)}. \tag{2.27}$$

Using this for $H = -\frac{\triangle_x}{2} + N^{-1/2}w(x-R)$ with $Z = N^{-1/2}w(x-R)$ and Ψ_0 the normalized constant function on $\mathbb{T}^d$, we have,

$$e_0\left(-\frac{\triangle_x}{2} + N^{-1/2}w(x-R)\right) \geq N^{-1/2}w_0 - N^{-1}(2\pi^2)^{-1}\int w^2. \tag{2.28}$$

This leads to

$$(\Psi, H_N - E_{\mathrm{H}}(N)\Psi) \geq (\Psi, \frac{T}{2}\Psi) - \left(\frac{N}{2(N-1)}(v(0)-v_0) + (2\pi^2)^{-1}\int w^2\right)\|\Psi\|^2. \tag{2.29}$$

Using that $N_+ \leq (2\pi)^{-2}T$, we see that the desired result holds. □

The second Lemma concerns the fluctuations of the condensate in the ground state, which are seen to be strongly suppressed due to the mean field scaling.

Lemma 2.2.2. *For all $N \geq 2$ we have the operator inequality*

$$N_+^2 \leq C(H_N - e_0(H_N))^2 + C. \tag{2.30}$$

Remark 2.6. Similarly as above, the Lemma immediately implies that if Ψ belongs to the spectral subspace of H_N corresponding to energy $E \leq e_0(N) + \xi$ with $\xi \geq 0$, then we have

$$(\Psi, N_+^2\Psi) \leq C\xi^2 + C \tag{2.31}$$

where the constants depend only on v and w but not on N. This will be of importance below.

Proof. Because $N_+ \leq \frac{1}{2\pi^2}(\frac{1}{2}T)$ and N_+ commutes with T, we find it convenient to give a bound on the operator $\frac{1}{2}N_+T$, as the latter can be directly linked to H_N. Writing

$$\frac{T}{2} = (H_N - e_0(H_N)) + S_1 + S \tag{2.32}$$

with

$$S_1 = -\frac{1}{N-1}\sum_{j=2}^{N} v(x_1 - x_j) - \frac{(-\triangle_1)}{2} - \frac{w(x_1 - R)}{\sqrt{N}} \tag{2.33}$$

and

$$S = e_0(H_N) - \frac{1}{N-1}\sum_{2\leq i\leq j\leq N} v(x_i - x_j) - \frac{1}{\sqrt{N}}\sum_{j=2}^{N} w(x_j - R) - \sum_{j=2}^{N}\frac{-\triangle_j}{2} - \frac{P^2}{2M} \tag{2.34}$$

we estimate the relevant terms. By the Cauchy–Schwarz inequality,

$$(\Psi, N_+(H_N - e_0(H_N))\Psi) \leq \sqrt{(\Psi, N_+^2\Psi)}\sqrt{(\Psi, (H_N - e_0(H_N))^2\Psi)}. \tag{2.35}$$

Note that $(S+S_1)\Psi$ is permutation symmetric in the Bose gas coordinates, so that $(\Psi, N_+(S+S_1)\Psi) = N(\Psi, \mathcal{Q}_1(S+S_1)\Psi)$, where $\mathcal{Q}_1 = 1 - \mathcal{P}_1$. Moreover, S is independent of x_1 hence it commutes with $\mathcal{Q}_1$. Using the inequality (2.25) (with N replaced with $N-1$) as well as Temple's inequality (2.28) and the upper bound on $e_0(H_N)$ in (2.22), we see that

$$S \leq \frac{v_0 + v(0)}{2} + \frac{w_0}{\sqrt{N}} + \frac{N-1}{N}\frac{\int w^2}{2\pi^2} =: \delta E'.$$

Since S commutes with $\mathcal{Q}_1$ we thus have

$$N(\Psi \mathcal{Q}_1 S \Psi) \leq \delta E'(\Psi, N_+\Psi). \tag{2.36}$$

The part of N_+S_1 not containing $-\triangle_1/2 + N^{-1/2}w(x_1-R)$ is equal to $-N(\Psi, \mathcal{Q}_1 v(x_1-x_2)\Psi)$. We introduce the short-hand v_{12} to denote $v(x_1-x_2)$. We write, following [26]

$$(\Psi, \mathcal{Q}_1 v_{12}\Psi) = (\Psi, \mathcal{Q}_1\mathcal{Q}_2 v_{12}\Psi) + (\Psi, \mathcal{Q}_1\mathcal{P}_2 v_{12}\mathcal{P}_2\Psi) + (\Psi, \mathcal{Q}_1\mathcal{P}_2 v_{12}\mathcal{Q}_2\Psi). \tag{2.37}$$

Observe that $(\Psi, \mathcal{Q}_1\mathcal{P}_2 v_{12}\mathcal{P}_2\Psi) = (\Psi, \mathcal{Q}_1\mathcal{P}_2 v_{12}\mathcal{P}_2\mathcal{Q}_1\Psi) + (\Psi, \mathcal{Q}_1\mathcal{P}_2 v_{12}\mathcal{P}_2\mathcal{P}_1\Psi)$, where the last term vanishes and the remaining one is positive. For the first term, we use $(\Psi, \mathcal{Q}_1\mathcal{Q}_2 v_{12}\Psi) \geq -\|v\|_\infty\sqrt{(\Psi \mathcal{Q}_1\mathcal{Q}_2\Psi)}$. Furthermore,

$$\begin{aligned}(\Psi, \mathcal{Q}_1\mathcal{P}_2 v_{12}\mathcal{Q}_2\Psi) &\geq -\frac{1}{2}(\Psi, \mathcal{Q}_2 v_{12}\mathcal{Q}_2\Psi) - \frac{1}{2}(\Psi, \mathcal{Q}_1\mathcal{P}_2 v_{12}\mathcal{P}_2\mathcal{Q}_1\Psi) \\ &\geq -\frac{\|v\|_\infty}{2}\left((\Psi, \mathcal{Q}_2\Psi) + (\Psi, \mathcal{Q}_1\mathcal{P}_2\mathcal{Q}_1\Psi)\right) \geq -\|v\|_\infty(\Psi, \mathcal{Q}_1\Psi)\end{aligned} \tag{2.38}$$

as $\mathcal{P}_2 \leq 1$ and $(\Psi, \mathcal{Q}_1\Psi) = (\Psi, \mathcal{Q}_2\Psi)$ due to the permutation symmetry. The remaining part of S_1 is bounded as

$$\left(\Psi, \mathcal{Q}_1\left(\frac{-\triangle_1}{2} + \frac{1}{\sqrt{N}}w(x_1-R)\right)\Psi\right) \geq -\frac{\|w\|_\infty}{2}\left(\frac{1}{N} + (\Psi, \mathcal{Q}_1\Psi)\right)$$

since $w \geq 0$.

We thus have

$$(\Psi, \mathcal{Q}_1 S_1\Psi) \leq \|v\|_\infty\sqrt{(\Psi, \mathcal{Q}_1\mathcal{Q}_2\Psi)} + (\|v\|_\infty + \tfrac{1}{2}\|w\|_\infty)(\Psi, \mathcal{Q}_1\Psi) + \frac{\|w\|_\infty}{2N}. \tag{2.39}$$

With $N^2(\Psi, \mathcal{Q}_1\mathcal{Q}_2\Psi) \leq (\Psi, N_+^2\Psi)$, this altogether implies

$$\frac{1}{2}(\Psi, N_+T\Psi) \leq \left(\|v\|_\infty + \sqrt{(\Psi, (H_N - e_0(H_N)^2\Psi)}\right)\sqrt{(\Psi, N_+^2\Psi)} + \alpha(\Psi, N_+\Psi) + \frac{\|w\|_\infty}{2}, \tag{2.40}$$

where the N-independent constant α equals $\alpha = \frac{1}{2}\|w\|_\infty + \|v\|_\infty + \delta E'$. As $N_+ \leq gT$, with $g = (2\pi)^2$ being the energy gap of the Laplacian on the torus, this implies

$$gN_+^2 \leq \frac{\|v\|_\infty^2}{\kappa} + \frac{(H_N - e_0(H_N))^2}{\lambda} + \frac{\alpha^2}{\epsilon} + \|w\|_\infty + (\kappa + \epsilon + \lambda)N_+^2$$

for any $\epsilon, \lambda, \kappa > 0$. By choosing $\epsilon = \lambda = \kappa = \frac{g}{4}$, we arrive at the desired result. □

The third and fourth Lemmas concern $\mathbb{H}^{\mathrm{F}}$. They will be of importance when proving the upper bound on the difference of eigenvalues in Theorem 3.

Lemma 2.2.3. *Let $\mathbb{H}_0^{\rm F} = \frac{P^2}{2M} + \sum_{p\neq 0}(p^2+v_p)a_p^\dagger a_p$ denote the particle-conserving part of the Fröhlich Hamiltonian* (2.9)*. Then there exist positive constants C_0, C_1, C_2 such that the inequalities*

$$N_+ \leq C_0 \mathbb{H}_0^{\rm F} \leq C_1 \mathbb{H}^{\rm F} + C_2 \tag{2.41}$$

hold true on $L^2(\mathbb{T}^d)\otimes\mathcal{F}_+$.

Proof. Clearly, as $v_p \geq 0$, one can take $C_0 = g^{-1} = (2\pi)^{-2}$. The particle non-conserving part of $\mathbb{H}^{\sf F}$ consists of the purely bosonic (v-dependent) part $V^{\rm OD}$and a w-dependent part $\tilde{W}$. The latter can be bounded by

$$\tilde{W} \geq -\epsilon \mathbb{H}_0^{\rm F} - \epsilon^{-1} \sum_{p\neq 0} \frac{|w_p|^2}{v_p + p^2} \tag{2.42}$$

for any $\epsilon > 0$. To see this, simply complete the square for a single mode using the inequality $(\eta a_p^\dagger + \eta^{-1} w_p e^{ipR})(\eta a_p + \eta^{-1} w_p e^{-ipR}) \geq 0$, then choose $\eta^2 = \epsilon(p^2+v_p)$ and sum over the modes. It is hence enough to show that the bosonic particle non-conserving part, given by

$$V^{\rm OD} = \frac{1}{2}\sum_{p\neq 0} v_p (a_p^\dagger a_{-p}^\dagger + a_p a_{-p}) \tag{2.43}$$

can be bounded below by $-c\mathbb{H}_0^{\rm F} - c'$ for $0<c<1$ and $c'>0$. By Cauchy–Schwarz,

$$\frac{v_p}{2}(a_p^\dagger a_{-p}^\dagger + a_p a_{-p}) \geq -\epsilon a_p^\dagger a_p - \frac{|v_p|^2}{4\epsilon} a_{-p}^\dagger a_{-p} - \frac{|v_p|^2}{4\epsilon} \tag{2.44}$$

for any $\epsilon > 0$. Now take $\epsilon = \lambda(p^2 + v_p)$ for some $\lambda > 0$ and define $\mu := \frac{\sup_{p\neq 0} v_p^2}{\sup_{p\neq 0} v_p^2 + \inf_{p \neq 0} p^2(p^2+2v_p)}$; then $0<\mu<1$ (recall that $p \in (2\pi\mathbb{Z})^d$) and $v_p^2 \leq \frac{\mu}{1-\mu} p^2(p^2+2v_p)$, or

$$\frac{v_p^2}{p^2+v_p} \leq \mu(p^2+v_p). \tag{2.45}$$

Consequently,

$$V^{\rm OD} \geq -(\lambda + \frac{\mu}{4\lambda})\mathbb{H}_0^{\rm F} - \sum_p \frac{v_p^2}{\lambda(p^2+v_p)}. \tag{2.46}$$

By choosing $\lambda = \frac{\sqrt{\mu}}{2}$, we have $\lambda + \frac{\mu}{4\lambda} = \sqrt{\mu} < 1$ and the desired result follows. □

Remark 2.7. Note that the above Lemma implies that $\mathbb{H}^{\rm F}$ is bounded from below.

The last Lemma relates N_+^2 to $(\mathbb{H}^{\rm F})^2$.

Lemma 2.2.4. *On $L^2(\mathbb{T}^d)\otimes\mathcal{F}_+$ we have*

$$N_+^2 \leq C(\mathbb{H}^{\rm F})^2 + C. \tag{2.47}$$

Proof. We will show that $N_+\mathbb{H}_0^{\rm F} \leq C(\mathbb{H}^{\rm F})^2 + C$, which implies the desired result by the previous lemma. As $[N_+, \mathbb{H}_0^{\rm F}] = 0$, we have

$$N_+\mathbb{H}_0^{\rm F} = \frac{1}{2}(N_+\mathbb{H}_0^{\rm F} + \mathbb{H}_0^{\rm F}N_+) = \frac{1}{2}(N_+\mathbb{H}^{\rm F} + \mathbb{H}^{\rm F}N_+) - \frac{1}{2}(N_+V^{\rm OD} + V^{\rm OD}N_+ + \tilde{W}N_+ + N_+\tilde{W}), \tag{2.48}$$

with $\tilde{W}$ and V^{OD} defined as in the proof of Lemma 2.2.3. Using the canonical commutation relations $[a_p, a_q^\dagger] = \delta_{p,q}$, we compute

$$N_+ V^{\mathrm{OD}} = \sum_{p\neq 0} a_p^\dagger V^{\mathrm{OD}} a_p + \sum_{p\neq 0} \frac{v_p}{2} a_p^\dagger a_{-p}^\dagger. \tag{2.49}$$

Since $V^{\mathrm{OD}} N_+ = (N_+ V^{\mathrm{OD}})^\dagger$ we have $V^{\mathrm{OD}} N_+ = \sum_{p\neq 0} a_p^\dagger V^{\mathrm{OD}} a_p + \sum_{p\neq 0} \frac{v_p}{2} a_p a_{-p}$ and finally

$$\frac{1}{2}(N_+ V^{\mathrm{OD}} + V^{\mathrm{OD}} N_+) = \sum_{p\neq 0} a_p^\dagger V^{\mathrm{OD}} a_p + \frac{1}{2} V^{\mathrm{OD}}. \tag{2.50}$$

Using (2.46) and the fact that $\sum_{p\neq 0} a_p^\dagger \mathbb{H}_0^{\mathrm{F}} a_p = \mathbb{H}_0^{\mathrm{F}}(N_+ - 1)$, we have

$$-\frac{1}{2}(N_+ V^{\mathrm{OD}} + V^{\mathrm{OD}} N_+) \leq \sqrt{\mu}\mathbb{H}_0^{\mathrm{F}} N_+ + \frac{\sqrt{\mu}}{2}\mathbb{H}_0^F + C \tag{2.51}$$

where $\mu < 1$. By Lemma 2.3 and the Cauchy–Schwarz inequality, the last two terms of the above are bounded by $C(\mathbb{H}^{\mathrm{F}})^2 + C$.

For $\tilde{W}$ we perform a computation analogous to (2.50), which yields

$$\frac{1}{2}(N_+ \tilde{W} + \tilde{W} N_+) = \sum_{p\neq 0} a_p^\dagger \tilde{W} a_p + \frac{1}{2}\tilde{W}. \tag{2.52}$$

By completing the square similarly as in Lemma 2.3, we have

$$\tilde{W} \geq -\lambda N_+ - \frac{1}{\lambda}\sum_{p\neq 0} |w_p|^2 \tag{2.53}$$

for any $\lambda > 0$. We obtain

$$-\frac{1}{2}(N_+ \tilde{W} + \tilde{W} N_+) \leq \lambda N_+(N_+ - 1) + \frac{\sum_{p\neq 0} |w_p|^2}{\lambda} N_+ + \frac{1}{2} N_+ + \frac{\sum_{p\neq 0} |w_p|^2}{2} \tag{2.54}$$

for any $\lambda > 0$. By Lemma 2.2.3 and $\mathbb{H}^{\mathrm{F}} \leq \frac{(\mathbb{H}^{\mathrm{F}})^2}{2} + \frac{1}{2}$, we can bound

$$-\frac{1}{2}(N_+ \tilde{W} + \tilde{W} N_+) \leq \lambda C_0 N_+ \mathbb{H}_0^{\mathrm{F}} + (\frac{1}{\lambda} + 1) C (\mathbb{H}^{\mathrm{F}})^2 + C. \tag{2.55}$$

Finally, using again the Cauchy–Schwarz inequality, we can bound

$$N_+ \mathbb{H}^{\mathrm{F}} + \mathbb{H}^{\mathrm{F}} N_+ \leq \epsilon N_+^2 + \frac{1}{\epsilon}(\mathbb{H}^{\mathrm{F}})^2 \tag{2.56}$$

for any $\epsilon > 0$. Invoking Lemma 2.3 again, we obtain for any $\epsilon > 0$ and $\lambda > 0$,

$$\left(1 - \sqrt{\mu} - \frac{1}{2} C_0(\epsilon + 2\lambda)\right) N_+ \mathbb{H}_0^{\mathrm{F}} \leq ((2\epsilon)^{-1} + \lambda^{-1}) C (\mathbb{H}^{\mathrm{F}})^2 + C. \tag{2.57}$$

By choosing ϵ and λ small enough, we arrive at the desired result. □

2.3 Comparing H_N and $\mathbb{H}^{\mathrm{F}}$

The estimates provided in the previous section concern the relation of the number of excitations operator N_+ (or its square) to the Hamiltonians H_N and $\mathbb{H}^{\mathrm{F}}$ independently. Now, making use of the LNSS transformation U introduced in Sec. 2.1.3, we give an important estimate relating $UH_NU^\dagger$ and $\mathbb{H}^{\mathrm{F}}$.

Proposition 2.3.1. *There exist positive constants α, β, independent of N, such that for every $\epsilon > 0$ and every Φ in $L^2(\mathbb{T}^d) \otimes \mathcal{F}_+^{\leq N}$ we have the inequality*

$$\left|\left(\Phi, \left(U(H_N - E_{\mathrm{H}}(N))U^\dagger - \mathbb{H}^{\mathrm{F}}\right)\Phi\right)\right| \leq \alpha\frac{(\Phi, N_+^2\Phi)}{N}\left(1+\frac{1}{\epsilon}\right) + \beta(\Phi, N_+\Phi)\left(\epsilon + \frac{1}{\sqrt{N}}\right). \tag{2.58}$$

The proof of the proposition is divided into two main steps. In step 1, we take care of the higher-order terms in the creation and annihilation operators that appear in the second quantization of H_N, but are absent in $\mathbb{H}^{\mathrm{F}}$. Let

$$\begin{aligned} H_N^{\mathrm{pre-F}} := \frac{P^2}{2M} + \sum_{p\neq 0} p^2 a_p^\dagger a_p + \frac{1}{2(N-1)}\sum_{p\neq 0} v_p(2a_p^\dagger a_p a_0^\dagger a_0 + a_p^\dagger a_0 a_0 a_{-p}^\dagger + a_p a_0^\dagger a_0^\dagger a_{-p}) \\ + \frac{1}{\sqrt{N}}\sum_{p\neq 0} w_p e^{-ipR}(a_p^\dagger a_0 + a_{-p} a_0^\dagger). \end{aligned} \tag{2.59}$$

viewed as an operator on $L^2(\mathbb{T}^d) \otimes \mathcal{H}_N$.

Lemma 2.3.2. *For any $\epsilon > 0$, one has the operator inequalities*

$$-E_\epsilon \leq H_N - E_{\mathrm{H}}(N) - H_N^{\mathrm{pre-F}} \leq F_\epsilon \tag{2.60}$$

where

$$E_\epsilon = \frac{N_+(N_+-1)}{2(N-1)}\left(v_0 + \frac{v(0)}{\epsilon}\right) + \epsilon v_0 \frac{2N-1}{N-1} N_+ \tag{2.61}$$

and

$$F_\epsilon = \frac{\|w\|_\infty}{\sqrt{N}} N_+ + \epsilon v_0 \frac{2N-1}{N-1} N_+ + \left(1+\frac{1}{\epsilon}\right)\frac{N_+(N_+-1)}{2(N-1)} v(0). \tag{2.62}$$

Proof. Using the Cauchy–Schwarz inequality and positivity of v viewed as a two-particle multiplication operator, we have

$$\begin{aligned} &\pm\left((\mathcal{P}\otimes\mathcal{Q} + \mathcal{Q}\otimes\mathcal{P})v(\mathcal{Q}\otimes\mathcal{Q}) + (\mathcal{Q}\otimes\mathcal{Q})v(\mathcal{P}\otimes\mathcal{Q} + \mathcal{Q}\otimes\mathcal{P})\right) \\ &\leq \epsilon(\mathcal{P}\otimes\mathcal{Q} + \mathcal{Q}\otimes\mathcal{P})v(\mathcal{P}\otimes\mathcal{Q} + \mathcal{Q}\otimes\mathcal{P}) + \frac{1}{\epsilon}(\mathcal{Q}\otimes\mathcal{Q})v(\mathcal{Q}\otimes\mathcal{Q}). \end{aligned} \tag{2.63}$$

By translation invariance $Q\otimes\mathcal{P}v\mathcal{P}\otimes\mathcal{P} = 0$. Moreover, the boundedness of v enables us to bound

$$\mathcal{Q}\otimes\mathcal{Q}v\mathcal{Q}\otimes\mathcal{Q} \leq v(0)\mathcal{Q}\otimes\mathcal{Q}. \tag{2.64}$$

Therefore, we have the bounds

$$\begin{aligned} v \geq\ &\mathcal{P}\otimes\mathcal{P}v\mathcal{P}\otimes\mathcal{P} + \mathcal{P}\otimes\mathcal{P}v\mathcal{Q}\otimes\mathcal{Q} + \mathcal{Q}\otimes\mathcal{Q}v\mathcal{P}\otimes\mathcal{P} \\ &+ (1-\epsilon)\left(\mathcal{P}\otimes\mathcal{Q} + \mathcal{Q}\otimes\mathcal{P}\right)v\left(\mathcal{P}\otimes\mathcal{Q} + \mathcal{Q}\otimes\mathcal{P}\right) - \epsilon^{-1}v(0)\mathcal{Q}\otimes\mathcal{Q} \end{aligned} \tag{2.65}$$

and

$$v \le \mathcal{P}\otimes\mathcal{P}v\mathcal{P}\otimes\mathcal{P} + \mathcal{P}\otimes\mathcal{P}v\mathcal{Q}\otimes\mathcal{Q} + \mathcal{Q}\otimes\mathcal{Q}v\mathcal{P}\otimes\mathcal{P} \\ + (1+\epsilon)\left(\mathcal{P}\otimes\mathcal{Q} + \mathcal{Q}\otimes\mathcal{P}\right) v \left(\mathcal{P}\otimes\mathcal{Q} + \mathcal{Q}\otimes\mathcal{P}\right) + (1+\epsilon^{-1})v(0)\mathcal{Q}\otimes\mathcal{Q}. \tag{2.66}$$

Similarly, treating $w(x-R)$ as a one-body multiplication operator parametrized by R, we have

$$0 \le w \le \mathcal{P}w\mathcal{P} + \mathcal{Q}w\mathcal{P} + \mathcal{P}w\mathcal{Q} + \|w\|_\infty \mathcal{Q}. \tag{2.67}$$

Taking into account that

$$(N-1)^{-1}\sum_{p\neq 0} v_p a_p^\dagger a_0^\dagger a_0 a_p \le v_0 N_+ \tag{2.68}$$

one easily arrives, after computing the relevant second quantization representations of the operators appearing in the bounds (2.65) and (2.67), at the desired result. Since this is essentially the same computation as in [26, Sec. 5], we omit the details. □

The operator inequalities in Lemma 2.3.2 quantify the effect of dropping the higher order terms in the creation and annihilation operators appearing in the original Hamiltonian. As a second step, we now estimate the effect of the Bogoliubov substitution of $a_0, a_0^\dagger$ by $\sqrt{N}\in\mathbb{R}$ via the unitary transform U, which replaces the $a_0, a_0^\dagger$ by an operator $\sqrt{N-N_+}$ acting on $\mathcal{F}_+^{\le N}$.

Lemma 2.3.3. *We have the following inequality for all $\Phi \in L^2(\mathbb{T}^d)\otimes\mathcal{F}_+^{\le N}$:*

$$|(\Phi, UH_N^{\mathrm{pre-F}}U^\dagger - \mathbb{H}^{\mathrm{F}}, \Phi)| \le \frac{\alpha'(\Phi, N_+^2\Phi) + \beta'\|\Phi\|^2}{(N-1)}, \tag{2.69}$$

where the positive constants α', β' do not depend on N.

Proof. By using the algebraic properties (2.15)–(3.27) of U we see that the expressions to estimate are the following. First, using (2.15),

$$\begin{aligned} &\left|\left(\Phi, \left[N^{-1/2}\sum_{p\neq 0} w_p e^{-ipR} U(a_p^\dagger a_0 + a_p a_0^\dagger)U^\dagger - \sum_{p\neq 0} w_p e^{-ipR}(a_p^\dagger + a_{-p})\right]\Phi\right)\right| \\ &= \left|\sum_{p\neq 0}\left(\Phi, w_p\left(a_p^\dagger e^{-ipR}\left(1-\sqrt{\frac{N-N_+}{N}}\right) + \left(1-\sqrt{\frac{N-N_+}{N}}\right)a_{-p}e^{ipR}\right)\Phi\right)\right| \\ &\le \epsilon^{-1}\frac{(\Phi, N_+^2\Phi)}{N^2}\sum_p |w_p|^2 + \epsilon(\Phi, N_+\Phi) \end{aligned} \tag{2.70}$$

which gives an expression of the type claimed Proposition 2.3.1 for $\epsilon^{-1} = N^2/(N-1)$. In the above, we used the Cauchy–Schwarz inequality

$$AB + BA^\dagger \le \epsilon A^\dagger A + \epsilon^{-1}B^2 \tag{2.71}$$

for $A = a_p^\dagger e^{-ipR}$ and $B = w_p(1-\sqrt{(N-N_+)/N})$, and used the bound

$$B^2 = w_p^2 N^{-1}(\sqrt{N} + \sqrt{N-N_+})^{-2} N_+^2 \le w_p^2 N_+^2/N^2.$$

Similarly, from (3.27), we arrive at the second term to estimate:

$$\begin{aligned}
&\left|\sum_{p\neq 0}(\Phi, (v_p a_p^\dagger a_{-p}^\dagger \left(\frac{\sqrt{(N-N_+)(N-N_+-1)}}{N-1}-1\right)+h.c.)\Phi)\right| \\
&\leq \epsilon^{-1}\sum_{p\neq 0}|v_p|^2\frac{(\Phi,(N_++1)^2\Phi)}{(N-1)^2}+\sum_{p\neq 0}\epsilon(\Phi, a_p^\dagger a_{-p}^\dagger a_{-p}a_p\Phi) \\
&\leq C\frac{(\Phi,(N_++1)^2\Phi)}{N-1}+\frac{(\Phi,N_+(N_+-1)\Phi)}{N-1}
\end{aligned} \tag{2.72}$$

for $\epsilon^{-1}=N-1$. We used (2.71) for $A=a_p^\dagger a_{-p}^\dagger$ and

$$B=v_p\left(\frac{\sqrt{(N-N_+)(N-N_+-1)}}{N-1}-1\right),$$

whose square is bounded by $v_p^2(\frac{N_++1}{N-1})^2$. Additionally,

$$\sum_{p\neq 0}a_p^\dagger a_{-p}^\dagger a_{-p}a_p \leq \sum_{p\neq 0}a_p^\dagger N_+ a_p = N_+^2 - N_+. \tag{2.73}$$

Similarly,

$$\begin{aligned}
&\left|(\Phi,\left[(N-1)^{-1}v_pU(a_p^\dagger a_p a_0^\dagger a_0+h.c.)U^\dagger-2a_p^\dagger a_p\right]\Phi)\right| \\
&=\left|(\Phi,(v_pa_p^\dagger a_p\left(\frac{N-N_+}{N-1}-1\right)+h.c.)\Phi)\right|\leq v_0\frac{(\Phi,N_+(N_+-1)\Phi)}{N-1}.
\end{aligned} \tag{2.74}$$

By combining these inequalities, we obtain the desired bound. □

The main result of this section, Proposition 2.3.1, is a direct consequence of the last two Lemmas.

2.4 Proof of Theorem 1

For brevity we denote $H_N - E_{\mathrm{H}}(N)$ by H_N'.

2.4.1 Lower bound

Let $\xi>0$ and consider i such that $e_i(H_N)-E_{\mathrm{H}}(N)\leq\xi$. Let G be the span of the $i+1$ lowest eigenvectors of H_N' (their existence is shown in Theorem 2; its proof relies on compactness arguments and does not exploit Theorem 3). For any normalized $\Psi\in G$, $(\Psi,H_N'\Psi)\leq e_i(H_N')$. For $\Psi\in G$, let $\Phi=U\Psi\in L^2(\mathbb{T}^d)\otimes\mathcal{F}_+^{\leq N}$. With the choice $\epsilon=\sqrt{\xi/N}$ in Proposition 2.3.1 it follows, by additionally invoking Lemma 2.2.2, that $(\Phi,UH_N'U^\dagger\Phi)\geq(\Phi,\mathbb{H}^{\mathsf{F}}\Phi)-\frac{C\xi^{3/2}}{\sqrt{N}}$ for some $C>0$. Thus clearly $e_i(H_N')+C\xi^{3/2}N^{-1/2}\geq\max_{\Psi\in G}(\Psi,U^\dagger\mathbb{H}^{\mathsf{F}}U\Psi)$ and, by the min-max principle,

$$e_i(H_N')+C\xi^{3/2}N^{-1/2}\geq e_i(\mathbb{H}^{\mathsf{F}}). \tag{2.75}$$

2.4.2 Upper bound

For the upper bound, we use *Fock space localization*. It is quantified by the following result [28, 48].

Proposition 2.4.1. *Let $A > 0$ be an operator on $\mathcal{F}$ with domain $D(A)$ such that for the projections $\bar{P}_j : \mathcal{F} \to \mathcal{H}_j$ we have $\bar{P}_j D(A) \subset D(A)$ and $\bar{P}_j A \bar{P}_i = 0$ for $|i-j| > \sigma$ for some constant $\sigma > 0$. Then, if $f, g \in C^\infty(\mathbb{R}, \mathbb{R}_{\geq 0})$ with $f^2 + g^2 \equiv 1$ and $f(x) = 1$ for $|x| \leq 1/2$ as well as $f = 0$ for $x > 1$, then we have the inequality*

$$-\frac{C\sigma^3}{M^2}\sum_{j=0}^{\infty} \bar{P}_j A \bar{P}_j \leq A - f_M A f_M - g_M A g_M \leq \frac{C\sigma^3}{M^2}\sum_{j=0}^{\infty} \bar{P}_j A \bar{P}_j \tag{2.76}$$

for all $M \in \mathbb{N}$. Here f_M denotes the operator

$$f_M := \sum_{j=0}^{\infty} f\left(\frac{j}{M}\right) \bar{P}_j \tag{2.77}$$

and analogously for g_M.

For the proof, which is based on an IMS-type argument, see [28, Appendix B]. Proposition 2.4.1 can be used to quantify the error made by constraining the states on Fock space to contain only up to M particles. From the Proposition, we deduce

Lemma 2.4.2. *We have*

$$\mathbb{H}^{\mathrm{F}} - f_M \mathbb{H}^{\mathrm{F}} f_M - g_M \mathbb{H}^{\mathrm{F}} g_M \geq -\frac{C}{M^2}(\mathbb{H}^{\mathrm{F}} + C) \tag{2.78}$$

for all $M \in \mathbb{N}$.

Proof. We apply Proposition 2.4.1 for $A = \mathbb{H}^{\mathrm{F}} - e_0(\mathbb{H}^{\mathrm{F}})$. From Lemma 2.2.3 it follows $e_0(\mathbb{H}^{\mathrm{F}}) \geq -C_2/C_1$ and further that $\sum_j \bar{P}_j(\mathbb{H}^{\mathrm{F}} - e_0(\mathbb{H}^{\mathrm{F}})\bar{P}_j = \mathbb{H}_0^{\mathrm{F}} - e_0(\mathbb{H}^{\mathrm{F}}) \leq C_1 C_0^{-1}\mathbb{H}^{\mathrm{F}} + (C_2 C_0^{-1} - e_0(\mathbb{H}^{\mathrm{F}}))$, which leads to the right hand side of the claimed inequality, with $\sigma = 2$. Using $f_M^2 + g_M^2 = \mathbb{I}$, we have $A - f_M A f_M - g_M A g_M = \mathbb{H}^{\mathrm{F}} - f_M \mathbb{H}^{\mathrm{F}} f_M - g_M \mathbb{H}^{\mathrm{F}} g_M$, which yields the left hand side of the desired result. □

Lemma 2.4.3. *Let $Y \subset L^2(\mathbb{T}^d) \otimes \mathcal{F}_+$ be the spectral subspace of $\mathbb{H}^{\mathrm{F}}$ corresponding to an energy window $[e_0(\mathbb{H}^{\mathrm{F}}), e_0(\mathbb{H}^{\mathrm{F}}) + \xi]$ for $\xi > 0$. Then $\dim f_N Y := \dim\{f_N \Psi : \Psi \in Y\} = \dim Y$ for N large enough and $\frac{\xi}{N}$ small enough.*

Proof. Suppose $\dim f_N Y < \dim Y$, in which case there exists $\Phi \in Y$ with $\|\Phi\| = 1$ such that $f_N \Phi = 0$. In particular, $\Phi = g_N \Phi$. From Lemma 2.2.3 we thus conclude that

$$e_0(\mathbb{H}^{\mathrm{F}}) + \xi \geq (\Phi, \mathbb{H}^{\mathrm{F}}\Phi) = (\Phi, g_N \mathbb{H}^{\mathrm{F}} g_N \Phi) \geq C(\Phi, g_N \mathcal{N}_+ g_N \Phi) - C \geq CN - C, \tag{2.79}$$

which is a contradiction for large N and small ξ/N. □

Let us now take $Y \subset L^2(\mathbb{T}^d) \otimes \mathcal{F}_+$ to be the spectral subspace of $\mathbb{H}^{\mathrm{F}}$ corresponding to energies $E \leq e_i(\mathbb{H}^{\mathrm{F}})$, and let $1 \leq \xi \leq N$. The bound (2.75) together with the upper bound of Lemma 2.2.1 implies that $e_i(\mathbb{H}^{\mathrm{F}}) \leq C\xi$, and hence also $(\Phi, (\mathbb{H}^{\mathrm{F}})^k \Phi) \leq C\xi^k$ for $k = 1, 2$ for any $\Phi \in Y$. By Lemma 2.4.2 and Proposition 2.3.1 (with the choice $\epsilon = \sqrt{\xi/N}$) we have

$$\mathbb{H}^{\mathsf{F}} \geq f_N U H_N' U^\dagger f_N + e_0(\mathbb{H}^{\mathrm{F}}) g_N^2 - \frac{C}{N^2}(\mathbb{H}^{\mathrm{F}} + K) - C\frac{f_N N_+^2 f_N}{\sqrt{N\xi}} - C\sqrt{\frac{\xi}{N}} f_N N_+ f_N. \quad (2.80)$$

By taking the expectation value in any normalized $\Phi \in Y$, we obtain, by Lemmas 2.2.3 and 2.2.4 and the simple inequalities $N_+^k \geq f_N N_+^k f_N$ for $k = 1, 2$, the bound

$$C\xi \left(\frac{\xi}{N}\right)^{1/2} + e_i(\mathbb{H}^{\mathrm{F}}) \geq (\Phi, f_N U H_N' U^\dagger f_N \Phi) + e_0(\mathbb{H}^{\mathrm{F}})(\Phi, g_N^2 \Phi). \quad (2.81)$$

Since $g^2(x) \leq 2x$, we have $g_N^2 \leq \frac{2N_+}{N} \leq \frac{C\mathbb{H}^{\mathrm{F}}+C}{N}$ by Lemma 2.2.3. For $Y \in \Phi$ we thus have $(\Phi, g_N^2 \Phi) \leq \frac{C\xi + C}{N}$. Hence $1 \geq (\Psi, f_N^2 \Psi) \geq 1 - \frac{C\xi+C}{N} > 0$ for large N and ξ/N small enough. By Lemma 2.4.3 and the min-max principle, the maximum over Y of the right hand side (2.81) is at least as large as $e_i(H_N') + O(\xi^2 N^{-1})$. This allows us to conclude that

$$C\xi \left(\frac{\xi}{N}\right)^{1/2} + e_i(\mathbb{H}^{\mathrm{F}}) \geq e_i(H_N') \quad (2.82)$$

for some $C > 0$, which is the desired bound.

2.5 Proof of Theorem 2

2.5.1 Existence of eigenvectors

We shall now conclude the existence of eigenvectors of H_N and $\mathbb{H}^{\mathsf{F}}$ by showing that these operators have compact resolvents. By the definition of compactness and the spectral theorem one easily sees that if $A \geq B > 0$, then the compactness of B^{-1} implies the compactness of A^{-1}. Since the particles are confined to the unit torus, for any $\epsilon > 0$ the operators $T + \epsilon$ and $P^2 + \epsilon$ are strictly positive and have purely discrete spectra with eigenvalues accumulating at infinity; therefore, they have a compact inverse. The same observation applies to the operator

$$\mathbb{H}_0 := \frac{P^2}{2M} + \sum_{p \neq 0} e_p b_p^\dagger b_p \quad (2.83)$$

since $\lim_{|p| \to \infty} e_p = \infty$ and $\inf_p e_p > 0$. Since $H_N \geq T + \frac{P^2}{2M}$, we conclude that H_N has compact resolvent, which, by the spectral theorem, implies that the spectrum of H_N is discrete and eigenvectors exist. On the other hand, by completing the square, as in Lemma 2.2.3, it is easy to see that

$$\mathbb{H}^{\mathsf{F}} \geq c\mathbb{H}_0 - d \quad (2.84)$$

for appropriate constants $c, d > 0$. The existence of eigenvectors of $\mathbb{H}^{\mathsf{F}}$, along with the fact that its spectrum is discrete, follows now from precisely the same reasoning as above. This proves the first part of Theorem 2.

2.5.2 Convergence of eigenvectors

Fix $\xi > 0$ and take any i such that $e_i(H_N') \leq \xi$, uniformly in N. Recall that from the proof of the lower bound in Theorem 3, we have $\sum_{j=0}^{i} e_j(\mathbb{H}^{\mathsf{F}}) \leq \sum_{j=0}^{i} (U\Psi_j, \mathbb{H}^{\mathsf{F}} U\Psi_j) \leq$

$\sum_{j=0}^{i} e_j(H'_N) + c_N$ with $\lim_N c_N = 0$ for i fixed. The upper bound (2.82) implies further that $e_j(H'_N) \leq e_j(\mathbb{H}^\mathsf{F}) + c'_N$ where again c'_N goes to zero as $N \to \infty$. Thus,

$$\lim_{N\to\infty} \sum_{j=0}^{i} (U\Psi_j, \mathbb{H}^\mathsf{F} U\Psi_j) = \sum_{j=0}^{i} e_j(\mathbb{H}^\mathsf{F}). \tag{2.85}$$

We first show the convergence for ground states. Recall that $\mathbb{P}_i$ denotes the orhogonal projection onto the eigenspace of $\mathbb{H}^\mathrm{F}$ corresponding to energy $e_i(\mathbb{H}^\mathrm{F})$. By writing $U\Psi_0 = a_N + b_N$, $a_N \in \mathrm{ran}\mathbb{P}_0$ and $b_N \perp a_N$, we have

$$(U\Psi_0, \mathbb{H}^\mathsf{F} U\Psi_0) \geq \|\Psi_0\|^2 e_0(\mathbb{H}^\mathsf{F}) + \left(\inf_{\Psi \in \ker \mathbb{P}_0} (\Psi, \mathbb{H}^\mathsf{F}\Psi) - e_0(\mathbb{H}^\mathsf{F}) \right) \|b_N\|^2. \tag{2.86}$$

By using (2.85) for $i = 0$ as well as the fact that $\inf_{\Psi\in\ker\mathbb{P}_0}(\Psi, \mathbb{H}^\mathsf{F}\Psi) > e_0(\mathbb{H}^\mathsf{F})$ by the discreteness of the spectrum of $\mathbb{H}^\mathsf{F}$, we have $\lim_{N\to\infty} \|b_N\| = 0$, which is the desired result for the ground states.

For higher eigenvectors, we apply a reasoning similar to the one in [49, Sec. 5]. Let us take any $k > 0$ such that $e_{k+1}(\mathbb{H}^\mathsf{F}) > e_k(\mathbb{H}^\mathsf{F})$. Consider the operator $\tilde{H} := \mathbb{H}^\mathsf{F}\tilde{\mathbb{P}}_k + e_k(\mathbb{H}^\mathsf{F})(1-\tilde{\mathbb{P}}_k)$ where $\tilde{\mathbb{P}}_k$ denotes the projection onto the $k+1$ lowest eigenvectors of the Fröhlich Hamiltonian $\mathbb{H}^\mathrm{F}$. $\tilde{H}$ acts on $L^2(\mathbb{T}^d) \otimes \mathcal{F}_+$ and has spectrum $\{e_0(\mathbb{H}^\mathsf{F}), ..., e_k(\mathbb{H}^\mathsf{F})\}$. Therefore, by the min-max principle,

$$\sum_{i=0}^{k} (U\Psi_i, \tilde{H} U\Psi_i) \geq \sum_{i=0}^{k} e_i(\mathbb{H}^\mathsf{F}). \tag{2.87}$$

Clearly, $\mathbb{H}^\mathsf{F} \geq \mathbb{H}^\mathsf{F}\tilde{\mathbb{P}}_k + e_{k+1}(\mathbb{H}^\mathsf{F})(1-\tilde{\mathbb{P}}_k)$ so that

$$\sum_{i=0}^{k} (U\Psi_i, \mathbb{H}^\mathsf{F} U\Psi_i) \geq \sum_{i=0}^{k} e_i(\mathbb{H}^\mathsf{F}) + (e_{k+1}(\mathbb{H}^\mathsf{F}) - e_k(\mathbb{H}^\mathsf{F})) \sum_{i=0}^{k} \|(1-\tilde{\mathbb{P}}_k)U\Psi_i\|^2, \tag{2.88}$$

which can be rewritten as

$$\sum_{i=0}^{k} (U\Psi_i, \tilde{\mathbb{P}}_k U\Psi_i) \geq k + 1 - \frac{\sum_{i=0}^{k} \left(e_i(\mathbb{H}^\mathsf{F}) - (\Psi_i, U^\dagger \mathbb{H}^\mathsf{F} U\Psi_i) \right)}{e_{k+1}(\mathbb{H}^\mathsf{F}) - e_k(\mathbb{H}^\mathsf{F})}. \tag{2.89}$$

Note that the last term converges to zero as $N \to \infty$ by (2.85). Take now l to be the largest integer such that $e_l(\mathbb{H}^\mathsf{F}) < e_k(\mathbb{H}^\mathsf{F})$. The dimension of the eigenspace corresponding to $e_k(\mathbb{H}^\mathsf{F})$ therefore equals $k - l$. We have the simple identity

$$\sum_{i=l+1}^{k} (U\Psi_i, \mathbb{P}_k U\Psi_i) = \sum_{i=0}^{k} (U\Psi_i, \tilde{\mathbb{P}}_k U\Psi_i) + \sum_{i=0}^{l} (U\Psi_i, \tilde{\mathbb{P}}_l U\Psi_i) - \sum_{i=0}^{k} (U\Psi_i, \tilde{\mathbb{P}}_l U\Psi_i) - \sum_{i=0}^{l} (U\Psi_i, \tilde{\mathbb{P}}_k U\Psi_i) \tag{2.90}$$

(note the presence of both tilded and untilded operators). For the first two terms, we can use (2.89) for a lower bound. Moreover, since the Ψ_i are orthonormal, we have $\sum_{i=0}^{k} (U\Psi_i, \tilde{\mathbb{P}}_l U\Psi_i) \leq \mathrm{Tr}\,\tilde{\mathbb{P}}_l = l + 1$. The last term in (2.90) is trivially bounded from below by $-(l+1)$. We thus conclude that

$$k - l \geq \sum_{i=l+1}^{k} (U\Psi_i, \mathbb{P}_k U\Psi_i) \geq k - l - C_N - D_N, \tag{2.91}$$

where the quantities $C_N > 0, D_N > 0$ can be read off from (2.89) and vanish as $N \to \infty$, because of (2.85). Therefore, $\sum_{i=l+1}^{k} (U\Psi_i, \mathbb{P}_k U\Psi_i) \to k - l$, but as each individual term in the sum is ≤ 1, we must have $\lim(U\Psi_i \mathbb{P}_k U\Psi_i) = 1$ for every eigenstate of H'_N with energy $e_k(H'_N)$. This is precisely the convergence result stated in Theorem 2, whose proof is now complete.

CHAPTER 3

Polaron models with regular interactions at strong coupling

This chapter contains the paper

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Abstract. We study a class of polaron-type Hamiltonians with sufficiently regular form factor in the interaction term. We investigate the strong-coupling limit of the model, and prove suitable bounds on the ground state energy as a function of the total momentum of the system. These bounds agree with the semiclassical approximation to leading order. The latter corresponds here to the situation when the particle undergoes harmonic motion in a potential well whose frequency is determined by the corresponding Pekar functional. We show that for all such models the effective mass diverges in the strong coupling limit, in all spatial dimensions. Moreover, for the case when the phonon dispersion relation grows at least linearly with momentum, the bounds result in an asymptotic formula for the effective mass quotient, a quantity generalizing the usual notion of the effective mass. This asymptotic form agrees with the semiclassical Landau–Pekar formula and can be regarded as the first rigorous confirmation, in a slightly weaker sense than usually considered, of the validity of the semiclassical formula for the effective mass.

3.1 Introduction and main results

3.1.1 The model

The polaron problem concerns the motion of a quantum particle of mass m exchanging energy and momentum with a large environment modeled by a bosonic field. The model has a long history tracing back to the thirties [77, 67, 9, 4] but due to its basic character it remains a model of reference in many problems, and is still under active investigation in condensed matter physics; we refer to [50, 1] for an overview and further references. The models under study here are defined by the Hamiltonian

$$\mathbb{H} = -\frac{1}{2m}\Delta_x + \int_{\mathbb{R}^d} \epsilon(k) a_k^\dagger a_k dk + \sqrt{\alpha}\int_{\mathbb{R}^d} \left(v(k) a_k e^{ik\cdot x} + \overline{v(k)} a_k^\dagger e^{-ik\cdot x}\right) dk. \tag{3.1}$$

This operator acts on $L^2(\mathbb{R}^d) \otimes \mathcal{F}$ with $\mathcal{F}$ the bosonic Fock space over $L^2(\mathbb{R}^d)$, and with $a_k, a_k^\dagger$ the usual annihilation and creation operators. The phonon *dispersion relation* ϵ is a positive function, v quantifies the interaction of the particle with the field modes and is referred to as the *form factor*, and α is a positive coupling constant, traditionally appearing in (3.1) under the square root. We assume that $\inf_{k\in\mathbb{R}^d} \epsilon(k) > 0$ and $v \in L^2(\mathbb{R}^d)$, in which case (3.1) is well-defined as a self-adjoint operator on the intersection of the domains of Δ_x and the field energy $\int \epsilon(k) a_k^\dagger a_k dk$, respectively. Moreover, we can then readily define two functions naturally related to this Hamiltonian: the *Pekar kernel*

$$h(x) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \frac{v(k)}{\sqrt{\epsilon(k)}} e^{ik\cdot x} dk \tag{3.2}$$

and the position space potential

$$\eta(x) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} v(k) e^{ik\cdot x} dk. \tag{3.3}$$

We shall impose further regularity assumptions on h and η, namely that h is in the Sobolev space $W^{2,2}(\mathbb{R}^d)$ and that η is in $W^{1,2}(\mathbb{R}^d)$. Equivalently, the functions $k \mapsto v(k)(1+k^2)\epsilon(k)^{-1/2}$ and $k \mapsto v(k)(1+k^2)^{1/2}$ are in $L^2(\mathbb{R}^d)$. For simplicity, we shall also assume that the form factor and the dispersion relation depend on $|k|$ only, and that the latter is a continuous function of $|k|$. If all these conditions are satisfied, we call $\mathbb{H}$ *regular*.

Our main interest lies in the strong-coupling limit of very large α, and its connection to the semiclassical limit described below. This problem has been studied in the mathematical physics literature [2, 58, 66] in the special case of the *Fröhlich model* corresponding to $d = 3$, $v(k) = (\sqrt{2}\pi|k|)^{-1}$ and $\epsilon(k) = 1$ in appropriate units. It corresponds to the original polaron problem addressing the important problem of electronic conductivity in ionic crystals. Our goal here is to analyze the strong-coupling limit in the regular case, where, on the one hand, one does need to worry about the UV divergences as in the Fröhlich model, but at the same time the useful scaling properties found therein are lost. We believe that performing the strong-coupling analysis for polaron models other than the original Fröhlich Hamiltonian may be of relevance as various versions of the polaron problem, with more general choices of the form factor and the dispersion relation, are being considered in the literature, mostly in the context of the physics of cold atoms, e.g. in the Bose polaron model and its analog, the angulon model [1, 5, 19, 34, 16]. The rigorous results obtained, even if proved for simplified versions of the problem, may be practically useful e.g. as a reference point for numerical calculations. At the same time, the regularity enables us to prove new results concerning the validity of the semiclassical approximation to the effective mass, which constitutes an outstanding open problem. Our result on the effective mass is applicable in the case of a dispersion relation growing at least linearly in $|k|$ as in the case of the Bose polaron, thus excluding the Fröhlich polaron, although we expect that our methods can serve as a starting point in future investigations on this problem also in this case.

3.1.2 Basic considerations and definitions

Because of translation invariance, the Hamiltonian (3.1) commutes with the total momentum

$$-i\nabla_x + \underbrace{\int k\, a_k^\dagger a_k\, dk}_{=:P_f} \tag{3.4}$$

and it can be cast, using a transformation due to Lee, Low and Pines [10], in the unitarily equivalent form

$$\frac{1}{2m}\left(-i\nabla_x - P_f\right)^2 + \mathbb{F} + \sqrt{\alpha}\mathbb{V} \tag{3.5}$$

where $\mathbb{F} = \int \epsilon(k) a_k^\dagger a_k dk$ and $\mathbb{V} = \int (v(k) a_k + \overline{v(k)} a_k^\dagger) dk$. This can be easily diagonalized in the L^2 part of the domain, so that one has the fiber decomposition $\mathbb{H} \simeq \int_\oplus \mathbb{H}_P dP$ with a family of Hamiltonians acting only on Fock space

$$\mathbb{H}_P := \frac{1}{2m}(P - P_f)^2 + \mathbb{F} + \sqrt{\alpha}\mathbb{V} \tag{3.6}$$

describing the system moving with momentum $P \in \mathbb{R}^d$. In this work, we are concerned with the ground state energies at fixed momentum,

$$E(P) := \inf \operatorname{spec} \mathbb{H}_P \tag{3.7}$$

and the absolute ground state energy

$$E_0 = \inf \operatorname{spec} \mathbb{H} = \inf_P E(P). \tag{3.8}$$

The following terminology concerning the dispersion relation will be useful below.

1. We say that ϵ is *massive* if $\Delta := \inf_k \epsilon(k) > 0$.
2. ϵ is *subadditive* if $\epsilon(k_1 + k_2) \leq \epsilon(k_1) + \epsilon(k_2)$ for all $k_1, k_2 \in \mathbb{R}^d$.
3. Moreover, we say that ϵ is of *superfluid type* if

   $$\inf_{k \in \mathbb{R}^d} \frac{\epsilon(k)}{|k|} =: c > 0. \tag{3.9}$$

   The number c is called the *critical velocity*.

Prime examples of the above are optical phonons (with constant dispersion relation) for a massive and subadditive field and acoustic phonons (where $\epsilon(k)$ is linear in $|k|$) for a field of superfluid type. Physically, the first case is encountered in the original Fröhlich polaron model, while a superfluid-type field is found in the Bose polaron. If the dispersion relation is massive and subadditive, $E(P)$ is an isolated, simple eigenvalue for $P^2 < 2m\Delta$. Moreover, $\inf_P E(P) = E(0)$, and $E(P)$ is an analytic function close to $P = 0$ [71, 90]. The *effective mass* is then defined as

$$M_{\text{eff}} := \frac{1}{2} \lim_{P \to 0} \left(\frac{E(P) - E(0)}{P^2} \right)^{-1}. \tag{3.10}$$

In other words, $E(P) \approx E(0) + \frac{P^2}{2M_{\text{eff}}}$ for small P, and the system is envisioned as behaving, for sufficiently small momenta, like a free particle of mass M_{eff} called the polaron, whence the entire model bears its name. We also introduce the function

$$M(P) = \frac{1}{2} \left(\frac{E(P) - E(0)}{P^2} \right)^{-1} \tag{3.11}$$

which we call *the effective mass quotient*. It is well-defined for all P s.t. $E(0) \neq E(P)$, and can be viewed as a *global* measure of the curvature of $E(P)$, in contrast to $M_{\text{eff}} = \lim_{P \to 0} M(P)$ which quantifies this curvature *locally* at $P = 0$. The validity of the polaron picture can be also expressed as a statement that $M(P)$ is asymptotically a constant function for sufficiently small momenta. We find this picture useful below, where we shall consider both the case of P vanishingly small as well as admitting values from a specified range.

3.1.3 Motivation and statements of the results

We shall provide bounds on the above quantities in the limit of large α. These bounds agree with the semi-classical approximation, which we now briefly recall. To do so, let us first observe from (3.6) that the presence of the particle induces non-trivial correlations between the modes of the field; if these are ignored, the problem is easily solvable. Indeed, in the case $m = \infty$, the spectrum of $\mathbb{H}_P$ is equal to that of the operator $\mathbb{F} - \alpha\|h\|^2$, with ground state energy $-\alpha\|h\|^2$. This corresponds to a free bosonic field fluctuating on top of a classical deformation profile induced by a point impurity. The ground state is simply the coherent state $|\phi\rangle$ with

$$a_k|\phi\rangle = -\sqrt{\alpha}\frac{\overline{v(k)}}{\epsilon(k)}|\phi\rangle \qquad \forall k \in \mathbb{R}^d. \tag{3.12}$$

The evaluation of $\mathbb{H}$ on pure tensor products of the form $\psi \otimes \phi$, where ϕ is a coherent state, amounts to replacing the creation and annihilation operators by complex numbers, which is equivalent to treating the boson field in a classical way. In fact, as is well known (we reproduce the argument in the proof of the upper bound in Theorem 3 below), this coherent state ansatz is optimal over all product trial states. In other words, for polaron models, *the adiabatic limit* (corresponding to a product trial state) *and the strong-coupling limit coincide*. The adiabatic limit can certainly be expected to be asymptotically correct if the mass of the particle is large. At the same time, it is well known that the adiabatic limit is asymptotically correct as $\alpha \to \infty$ in the Fröhlich case, indirectly through energy estimates [2] and also as far as the dynamics is concerned [81, 13]. If we were, therefore, to assume that the same conclusion is valid in more generality, our regular case included, we expect that

$$\lim_{\alpha\to\infty} \frac{E_0}{\alpha} = -\|h\|^2. \tag{3.13}$$

Moreover, one can readily postulate how the next order correction should look like: since the leading order corresponds to the picture of a classical point particle situated at the bottom of a potential well created by the phonons, the next order correction should stem from the zero-point oscillations in this well. If we replace the annihilation operators in $\mathbb{H}$ by the numbers $-\sqrt{\alpha}\frac{\overline{v(k)}}{\epsilon(k)}$ (and $a_k^\dagger$ by its complex conjugate) and expand the $e^{ik\cdot x}$ factors to second order, we arrive at the one-particle Schrödinger operator

$$-\frac{\Delta_x}{2m} + \frac{m\omega^2}{2}x^2 - \alpha\|h\|^2, \tag{3.14}$$

where

$$\omega = \sqrt{\frac{2\alpha}{dm}}\|\nabla h\|, \tag{3.15}$$

with well-known ground state energy $\frac{d\omega}{2} - \alpha\|h\|^2$. We hence expect the subleading term to be $d\omega/2$, and thus of order $\alpha^{1/2}$. That these considerations are correct is the content of our first theorem.

Ground state energy asymptotics

Theorem 3. *Let* $\mathbb{H}$ *be regular. Then we have*

$$\begin{aligned} -\alpha\|h\|^2 + \sqrt{\frac{d\alpha}{2m}}\|\nabla h\| \ &\geq\ \inf\operatorname{spec}\mathbb{H}\ \geq \\ \geq\ -\alpha\|h\|^2 + \sqrt{\frac{d\alpha}{2m}}\|\nabla h\| &- \frac{d}{2}\frac{\|\nabla\eta\|^2}{\|\nabla h\|^2} - \frac{d}{8m}\frac{\|\Delta h\|^2}{\|\nabla h\|^2}. \end{aligned} \tag{3.16}$$

In particular, for $E_0 = \inf \operatorname{spec} \mathbb{H}$*,* (3.13) *holds, and*

$$\lim_{\alpha\to\infty} \alpha^{-1/2}\left(E_0 + \alpha\|h\|^2\right) = \sqrt{\frac{d}{2m}}\|\nabla h\|. \tag{3.17}$$

Remark 3.1. As recalled in detail in the proof, the semiclassical limit naturally gives rise to the *Pekar functional*

$$\mathcal{E}_\alpha^{\mathrm{Pek}}(\psi) = \frac{1}{2m}\int |\nabla\psi(x)|^2 dx - \alpha \iint |\psi(x)|^2 g(x-y)|\psi(y)|^2 dxdy, \tag{3.18}$$

where

$$g(x) = \int \frac{|v(k)|^2}{\epsilon(k)} e^{ik\cdot x} dk = (\bar{h} * h)(x), \tag{3.19}$$

and

$$E_0 \leq E^{\mathrm{Pek}} := \inf_{\psi:\|\psi\|=1} \mathcal{E}_\alpha^{\mathrm{Pek}}(\psi). \tag{3.20}$$

In the Fröhlich case, where $g(x) = \frac{1}{|x|}$, one has $\inf \mathcal{E}_\alpha^{\mathrm{Pek}}(\psi) = \alpha^2 \inf \mathcal{E}_1^{\mathrm{Pek}}(\psi) \equiv \alpha^2 e^{\mathrm{Pek}}$, in particular the contribution of the kinetic energy $\int |\nabla\psi|^2$ to $\mathcal{E}_\alpha^{\mathrm{Pek}}$ is *not* negligible in this limit. Existing results [2] show that in this particular case

$$e^{\mathrm{Pek}} \geq \alpha^{-2} E_0 \geq e^{\mathrm{Pek}} - C\alpha^{-1/5} \tag{3.21}$$

for some $C > 0$ and α large. If instead of $\mathbb{R}^d$ one considers a sufficiently regular subset Ω thereof (suitably rescaled to be of linear size α^{-1}), with the corresponding modification of η involving the Laplacian on Ω, then also the subleading correction to E_0, being of order α^0, has been rigorously established [66, 7]. Adapting some of the methods in that proof to improve the control on the UV divergence of the model, the exponent $-1/5$ in the lower bound (3.21) can be slightly improved to $-20/73$ [6].
In our case, we lose the scaling properties of the original Fröhlich model, and the semiclassical energy is a more general function of α; our result captures the first two terms that emerge from the expansion of the kernel (3.19) of the Pekar functional around its maximum.

Remark 3.2. It can be argued that the $O(1)$ correction in (3.16) is optimal as far as the order of magnitude is concerned. These $O(1)$ corrections can be attributed to two sources: the quantum fluctuations of the field and a purely classical effect of anharmonicity of the actual potential well that accompanies the particle's motion. We do not know how to obtain the sharp $O(1)$ correction to E_0, however.

Remark 3.3. While the lower bound in Theorem 3 holds for all values of the parameters in the problem, it is optimal only in our case of interest, i.e., for large α with m fixed. However, our analysis leads to a distinct result in the opposite regime with m large at α fixed. In this case our technique yields a positive term $\frac{\alpha}{4m}\frac{\|\nabla h\|^4}{\|\nabla\eta\|^2}$ as a leading-order finite mass correction to the exact ground state energy at infinite mass $-\alpha\|h\|^2$ in the lower bound. Perturbation theory predicts here $-\alpha\|h\|^2 + \frac{\alpha}{2m}\int \frac{k^2|v(k)|^2}{\epsilon(k)^2}dk + o(m^{-1})$. Clearly $\|\nabla h\|^4 \leq \|\nabla\eta\|^2 \left(\int k^2 \frac{|v(k)|^2}{\epsilon(k)^2}dk\right)$, with equality in the case a constant dispersion relation, but even in this case the resulting correction is off by a factor of two with respect to the result from perturbation theory.

The proof of Theorem 3 will be given in Section 3.2.1. The upper bound relies on a straightforward expansion of the kernel of the Pekar functional. For the lower bound we closely follow the approach of Lieb and Yamazaki [3] in their analysis of the Fröhlich model. In the regular case considered here, the obtained bounds turn out to be sharp, however.

Divergence of the effective mass

Our further results concern the effective mass problem (for other rigorous work concerning this problem, we refer to [14, 59, 15, 85] and references therein). First, we present a generalization of [85] by showing that the effective mass diverges as $\alpha \to \infty$, in all spatial dimensions, and for all regular polaron models with massive fields. This is to be expected from the fact that the strong-coupling limit and the adiabatic limit coincide: while the particle's mass is fixed, the relevant dynamical degrees of freedom behave like a free particle with very large mass, which leads to the effective separation of timescales of the field and of the particle.

Theorem 4. *Let $\mathbb{H}$ satisfy the assumptions of Theorem 3, with a dispersion relation that is massive and subadditive. Then there exists a constant $C > 0$ s.t. for all $\alpha \gg 1$ we have*

$$M_{\text{eff}} \geq C\alpha^{1/4}. \tag{3.22}$$

Remark 4.1. The assumption of subadditivity of ϵ is only used to ensure the existence of a ground state of $\mathbb{H}_0$, which is proved in [90].

Remark 4.2. We emphasize that the result holds regardless of the spatial dimension, assuming, of course, the required regularity of $\mathbb{H}$. On the other hand, in the physics literature the effective mass of a polaron has been investigated numerically also for various different polaron-type models [16, 18, 34], and it appears that for some of these models one can expect different behavior of the effective mass in different dimensions.

Our proof takes the formula for the inverse of the effective mass from second-order perturbation theory as a starting point, and provides an upper bound on this quantity. The proof of this bound relies heavily on Theorem 3. It can be shown that the same conclusion can be reached with the method from [85]. The regularity enables us to simplify the argument, and also to provide an explicit estimate on the rate of the divergence. However, based on the semiclassical analysis, we expect that the effective mass should actually, in the regular case, diverge much faster, namely linearly in α. We perform this semiclassical analysis subsequently (see also [5]) before stating our last result, which addresses the effective mass quotient at non-zero P.

Semiclassical analysis of the effective mass

As discussed above, the behavior of the system at strong coupling can be expected to be inferable from the semiclassical functional

$$\frac{1}{2m}\int |\nabla\psi(x)|^2 dx + 2\sqrt{\alpha}\mathfrak{Re}\int v(p)\varphi(p)\rho_\psi(p)dp + \int \epsilon(p)|\varphi(p)|^2 dp \tag{3.23}$$

with $\rho_\psi(p) = \int |\psi(x)|^2 e^{ip\cdot x}dx$ and $\varphi : \mathbb{R}^d \to \mathbb{C}$ the classical field, which carries momentum $\int p|\varphi(p)|^2 dp$. We wish to minimize (3.23) under the constraint that the total momentum of the system be P. With u a Lagrange multiplier (which can be interpreted as the velocity), the relevant functional to be minimized is thus

$$\begin{aligned}\mathcal{H}_P(\psi,\varphi,u) = &\int \epsilon(p)|\varphi(p)|^2 dp + \frac{1}{2m}\int p^2|\hat{\psi}(p)|^2 dp + \\ &+ 2\sqrt{\alpha}\mathfrak{Re}\int v(p)\varphi(p)\rho_\psi(p)dp + u\cdot\left(P - \int p\left(|\varphi(p)|^2 + |\hat{\psi}(p)|^2\right)dp\right).\end{aligned} \tag{3.24}$$

We expect continuity and accordingly $u \to 0$ as $P \to 0$; we also suppose that to leading order in $|u|$, the particle moves with velocity u while maintaining its waveform, i.e., the ψ minimizing (3.24) is approximately

$$\hat{\psi}_u(p) = \widehat{e^{imu\cdot x}\psi_\alpha^{\mathrm{Pek}}}(p) = \hat{\psi}_\alpha^{\mathrm{Pek}}(p - mu) \tag{3.25}$$

where $\psi_\alpha^{\mathrm{Pek}}$ minimizes (3.18). Plugging this into (3.24), we minimize with respect to the field, with the result that

$$\varphi_u(p) = -\sqrt{\alpha}\frac{\overline{\rho_\alpha^{\mathrm{Pek}}(p)v(p)}}{\epsilon(p) - u\cdot p} \tag{3.26}$$

with $\rho_\alpha^{\mathrm{Pek}} = \rho_{\psi_\alpha^{\mathrm{Pek}}}$. Accordingly, the Lagrange multiplier u has to be chosen such that

$$P = mu + \alpha \int p \frac{|v(p)|^2|\rho_\alpha^{\mathrm{Pek}}(p)|^2}{(\epsilon(p) - u\cdot p)^2} dp. \tag{3.27}$$

Expanding this to leading order in u, we have

$$P = \left(m + \frac{2\alpha}{d}\int p^2 \frac{|v(p)|^2|\rho_\alpha^{\mathrm{Pek}}(p)|^2}{\epsilon(p)^3}\right) u. \tag{3.28}$$

We further evaluate the energy $\mathcal{H}_P(\psi_u, \varphi_u, u)$ and expand it to second order in P, with the result that

$$\mathcal{H}_P(\psi_u,\varphi_u,u) \approx E^{\mathrm{Pek}} + \left(2m + \frac{4\alpha}{d}\int p^2 \frac{|v(p)|^2|\rho_\alpha^{\mathrm{Pek}}(p)|^2}{\epsilon(p)^3} dp\right)^{-1} P^2 \tag{3.29}$$

with E^{Pek} defined in (3.20). We are thus led to the definition of the *Pekar mass formula*

$$M_\alpha^{\mathrm{Pek}} := \frac{2\alpha}{d}\iint |\psi_\alpha^{\mathrm{Pek}}(x)|^2 R(x-y)|\psi_\alpha^{\mathrm{Pek}}(y)|^2 dxdy = \frac{2}{d}\int p^2 \frac{|\varphi_\alpha^{\mathrm{Pek}}(p)|^2}{\epsilon(p)} dp \tag{3.30}$$

where $R(x) := \int \frac{p^2|v(p)|^2}{\epsilon(p)^3} e^{ip\cdot x} dp$, $\psi_\alpha^{\mathrm{Pek}}$ minimizes (3.18) and $\varphi_\alpha^{\mathrm{Pek}}$ is the corresponding minimizing field. If we evaluate the above expression for the original Fröhlich model, in which case $\psi_\alpha^{\mathrm{Pek}}(x) = \alpha^{3/2}\psi_1^{\mathrm{Pek}}(\alpha x)$ and $R(x) = 4\pi\delta(x-y)$, we obtain the celebrated *Landau–Pekar mass formula* [8]

$$M^{\mathrm{LP}} = \frac{8\pi}{3}\alpha^4 \|\psi_1^{\mathrm{Pek}}\|_4^4. \tag{3.31}$$

In the regular case we expect, given Theorem 3, that $|\psi_\alpha^{\mathrm{Pek}}|^2$ tends to a δ-function as $\alpha \to \infty$, and accordingly that

$$\lim_{\alpha\to\infty} \alpha^{-1} M_\alpha^{\mathrm{Pek}} = \frac{2}{d}\int p^2 \frac{|v(p)|^2}{\epsilon(p)^3} dp =: M^{\mathrm{Pek}} \tag{3.32}$$

holds true. This leads us to the following

Conjecture. *Let $\mathbb{H}$ be regular. Then*

$$\lim_{\alpha\to\infty} \alpha^{-1} M_{\mathrm{eff}} = M^{\mathrm{Pek}} = \frac{2}{d}\int \frac{p^2|v(p)|^2}{\epsilon(p)^3} dp. \tag{3.33}$$

This conjecture generalizes the one for the original Fröhlich model, where one expects that $\lim_{\alpha\to\infty}\alpha^{-4}M_{\text{eff}} = \frac{8\pi}{3}\|\psi_1^{\text{Pek}}\|_4^4$, c.f. Eq. (3.31), as suggested by a calculation by Landau and Pekar [8]. A proof of this prediction remains an outstanding open problem. In the physics literature one also encounters discussions beyond the Fröhlich case that lead to Conjecture 3.1.3 [5] (see also [19, Eq. 12]) and also to the linear dependence of the effective mass on α at strong coupling [1].

While we are unable to prove Conjecture 3.1.3, we are able to prove a related result that can be regarded as a confirmation of the validity of the semiclassical approximation in the effective mass problem. Recall the definition of the effective mass quotient in (3.11). Instead of the limit $\lim_{\alpha\to\infty}\alpha^{-1}\lim_{P\to 0}M(P)$, we consider the combined limit

$$\alpha\to\infty,\quad |P|\to\infty \quad \text{with} \quad |P|/\alpha\to 0,\quad |P|/\alpha^{1/2}\to\infty. \tag{3.34}$$

which we denote as

$$\lim_{\substack{\alpha\to\infty\\ \alpha^{1/2}\ll|P|\ll\alpha}} .$$

Then we have

Theorem 5. *Let $\mathbb{H}$ be regular, and assume that ϵ is massive and of superfluid type. Then*

$$\lim_{\substack{\alpha\to\infty\\ \alpha^{1/2}\ll|P|\ll\alpha}} \alpha^{-1}M(P) = M^{\text{Pek}} \tag{3.35}$$

with M^{Pek} defined in (3.32). *In particular, we have for $\mathbb{H}$ satisfying the assumptions of Theorem 3 and for all P with $|P|\leq C\alpha$ for some $C>0$ independent of P and α,*

$$E(P)\leq -\alpha\|h\|^2+\frac{d\omega}{2}+\frac{P^2}{2\alpha M^{\text{Pek}}}+O(|P|\alpha^{-1}), \tag{3.36}$$

where ω is defined in (3.15). *If in addition the dispersion relation is assumed to be of superfluid type, we have for all P such that $|P|\leq C'\alpha$ with $C'>0$ small enough,*

$$E(P)\geq -\alpha\|h\|^2+\frac{d\omega}{2}+\frac{P^2}{2\alpha M^{\text{Pek}}}-\frac{d}{2}\frac{\|\nabla\eta\|^2}{\|\nabla h\|^2}-\frac{d}{8m}\frac{\|\Delta h\|^2}{\|\nabla h\|^2}-O(P^2\alpha^{-3/2}+|P|^3\alpha^{-2}). \tag{3.37}$$

Note that (3.36) and (3.37) are non-zero momentum analogs of the bounds in Theorem 3. In combination, they readily imply (3.35). We conjecture that (3.35) holds without the restriction that $|P|\gg\alpha^{1/2}$ (and hence, in particular, in the case when $P\to 0$ before $\alpha\to\infty$).

Since the limit (3.34) may at first sight appear artificial, let us briefly explain its origin. Theorem 5 states that $E(P)-E(0)$ is, for large α, and in a suitable window of momenta, asymptotically a parabolic curve with a coefficient determined by the semiclassical approximation. This can be regarded as a statement on the global curvature of $E(P)-E(0)$, in contrast to the *local* curvature at $P=0$ described by the effective mass. The size of the window of momenta for which this asymptotic form holds depends on α: the lower margin $|P|\gg\alpha^{1/2}$ ensures that we look at $E(P)$ in the regime when the kinetic energy of the center-of-mass motion is much larger than the $O(1)$ energetic error determining the accuracy of our knowledge of the ground state energy, as expressed in Theorem 3 and the bounds (3.36) and (3.37). The upper margin $|P|\ll\alpha$ is natural in view of the following discussion. Typically, one can expect that $E(P)$ has a parabolic shape for sufficiently small momenta, and this parabolic shape is in general lost when $E(P)$ approaches the bottom of the essential spectrum $E_{\text{ess}}(P)$. There is a formula for the latter [90, 71],

$$E_{\text{ess}}(P) = \inf_{k} \left(E(P-k) + \epsilon(k) \right), \tag{3.38}$$

and in particular $E_{\text{ess}}(P) \leq E(0) + \epsilon(P)$. Hence $E(P) \approx E(0) + \frac{P^2}{2M_{\text{eff}}}$ certainly ceases to be valid for $P^2 \gtrsim M_{\text{eff}}\epsilon(P)$. Since $\epsilon(P) \geq c|P|$ by assumption, this is thus the case if $|P| \gtrsim M_{\text{eff}} \sim \alpha$.

Theorem 5 may be regarded as our principal novel contribution to the existing literature. Its proof utilizes, in particular, a new trial state in order to obtain the upper bound (3.36), which is essentially the extension of the very simple bound $E(0) \leq \inf_\psi \mathcal{E}_\alpha^{\text{Pek}}(\psi)$ to non-zero momenta. The lower bound relies, on the other hand, on an extension of the techniques used in the lower bound of Theorem 3, and is thus also ultimately rooted in [3].

In the remainder of the article we give the proofs of our results. The symbol C denotes a positive constant, independent of α and P, whose exact value may change from one instance to the other.

3.2 Proofs

3.2.1 Proof of Theorem 3

Upper bound

Proof. For any normalized $\phi \in \mathcal{F}$, we have

$$\langle \phi | a_k^\dagger a_k | \phi \rangle \geq |\langle \phi | a_k | \phi \rangle|^2 \qquad \forall k \in \mathbb{R}^d \tag{3.39}$$

with equality if and only if ϕ is a coherent state, i.e., an eigenstate of all the a_k. Thus

$$\inf_{\phi,\psi} \langle \psi \otimes \phi | \mathbb{H} | \psi \otimes \phi \rangle = \inf_{\varphi,\psi} \mathcal{H}(\psi, \varphi) \tag{3.40}$$

where $\mathcal{H}$ is the classical functional

$$\mathcal{H}(\psi, \varphi) = \frac{1}{2m} \int |\nabla \psi(x)|^2 dx + 2\sqrt{\alpha} \mathfrak{Re} \int v(p)\varphi(p)\rho_\psi(p)dp + \int \epsilon(p)|\varphi(p)|^2 dp \tag{3.41}$$

with $\rho_\psi(p) = \int |\psi(x)|^2 e^{ip\cdot x}dx$. Minimizing with respect to the field φ and passing to position space, we obtain the *Pekar functional*

$$\mathcal{E}_\alpha^{\text{Pek}}(\psi) = \frac{1}{2m} \int |\nabla \psi(x)|^2 dx - \alpha \iint |\psi(x)|^2 g(x-y) |\psi(y)|^2 dx dy, \tag{3.42}$$

with $g(x) = \int \frac{|v(k)|^2}{\epsilon(k)} e^{ik\cdot x} dk$. Since $\mathbb{H}$ is isotropic, $g(x) = \int \frac{|v(k)|^2}{\epsilon(k)} \cos(k\cdot x)dk$. By the elementary inequality $\cos x \geq 1 - \frac{x^2}{2}$ we have

$$\mathcal{E}_\alpha^{\text{Pek}}(\psi) \leq -\alpha \|h\|^2 + \mathcal{L}_\alpha(\psi) \tag{3.43}$$

with the functional

$$\begin{aligned} \mathcal{L}_\alpha(\psi) &= \frac{1}{2m} \int |\nabla \psi(x)|^2 dx + \frac{\alpha \|\nabla h\|^2}{2d} \iint |\psi(x)|^2 (x-y)^2 |\psi(y)|^2 dx dy \\ &= \frac{1}{2m} \int |\nabla \psi(x)|^2 dx + \frac{\alpha \|\nabla h\|^2}{d} \left(\int |\psi(x)|^2 x^2 - \left(\int x |\psi(x)|^2 dx \right)^2 \right). \end{aligned} \tag{3.44}$$

It follows from the Heisenberg uncertainty principle that the infimum of $\mathcal{L}_\alpha$ equals $d\omega/2$, with ω in (3.15). This leads to the claimed upper bound. □

Lower bound

Proof. Our starting point is the inequality, valid for all $\lambda \in \mathbb{R}$ and all $R \in \mathbb{R}^d$,

$$\sqrt{\alpha}\lambda[P_f + R, [\mathbb{V}, P_f + R]] \leq \frac{1}{2m}(P_f + R)^2 - 2m\lambda^2\alpha[P_f + R, \mathbb{V}]^2 \tag{3.45}$$

which can be easily proved using the Cauchy–Schwarz inequality (the minus sign on the right-hand side stems from the fact that $[P_f, \mathbb{V}]$ is anti-hermitian). We have the identity

$$\lambda[P_f + R, [\mathbb{V}, P_f + R]] = \lambda[P_f, [\mathbb{V}, P_f] = -\lambda \int k^2 \left(\overline{v(k)}a_k^\dagger + v(k)a_k\right) dk. \tag{3.46}$$

We conclude that for all $P \in \mathbb{R}^d$, the operators $\mathbb{H}_P$ in (3.6) are bounded below, uniformly in P, by

$$\mathbb{H}_P \geq \mathbb{H}'_\lambda := \mathbb{F} + \sqrt{\alpha}\mathbb{W}_\lambda + 2m\lambda^2\alpha[P_f, \mathbb{V}]^2 \tag{3.47}$$

with

$$\mathbb{W}_\lambda = \int (1 - \lambda k^2)\left(v(k)a_k + \overline{v(k)}a_k^\dagger\right) dk. \tag{3.48}$$

Given that $\mathbb{H}$ is unitarily equivalent to $\int_\oplus \mathbb{H}_P dP$, this clearly implies that

$$\inf \operatorname{spec} \mathbb{H} \geq \sup_\lambda \ \inf \operatorname{spec} \mathbb{H}'_\lambda. \tag{3.49}$$

Let

$$w_\lambda(k) := (1 - \lambda k^2)v(k) \tag{3.50}$$

and observe that our assumptions on v and ϵ, i.e., $h \in W^{2,2}(\mathbb{R}^d)$ and ϵ massive, imply that $w_\lambda \epsilon^{-1} \in L^2(\mathbb{R}^d)$. We may thus apply the unitary shift operator U with the property that $Ua_kU^\dagger = a_k - \sqrt{\alpha}\frac{\overline{w_\lambda(k)}}{\epsilon(k)}$ for all $k \in \mathbb{R}^d$ to $\mathbb{H}_\lambda$. We obtain

$$U\left(\mathbb{F} + \sqrt{\alpha}\mathbb{W}_\lambda\right)U^\dagger = \mathbb{F} - \alpha\|h\|^2 + 2\lambda\alpha\|\nabla h\|^2 - \lambda^2\alpha\|\Delta h\|^2. \tag{3.51}$$

Furthermore

$$\begin{aligned} U[P_f, \mathbb{V}]U^\dagger &= \int kv(k)\left(a(k) - \alpha^{1/2}\overline{w_\lambda(k)}\epsilon(k)^{-1}\right) dk - \int k\left(\overline{v(k)}a_k^\dagger - \alpha^{1/2}w_\lambda(k)\epsilon(k)^{-1}\right) dk \\ &= [P_f, \mathbb{V}] \end{aligned} \tag{3.52}$$

since $\int kv(k)\overline{w_\lambda(k)}\epsilon(k)^{-1}dk \in \mathbb{R}$. We are thus left with providing a lower bound to the operator

$$\mathbb{F} + 2m\lambda^2\alpha[P_f, \mathbb{V}]^2. \tag{3.53}$$

Since $\eta \in W^{1,2}(\mathbb{R}^d)$ by assumption, we can introduce the bosonic operators, for $i = 1, \ldots, d$,

$$b_i = \frac{\sqrt{d}}{\|\nabla\eta\|}\int k_i v(k)a_k dk \tag{3.54}$$

with $[b_i, b_j^\dagger] = \delta_{ij}$. Then

$$[P_f, \mathbb{V}]^2 = \frac{\|\nabla\eta\|^2}{d}\sum_{i=1}^d (b_i - b_i^\dagger)^2. \tag{3.55}$$

Let

$$E = \frac{\|\nabla\eta\|^2}{\|\nabla h\|^2}. \tag{3.56}$$

We claim that

$$\mathbb{F} \geq E \sum_{i=1}^{d} b_i^\dagger b_i. \tag{3.57}$$

To prove this, it is enough to show that for every one-phonon vector $\Phi \in L^2(\mathbb{R}^d)$

$$\int \epsilon(k)|\Phi(k)|^2 dk \geq \frac{dE}{\|\nabla\eta\|^2} \sum_{i=1}^{d} \left| \int k_i \overline{v(k)} \Phi(k) dk \right|^2. \tag{3.58}$$

For any $\psi \in L^2(\mathbb{R}^d)$ and d orthonormal functions ϕ_i we have by Bessel's inequality

$$\int |\psi(k)|^2 dk \geq \sum_{i=1}^{d} \left| \int \overline{\phi_i(k)} \psi(k) dk \right|^2. \tag{3.59}$$

Using this for $\psi(k) = \sqrt{\epsilon(k)}\Phi(k)$ and $\phi_i(k) = (d^{-1/2}\|\nabla h\|)^{-1} k_i \frac{v(k)}{\sqrt{\epsilon(k)}}$ yields (3.58). Moreover, since

$$(b_i - b_i^\dagger)^2 = (b_i + b_i^\dagger)^2 - 4b_i^\dagger b_i - 2 \geq -4b_i^\dagger b_i - 2 \tag{3.60}$$

we conclude that (3.53) is bounded below by $-4m\lambda^2\alpha\|\nabla\eta\|^2$ provided that

$$|\lambda| \leq \lambda_0 = \sqrt{\frac{d}{8m\alpha\|\nabla h\|^2}} = \frac{1}{2m\omega}. \tag{3.61}$$

In particular,

$$\inf \operatorname{spec} \mathbb{H} \geq -\alpha\|h\|^2 + \alpha \sup_{|\lambda| \leq \lambda_0} \left(2\lambda\|\nabla h\|^2 - \lambda^2\|\Delta h\|^2 - 4m\lambda^2\|\nabla\eta\|^2 \right). \tag{3.62}$$

The choice $\lambda = \lambda_0$ yields the lower bound in (3.16). This choice for λ is in fact optimal as long as

$$\alpha \geq \alpha_m := \frac{d}{8m} \left(\frac{4m\|\nabla\eta\|^2 + \|\Delta h\|^2}{\|\nabla h\|^3} \right)^2. \tag{3.63}$$

For $\alpha < \alpha_m$, the optimal choice of λ is rather $\lambda = \|\nabla h\|^2(4m\|\nabla\eta\|^2 + \|\Delta h\|^2)^{-1}$, which yields the improved lower bound mentioned in Remark 3.3 in this case. □

3.2.2 Proof of Theorem 4

Proof. Under the stated assumptions on v and ϵ, there exists an isolated eigenvalue at the bottom of the spectrum of $\mathbb{H}_0$, and a unique corresponding ground state ϕ_0 [90]. Using second-order perturbation theory and rotation invariance, one arrives at the formula

$$\frac{1}{2M_{\text{eff}}} = \frac{1}{2m} - \frac{1}{dm^2} \langle \phi_0 | P_f \frac{1}{\mathbb{H}_0 - E_0} P_f | \phi_0 \rangle \tag{3.64}$$

for the effective mass M_{eff} defined in (3.10). Note that $\langle \phi_0 | P_f | \phi_0 \rangle = 0$, hence $QP_f|\phi_0\rangle = P_f|\phi_0\rangle$, where Q is the projection onto the orthogonal complement of the ground state of $\mathbb{H}_0$, and $\mathbb{H}_0 - E_0$ is strictly positive and invertible on the range of Q. Therefore, by the Cauchy-Schwarz inequality,

$$\frac{m}{M_{\text{eff}}} \leq 1 - \frac{2}{dm} \frac{\langle \phi_0 | P_f^2 | \phi_0 \rangle^2}{\langle \phi_0 | P_f (\mathbb{H}_0 - E_0) P_f | \phi_0 \rangle}. \tag{3.65}$$

We exploit the fact that ϕ_0 is the ground state of $\mathbb{H}_0$ and arrive at the identity

$$\langle\phi_0|P_f(\mathbb{H}_0 - E_0)P_f|\phi_0\rangle = \frac{1}{2}\langle\phi_0|[P_f,[\mathbb{H}_0,P_f]]|\phi_0\rangle. \tag{3.66}$$

A simple computation shows that the double commutator equals

$$\frac{1}{2}[P_f,[\mathbb{H}_0,P_f]] = \mathbb{W} := -\frac{\sqrt{\alpha}}{2}\int k^2\left(v(k)a_k + \overline{v(k)}a_k^\dagger\right)dk. \tag{3.67}$$

Define for $\lambda > -\frac{1}{2m}$ and $\mu \in \mathbb{R}$

$$\mathbb{H}(\lambda,\mu) := \mathbb{H}_0 + \lambda P_f^2 + \mu\mathbb{W}, \quad E_0(\lambda,\mu) = \inf\operatorname{spec}\mathbb{H}(\lambda,\mu). \tag{3.68}$$

By the variational principle,

$$E_0(\lambda,\mu) \le E_0 + \lambda\langle\phi_0|P_f^2|\phi_0\rangle + \mu\langle\phi_0|\mathbb{W}|\phi_0\rangle. \tag{3.69}$$

We have the lower bound

$$E_0(0,\mu) \ge -\alpha\int\left(1-\frac{\mu k^2}{2}\right)^2\frac{|v(k)|^2}{\epsilon(k)}dk \tag{3.70}$$

which is finite because of our assumption $h \in W^{2,2}(\mathbb{R}^d)$. Combining the last two inequalities with the upper bound on E_0 from Theorem 3, we conclude that for all negative μ

$$\langle\phi_0|\mathbb{W}|\phi_0\rangle \le \frac{dm\omega^2}{2} - \alpha\frac{\mu}{4}\int k^4\frac{|v(k)|^2}{\epsilon(k)}dk - \mu^{-1}\frac{d\omega}{2}. \tag{3.71}$$

Optimizing over $\mu < 0$ yields the bound

$$\langle\phi_0|\mathbb{W}|\phi_0\rangle \le \frac{dm\omega^2}{2}\left(1 + C\alpha^{-1/4}\right) \tag{3.72}$$

for $C = \|\Delta h\| m^{-1/4}(d/2)^{1/4}\|\nabla h\|^{-3/2}$.

In a similar fashion we conclude from (3.69) that for all $\lambda > -\frac{1}{2m}$

$$\lambda\langle\phi_0|P_f^2|\phi_0\rangle \ge E_0(\lambda,0) - E_0 \ge E_0(\lambda,0) + \alpha\int\frac{|v(k)|^2}{\epsilon(k)}dk - \frac{d\omega}{2} \tag{3.73}$$

where we again used the upper bound from Theorem 3. Now, a lower bound on $E_0(\lambda,0)$ is provided by Theorem 3 for a particle with mass $\frac{m}{(1+2\lambda m)}$:

$$E_0(\lambda,0) \ge -\alpha\int\frac{|v(k)|^2}{\epsilon(k)}dk + \frac{d\omega}{2}\sqrt{1+2\lambda m} - \frac{d}{2}\frac{\|\nabla\eta\|^2}{\|\nabla h\|^2} - \frac{d(1+2\lambda m)}{8m}\frac{\|\Delta h\|^2}{\|\nabla h\|^2}. \tag{3.74}$$

In particular, for any $\lambda > 0$,

$$\langle\phi_0|P_f^2|\phi_0\rangle \ge \frac{dm\omega}{2} + \left(\frac{d\omega}{2}\left(\frac{\sqrt{1+2m\lambda}-1}{\lambda} - m\right)\right) - C\frac{1+\lambda}{\lambda} \tag{3.75}$$

for suitable $C > 0$. For small λ, the second term on the right-hand side behaves like $\omega\lambda$, hence the optimal choice of λ is of the order $\omega^{-1/2} \sim \alpha^{-1/4}$, and we arrive at the bound

$$\langle\phi_0|P_f^2|\phi_0\rangle \ge \frac{dm\omega}{2}\left(1 - C\alpha^{-1/4}\right) \qquad \text{for } \alpha \gg 1. \tag{3.76}$$

Combining (3.65), (3.72) and (3.76), we arrive at the claimed lower bound on the effective mass. □

3.2.3 Proof of Theorem 5

Lower bound

Proof. Recall our assumption $\epsilon(k) \geq c|k|$ for some $c > 0$. Pick $u \in \mathbb{R}^d$ with $|u| < c$, and write

$$\mathbb{H}_P = P \cdot u - \frac{m}{2}u^2 + \frac{(P_f - P + mu)^2}{2m} + \tilde{\mathbb{F}}_u + \sqrt{\alpha}\mathbb{V} \tag{3.77}$$

where

$$\tilde{\mathbb{F}}_u = \int (\epsilon(k) - u \cdot k)\, a_k^\dagger a_k dk. \tag{3.78}$$

We proceed as in the proof of Theorem 3 and use (3.45), this time for $R = P - mu$. This gives the lower bound

$$\begin{aligned} E(P) \geq\ & P \cdot u - \frac{m}{2}u^2 - \alpha\|h_u\|^2 \\ & + \sup_{\lambda \in \mathbb{R}} \left[\inf \operatorname{spec}\{\tilde{\mathbb{F}}_u + 2m\alpha\lambda^2[P_f, \mathbb{V}]^2\} + 2\lambda\alpha\|\nabla h_u\|^2 - \lambda^2\alpha\|\Delta h_u\|^2\right] \end{aligned} \tag{3.79}$$

with

$$h_u(x) = \frac{1}{(2\pi)^{d/2}} \int \frac{v(k)}{\sqrt{\epsilon(k) - u \cdot k}} e^{ik\cdot x} dk. \tag{3.80}$$

Without loss of generality, we can assume that $P = |P|e_1$, where e_1 is the unit vector pointing in the first coordinate direction, and we shall also pick u to point along e_1. The functions

$$\phi_i^u(k) = \frac{k_i v(k)}{\sqrt{\epsilon(k) - u \cdot k}} = \frac{k_i v(k)}{\sqrt{\epsilon(k) - |u|k_1}} \tag{3.81}$$

are then orthogonal, and

$$\begin{aligned} \|\phi_i^u\|^2 &= \frac{1}{d}\int \frac{k^2|v(k)|^2}{\epsilon(k)} dk + u^2 \int \frac{k_i^2 k_1^2 |v(k)|^2}{\epsilon(k)^2(\epsilon(k) - |u|k_1)} dk \\ &\leq \frac{1}{d}\int \frac{k^2|v(k)|^2}{\epsilon(k)} dk \left(1 + \frac{u^2}{c(c-|u|)}\right) \end{aligned} \tag{3.82}$$

where we used $\epsilon(k) \geq c|k| \geq c|k_1|$ in the last step. Bessel's inequality

$$\int |\psi(k)|^2 dk \geq \sum_{i=1}^d \left| \frac{1}{\|\phi_i^u\|} \int \overline{\phi_i^u(k)} \psi(k) dk \right|^2 \tag{3.83}$$

thus yields

$$\tilde{\mathbb{F}}_u \geq \left(1 + \frac{u^2}{c(c-|u|)}\right)^{-1} E \sum_{i=1}^d b_i^\dagger b_i \tag{3.84}$$

with E defined in (3.56). Arguing as in the proof of the lower bound in Theorem 3, we conclude that

$$\inf \operatorname{spec}\{\tilde{\mathbb{F}}_u + 2m\alpha\lambda^2[P_f, \mathbb{V}]^2\} \geq -4m\lambda^2\alpha\|\nabla\eta\|^2 \tag{3.85}$$

as long as

$$|\lambda| \leq \left(1 + \frac{u^2}{c(c-|u|)}\right)^{-1/2} \frac{1}{2m\omega}. \tag{3.86}$$

We choose the maximally allowed value of λ (i.e., equality in (3.86)), and arrive at the lower bound

$$E(P) \geq P \cdot u - \frac{m}{2} u^2 - \alpha \|h_u\|^2 + \left(1 + \frac{u^2}{c(c-|u|)}\right)^{-1/2} \sqrt{\frac{\alpha d}{2m} \|\nabla h_u\|^2 - \frac{d}{2} \frac{\|\nabla \eta\|^2}{\|\nabla h\|^2} - \frac{d}{8m} \frac{\|\Delta h_u\|^2}{\|\nabla h\|^2}}. \tag{3.87}$$

We are left with estimating the norms appearing in (3.87). We have

$$\|h_u\|^2 = \int \frac{|v(k)|^2}{\epsilon(k)} \left(1 + \frac{(u \cdot k)^2}{\epsilon(k)\,(\epsilon(k) - u \cdot k)}\right) dk \leq \|h\|^2 + u^2 \frac{M^{\mathrm{Pek}}}{2(1 - |u|/c)} \tag{3.88}$$

where we used the definition of M^{Pek} in (3.32) and $\epsilon(k) \geq c|k|$. Similarly,

$$\|\Delta h_u\|^2 = \int \frac{|k|^4 |v(k)|^2}{\epsilon(k)} \left(1 + \frac{(u \cdot k)^2}{\epsilon(k)\,(\epsilon(k) - u \cdot k)}\right) dk \leq \|\Delta h\|^2 \left(1 + \frac{u^2}{c(c-|u|)}\right). \tag{3.89}$$

For the remaining term, we simply bound

$$\|\nabla h_u\|^2 = \int \frac{k^2 |v(k)|^2}{\epsilon(k)} \left(1 + \frac{(u \cdot k)^2}{\epsilon(k)\,(\epsilon(k) - u \cdot k)}\right) dk \geq \|\nabla h\|^2. \tag{3.90}$$

We are still free to choose u (subject to the constraint $|u| < c$) and the leading terms to optimize are simply $P \cdot u - \alpha u^2 M^{\mathrm{Pek}}/2$. We therefore choose

$$u = \frac{P}{\alpha M^{\mathrm{Pek}}} \tag{3.91}$$

which yields the desired bound (3.37). □

Remark 5.1. By choosing u simply $O(1)$, the bound (3.87) implies that under the same assumptions on v and ϵ, there exist $\gamma > 0$ and $F_\alpha \in \mathbb{R}$ such that for all $P \in \mathbb{R}^d$,

$$E(P) \geq \gamma |P| + F_\alpha. \tag{3.92}$$

From this and from the analyticity of $E(P)$ in a neighborhood of its global minimum at $P = 0$ one can deduce that there exists a $P^* > 0$ such that

$$E(P) = E^*(P), \quad \forall P : 0 \leq |P| \leq P^*, \tag{3.93}$$

where E^* denotes the convex envelope of E, i.e., the largest convex function not exceeding E. One can verify that

$$E^*(P) = \sup_{s \in \mathbb{R}^d} \left(sP + \inf_{Q \in \mathbb{R}^d} (E(Q) - sQ)\right); \tag{3.94}$$

using the Lee-Low-Pines transformation, this can be cast into the form

$$E^*(P) = \sup_{s \in \mathbb{R}^d} \left(s \cdot P + \inf \operatorname{spec}\ (\mathbb{H} - s \cdot P_{\mathrm{tot}})\right) \tag{3.95}$$

where $P_{\mathrm{tot}} = -i\nabla_x + P_f$. In particular, for any $\varphi \in L^2(\mathbb{R}^d)$ and any L^2-normalized $\psi \in H^1(\mathbb{R}^d)$ we have $E^*(P) \leq \sup_s \mathcal{H}_P(\psi, \varphi, s)$, where $\mathcal{H}_P(\psi, \varphi, s)$ is defined in (3.24). Choosing

$$\psi = \psi_\alpha^{\mathrm{Pek}}, \quad \varphi(p) = \varphi_\alpha^{\mathrm{Pek}}(p) \left(1 + \frac{p \cdot P}{\epsilon(p) M_\alpha^{\mathrm{Pek}}}\right) \tag{3.96}$$

one easily arrives at

$$E^*(P) \leq E^{\mathrm{Pek}} + \frac{P^2}{2M_\alpha^{\mathrm{Pek}}} \qquad \forall P \in \mathbb{R}^d, \tag{3.97}$$

and hence

$$E(P) \leq E^{\mathrm{Pek}} + \frac{P^2}{2M_\alpha^{\mathrm{Pek}}} \qquad \forall P \text{ with } |P| \leq P^*, \tag{3.98}$$

where E^{Pek} is the infimum of the Pekar functional (3.18), and M_α^{Pek} is given by the Pekar mass formula (3.30). If we knew that $|P^*| \sim \alpha$, we could already deduce the main statement of Theorem 5, Eq. (3.35). Without this knowledge, we need to find an upper bound directly on $E(P)$ by using an appropriate trial state for $\mathbb{H}_P$, with is the topic of the next section. The resulting bound holds for all $|P| \lesssim \alpha$, and is hence sufficient for our purpose. Let us also emphasize that for the upper bound in (3.98) via the equality (3.93) the superfluid property of ϵ is crucial. In fact, for a constant dispersion relation (and hence, in particular, in the Fröhlich case) $E^*(P) \equiv E(0)$ and hence $P^* = 0$. On the other hand, the proof of the upper bound that we shall now give holds for all regular polaron Hamiltonians, without the restriction that ϵ be superfluid.

Upper bound

Proof. <u>*The trial state*</u>: Let $\psi \in L^2(\mathbb{R}^d)$ be real-valued, with Fourier transform in $H^1(\mathbb{R}^d)$, and let $\varphi \in L^2(\mathbb{R}^d)$. We denote by $|\varphi\rangle$ the coherent state corresponding to φ, satisfying $a_k|\varphi\rangle = \varphi(k)|\varphi\rangle$ for all $k \in \mathbb{R}^d$. Explicitly, $|\varphi\rangle = e^{a^\dagger(\varphi)-a(\varphi)}|\Omega\rangle$ with $|\Omega\rangle$ – the vacuum on $\mathcal{F}$. We choose a trial state (on $\mathcal{F}$) of the form (comp. [11, 12])

$$|\phi_P\rangle = \psi(P - P_f)|\varphi\rangle. \tag{3.99}$$

This state corresponds to the P-momentum fiber of the product state $\psi \otimes |\varphi\rangle$. It appears that this particular form of a trial state for $\mathbb{H}_P$ was first considered, for the case $P = 0$, by Nagy [11], who in this way obtained the bound $E(0) \leq E^{\mathrm{Pek}}$ directly on $\mathcal{F}$. This form is also behind the intuition of the trial state in [12], where its linearized version is considered. In these cases ψ and φ were chosen to be the momentum space minimizers of the Pekar functional. We shall rather choose functions related to the ones mentioned in the preceding Remark, i.e., (3.96), in particular φ will have an additional explicit P-dependence. Thanks to the regularity, we can sligthly simplify their form using the intuition from Theorem 3, which facilitates the computations. Note that (3.99) induces non-trivial correlations between different modes of the field, in contrast to the full product state. One of the main points of the analysis below is to show that these correlations lead to subleading corrections to the desired energy expression, which naturally appears for our choice of ψ and φ. We proceed with the details and start by rewriting the expected value of the energy and the norm of our trial state in a suitable way.

<u>*Preliminary computations*</u>: We have the identity

$$a_p\psi(P - P_f) = \psi(P - p - P_f)a_p \tag{3.100}$$

whence we deduce the relations

$$\psi(P - P_f)\mathbb{V}\psi(P - P_f) = \int dp\ v(p)\psi(P - P_f - p)\psi(P - P_f)a_p + \text{h.c.} \tag{3.101}$$

as well as

$$\psi(P - P_f)\mathbb{F}\psi(P - P_f) = \int \epsilon(p)a_p^\dagger\psi(P - P_f - p)^2 a_p dp. \tag{3.102}$$

Consequently

$$\langle \phi_P | \mathbb{H}_P | \phi_P \rangle = \frac{1}{2m} \langle \varphi | (P - P_f)^2 \psi (P - P_f)^2 | \varphi \rangle + \int dp \; \epsilon(p) |\varphi(p)|^2 \langle \varphi | \psi (P - P_f - p)^2 | \varphi \rangle$$
$$+ 2\sqrt{\alpha} \mathfrak{Re} \int dp \; v(p) \varphi(p) \langle \varphi | \psi(P - P_f - p) \psi(P - P_f) | \varphi \rangle. \tag{3.103}$$

Define

$$G_{\psi,\varphi}(R) = \langle \varphi | \psi(R - P_f)^2 | \varphi \rangle. \tag{3.104}$$

In particular, $\langle \phi_P | \phi_P \rangle = G_{\psi,\varphi}(P)$. Using the properties of the Weyl operator $e^{a^\dagger(\varphi) - a(\varphi)}$, we compute

$$\langle \varphi | e^{-ix \cdot P_f} | \varphi \rangle = \exp \left(\int |\varphi(p)|^2 (e^{-ip \cdot x} - 1) dp \right) \tag{3.105}$$

and obtain

$$G_{\psi,\varphi}(R) = \frac{1}{(2\pi)^d} \int dx \; \rho_\psi(x) e^{F(x) - F(0) + iR \cdot x} \tag{3.106}$$

where

$$\rho_\psi(x) = \int |\psi(k)|^2 e^{-ik \cdot x} \; dk \tag{3.107}$$

and

$$F(x) := \rho_\varphi(x) = \int |\varphi(p)|^2 e^{-ip \cdot x} dp. \tag{3.108}$$

In a similar fashion, we obtain

$$G^{(2)}_{\psi,\varphi}(R, S) := \langle \varphi | \psi(R - P_f) \psi(S - P_f) | \varphi \rangle = \frac{1}{(2\pi)^d} \int \rho^{(2)}_\psi(x; R - S) e^{iR \cdot x} e^{F(x) - F(0)} dx \tag{3.109}$$

with

$$\rho^2_\psi(x; y) = \int \psi(k) \psi(k - y) e^{-ik \cdot x} dk. \tag{3.110}$$

Finally,

$$\frac{1}{2m} \langle \varphi | (P - P_f)^2 \psi (P - P_f)^2 | \varphi \rangle = \frac{1}{(2\pi)^d} \int \tau_\psi(x) e^{iP \cdot x} e^{F(x) - F(0)} dx \tag{3.111}$$

where

$$\tau_\psi(x) = \frac{1}{2m} \int k^2 \psi(k)^2 e^{-ik \cdot x} dk. \tag{3.112}$$

We shall now specify our choice of ψ and φ. We choose

$$\psi(k) = e^{-\frac{k^2}{2m\omega}} \tag{3.113}$$

where ω is defined in (3.15). With this choice of ψ, we have

$$\rho^2_\psi(x; p) = (m\pi\omega)^{d/2} \, e^{-\frac{1}{4m\omega} p^2} e^{-\frac{ip \cdot x}{2}} e^{-\frac{m\omega}{4} x^2}, \tag{3.114}$$

$$\rho_\psi(x) = \rho^2_\psi(x; 0) = (m\pi\omega)^{d/2} \, e^{-\frac{m\omega}{4} x^2}, \tag{3.115}$$

and

$$\tau_\psi(x) = (m\pi\omega)^{d/2} \left(\frac{d\omega}{4} - \frac{m\omega^2}{8} x^2 \right) e^{-\frac{m\omega}{4} x^2}. \tag{3.116}$$

For φ, we choose

$$\varphi(p) = -\frac{\sqrt{\alpha} \overline{v(p)}}{\epsilon(p)} \left(1 + \frac{p \cdot P}{\alpha M^{\text{Pek}} \epsilon(p)} \right). \tag{3.117}$$

In particular, by the definition of M^{Pek} in (3.32),

$$\int p|\varphi(p)|^2 dp = P \tag{3.118}$$

and

$$\int \epsilon(p)|\varphi(p)|^2 dp = \alpha \int \frac{|v(p)|^2}{\epsilon(p)} dp + \frac{P^2}{2\alpha M^{\mathrm{Pek}}}. \tag{3.119}$$

Furthermore, for this choice of φ we have

$$\mathfrak{Re} F(x) = \alpha J(x) + \frac{1}{\alpha} K_P(x) \tag{3.120}$$

where

$$J(x) := \int \frac{|v(p)|^2}{\epsilon(p)^2} \cos(p \cdot x)\, dp \tag{3.121}$$

and

$$K_P(x) := \frac{1}{(M^{\mathrm{Pek}})^2} \int \frac{|v(p)|^2}{\epsilon(p)^4} (P \cdot p)^2 \cos(p \cdot x)\, dp \tag{3.122}$$

as well as

$$\mathfrak{Im} F(x) = -P \cdot x - \frac{2}{M^{\mathrm{Pek}}} \int \frac{|v(p)|^2}{\epsilon(p)^3} (p \cdot P) \left(\sin(p \cdot x) - p \cdot x\right) dp \equiv -P \cdot x + A(x) \tag{3.123}$$

where we used (3.118). As a consequence,

$$\begin{aligned} G_{\psi,\varphi}(R) &= N_\alpha \int e^{-\frac{m}{4}\omega x^2} e^{\mathfrak{Re} F(x)} e^{i((R-P)\cdot x + A(x))}\, dx \\ &= N_\alpha \int e^{-\frac{m}{4}\omega x^2} e^{\mathfrak{Re} F(x)} \cos\left((R-P)\cdot x + A(x)\right)\, dx \end{aligned} \tag{3.124}$$

where

$$N_\alpha := \frac{1}{(2\pi)^d} (m\pi\omega)^{d/2} e^{-F(0)}. \tag{3.125}$$

We finally evaluate

$$G^{(2)}_{\psi,\varphi}(R,S) = N_\alpha \int e^{-\frac{1}{2\omega}(R-S)^2} e^{-\frac{m\omega}{4}x^2} e^{\mathfrak{Re} F(x)} \cos\left(A(x) + (R-P)\cdot x - \frac{(R-S)\cdot x}{2}\right) dx. \tag{3.126}$$

In the next step, we perform an asymptotic analysis of the integrals appearing in the definitions of $G, G^{(2)}$ for large values of α.

Estimation of the weight integrals: Let

$$I := N_\alpha \int e^{-\frac{m}{4}\omega x^2} e^{\mathfrak{Re} F(x)}\, dx; \tag{3.127}$$

since $\mathfrak{Re} F(x) \leq \mathfrak{Re} F(0)$, this integral is well-defined. We can hence introduce the probability measure

$$m(x)dx = \frac{N_\alpha e^{-\frac{m}{4}\omega x^2} e^{\mathfrak{Re} F(x)}}{I} dx. \tag{3.128}$$

Note that all moments of this distribution exist. We denote the expectation value with respect to this distribution by $\langle \cdot \rangle$, which should not be confused with the usual Dirac notation also employed here. The following lemma shows that $m(x)$ is essentially a Gaussian distibution with effective support on a lengthscale $x \sim \alpha^{-1/2}$ dictated by the $F(x)$.

Lemma 3.2.1. *For all $r \geq 0$ there exist positive constants $C_1^{(r)}, C_2^{(r)}$ such that for all α large enough and all P with $|P|/\alpha$ small enough we have*

$$C_1^{(r)} \alpha^{-(r+d)/2} \leq e^{-F(0)} \int |x|^r e^{-\frac{m}{4}\omega x^2} e^{\mathfrak{Re} F(x)} dx \leq C_2^{(r)} \alpha^{-(r+d)/2}. \tag{3.129}$$

Proof. As $\cos x \leq 1 - \frac{1}{2}x^2 + \frac{1}{24}x^4$, we clearly have, with J defined in (3.121),

$$J(x) \leq J(0) - \lambda x^2 + \theta |x|^4 \tag{3.130}$$

with $\lambda = \frac{1}{2d} \int \frac{p^2 |v(p)|^2}{\epsilon(p)^2} dp$ and $\theta = \frac{1}{24d} \int \frac{|p|^4 |v(p)|^2}{\epsilon(p)^2} dp$. These integrals are finite by our assumptions on v and ϵ. Moreover the function K_P, defined in (3.122), satisfies $K_P(x) \leq K_P(0)$ and hence

$$\mathfrak{Re} F(x) \leq F(0) - \alpha \lambda x^2 + \alpha \theta |x|^4. \tag{3.131}$$

Let us choose ε such that $0 < \varepsilon < \lambda$, and let $\delta = \sqrt{\frac{\varepsilon}{\theta}}$. We have that $J(x) < J(0)$ for any x with $|x| > \delta$. By the Riemann–Lebesgue Lemma, J is continuous and vanishes at infinity. It follows that there exists $\xi > 0$ such that

$$J(x) \leq J(0) - \xi, \quad \forall x : |x| > \delta. \tag{3.132}$$

Note that since J is independent of α and P, so are δ and ξ. From (3.132) and from $K_P(x) \leq K_P(0)$ we conclude that

$$\mathfrak{Re} F(x) \leq F(0) - \alpha \xi \quad \forall x : |x| > \delta. \tag{3.133}$$

We thus obtain the upper bound

$$\begin{aligned} &\int |x|^r e^{-\frac{m}{4}\omega x^2} e^{\mathfrak{Re} F(x)} dx = \int_{|x| \leq \delta} |x|^r e^{-\frac{m}{4}\omega x^2} e^{\mathfrak{Re} F(x)} dx + \int_{|x| > \delta} |x|^r e^{-\frac{m}{4}\omega x^2} e^{\mathfrak{Re} F(x)} dx \\ &\leq e^{F(0)} \int_{\mathbb{R}^d} |x|^r e^{-\alpha(\lambda - \varepsilon) x^2 - \frac{m}{4}\omega x^2} dx + e^{F(0) - \alpha \xi} \int_{\mathbb{R}^d} |x|^r e^{-\frac{m}{4}\omega x^2} dx \\ &= e^{F(0)} \mathcal{C}_r \left(\left(\alpha(\lambda - \varepsilon) + \frac{m\omega}{4} \right)^{-(r+d)/2} + e^{-\alpha \xi} \left(\frac{m\omega}{4} \right)^{-(r+d)/2} \right) \end{aligned} \tag{3.134}$$

where $\mathcal{C}_r = \int_{\mathbb{R}^d} |u|^r e^{-u^2} du = 2\pi^{d/2} \Gamma(\frac{r+d}{2}) / \Gamma(\frac{d}{2})$. Since $\omega \sim \sqrt{\alpha}$ and $\xi > 0$, the desired upper bound follows.

For a lower bound we simply use $\cos x \geq 1 - \frac{1}{2}x^2$, and consequently

$$\mathfrak{Re} F(x) \geq F(0) - \left(\alpha \lambda + \frac{P^2}{\alpha} \mu \right) x^2 \tag{3.135}$$

where

$$\mu = \frac{1}{2d (M^{\text{Pek}})^2} \int |p|^4 \frac{|v(p)|^2}{\epsilon(p)^4} dp. \tag{3.136}$$

Thus we can directly bound

$$\int |x|^r e^{-\frac{m}{4}\omega x^2} e^{\mathfrak{Re} F(x)} dx \geq \frac{e^{F(0)} \mathcal{C}_r}{\left(\alpha \lambda + \frac{P^2}{\alpha} \mu + \frac{m}{4}\omega \right)^{\frac{r+d}{2}}}. \tag{3.137}$$

Again, since $\omega \sim \sqrt{\alpha}$, and since $|P| \leq C\alpha$ by assumption, we arrive at the desired conclusion. □

The lemma implies the bounds

$$\frac{C_1^{(r)}}{C_2^{(0)}}\alpha^{-r/2} \leq \langle |x|^r \rangle \leq \frac{C_2^{(r)}}{C_1^{(0)}}\alpha^{-r/2}. \tag{3.138}$$

With these preliminary computations and results at hand, we shall now estimate the various terms in (3.103), as well as the norm of ϕ_P.

<u>*Bound on the norm*</u>: Note that for all $R \in \mathbb{R}^d$

$$G_{\psi,\varphi}(R) = N_\alpha \int e^{-\frac{m}{4}\omega x^2} e^{\mathfrak{Re} F(x)} \cos\left((R-P)\cdot x + A(x)\right)\ dx \leq I \tag{3.139}$$

with I defined in (3.127). Since $\langle \phi_P|\phi_P\rangle = G_{\psi,\varphi}(P)$, $G_{\psi,\varphi}(P)$ is positive. Using $\cos x \geq 1 - \frac{1}{2}x^2$ again, we have

$$G_{\psi,\varphi}(P) \geq I - \mathcal{J} \tag{3.140}$$

where

$$\mathcal{J} := \frac{1}{2} N_\alpha \int e^{-\frac{m}{4}\omega x^2} e^{\mathfrak{Re} F(x)} A(x)^2\, dx. \tag{3.141}$$

Since $|\sin x - x| \leq C|x|^3$ and $\int \frac{|v(p)|^2}{\epsilon(p)^2}|p|^4\, dp$ is finite, we have

$$|A(x)| \leq C_A |P||x|^3 \tag{3.142}$$

for some constant $C_A > 0$, independent of P and α. Therefore

$$\frac{\mathcal{J}}{I} \leq \frac{C_A^2 P^2}{2}\langle |x|^6 \rangle \leq C\frac{P^2}{\alpha^3} \tag{3.143}$$

by (3.138). Hence, if α is large and $|P| \lesssim \alpha$, $\mathcal{J}/I$ is small and we can conclude that

$$\frac{1}{\langle \phi_P|\phi_P\rangle} = \frac{1}{G_{\psi,\varphi}(P)} \leq \frac{1}{I}\left(1 + C\frac{P^2}{\alpha^3}\right) \tag{3.144}$$

for suitable $C > 0$. This bound on the norm is sufficient for our purpose.

<u>*Bound on the field energy*</u>: Using the definitions, we can express the expected value of the field energy in our trial state as

$$\frac{\langle \phi_P|\mathbb{F}|\phi_P\rangle}{\langle \phi_P|\phi_P\rangle} = \int \epsilon(p)|\varphi(p)|^2 \frac{G_{\psi,\varphi}(P-p)}{G_{\psi,\varphi}(P)}\ dp. \tag{3.145}$$

Using now (3.139), (3.140) and (3.143), we have

$$\frac{G_{\psi,\varphi}(P-p)}{G_{\psi,\varphi}(P)} \leq 1 + C\frac{P^2}{\alpha^3}, \tag{3.146}$$

and hence

$$\frac{\langle \phi_P|\mathbb{F}|\phi_P\rangle}{\langle \phi_P|\phi_P\rangle} \leq \alpha \int \frac{|v(p)|^2}{\epsilon(p)} dp + \frac{P^2}{2\alpha M^{\mathrm{Pek}}} + C\frac{P^2}{\alpha^2} \tag{3.147}$$

for $|P| \lesssim \alpha$, where we used (3.119).

Bound on the interaction energy: We have

$$\langle\phi_P|\mathbb{V}|\phi_P\rangle = 2\,\mathfrak{Re}\int v(p)\varphi(p)G^{(2)}_{\psi,\varphi}(P-p,P)\,dp. \tag{3.148}$$

By plugging in (3.114), we obtain

$$\langle\phi_P|\mathbb{V}|\phi_P\rangle = 2N_\alpha \iint v(p)\varphi(p)e^{-\frac{1}{4m\omega}p^2}e^{-\frac{m\omega}{4}x^2}\cos\left(A(x)-\frac{p\cdot x}{2}\right)e^{\mathfrak{Re}F(x)}\,dxdp. \tag{3.149}$$

Let $\tilde{V}$ denote the above expression without the coupling between p and x under the cosine, i.e.,

$$\tilde{V} = 2N_\alpha\int v(p)\varphi(p)e^{-\frac{1}{4m\omega}p^2}dp\int e^{-\frac{m\omega}{4}x^2}e^{\mathfrak{Re}F(x)}\cos A(x)\,dx. \tag{3.150}$$

Using the definition of $G_{\psi,\varphi}$ and plugging in our choice of φ, we obtain

$$\tilde{V} = -2G_{\psi,\varphi}(P)\sqrt{\alpha}\int\frac{|v(p)|^2}{\epsilon(p)}e^{-\frac{p^2}{4m\omega}}\,dp. \tag{3.151}$$

Note that the contribution of the P-dependent part of φ vanishes here by rotation invariance. By $e^{-x}\geq 1-x$ and the definition of ω in (3.15), this gives

$$\frac{\sqrt{\alpha}\tilde{V}}{\langle\phi_P|\phi_P\rangle} \leq -2\alpha\int\frac{|v(p)|^2}{\epsilon(p)}\,dp + \frac{d\omega}{4}. \tag{3.152}$$

We are left with estimating the difference $|G_{\psi,\varphi}(P)^{-1}(\langle\phi_P|\mathbb{V}|\phi_P\rangle - \tilde{V})|$. We apply the elementary inequality

$$\begin{aligned}&\left|\cos\left(A(x)-\frac{p\cdot x}{2}\right)-\cos A(x)\right| \leq |\cos(A(x))||\cos(p\cdot x/2)-1| + |\sin A(x)||\sin(p\cdot x/2)|\\ &\leq \frac{(p\cdot x)^2}{8} + |A(x)|\frac{|p||x|}{2}\end{aligned} \tag{3.153}$$

where we used $|\cos z - 1| = 2|\sin^2 z/2| \leq z^2/2$. Recalling our choice of φ in (3.117), this gives

$$\sqrt{\alpha}G(P)^{-1}\left(\langle\phi_P|\mathbb{V}|\phi_P\rangle - \tilde{V}\right) \leq I_a + I_b + II_a + II_b \tag{3.154}$$

with the following terms to estimate:

$$\begin{aligned}I_a &= \frac{2\alpha N_\alpha}{G(P)}\iint\frac{|v(p)|^2}{\epsilon(p)}e^{-\frac{1}{4m\omega}p^2}e^{-\frac{m\omega}{4}x^2}e^{\mathfrak{Re}F(x)}\frac{(p\cdot x)^2}{8}dxdp\\ &\leq \frac{\alpha N_\alpha}{4Id}\int\frac{p^2|v(p)|^2}{\epsilon(p)}dp\int x^2e^{-\frac{m\omega}{4}x^2}e^{\mathfrak{Re}F(x)}dx\left(1+C\frac{P^2}{\alpha^3}\right) = \frac{m\omega^2}{8}\langle x^2\rangle\left(1+C\frac{P^2}{\alpha^3}\right)\end{aligned} \tag{3.155}$$

where we have used (3.144), the rotation-invariance of $|v|^2/\epsilon$, and the definition of ω in (3.15);

$$\begin{aligned}I_b &= \frac{2N_\alpha}{G(P)}\iint\frac{|P\cdot p|\;|v(p)|^2}{M^{\mathrm{Pek}}\epsilon(p)^2}e^{-\frac{1}{4m\omega}p^2}e^{-\frac{m\omega}{4}x^2}e^{\mathfrak{Re}F(x)}\frac{(p\cdot x)^2}{8}dxdp\\ &\leq \frac{|P|\;\langle x^2\rangle}{4M^{\mathrm{Pek}}}\left(\int\frac{|p|^3|v(p)|^2}{\epsilon(p)^2}dp\right)\left(1+C\frac{P^2}{\alpha^3}\right)\leq C\frac{|P|}{\alpha}\end{aligned} \tag{3.156}$$

by (3.138);

$$\begin{aligned} II_a &= \frac{2\alpha N_\alpha}{G(P)} \iint \frac{|v(p)|^2}{\epsilon(p)} e^{-\frac{1}{4m\omega}p^2} e^{-\frac{m\omega}{4}x^2} e^{\Re\mathfrak{e} F(x)} |A(x)| \frac{|p||x|}{2} dx dp \\ &\leq C_A \alpha |P| \, \langle |x|^4 \rangle \, \left(\int \frac{|p||v(p)|^2}{\epsilon(p)} \, dp \right) \left(1 + C\frac{P^2}{\alpha^3} \right) \leq C \frac{|P|}{\alpha} \end{aligned} \tag{3.157}$$

by (3.142) and again (3.138); finally

$$\begin{aligned} II_b &= \frac{2N_\alpha}{G(P)} \iint \frac{|P \cdot p| \; |v(p)|^2}{M^{\text{Pek}} \epsilon(p)^2} e^{-\frac{1}{4m\omega}p^2} e^{-\frac{m\omega}{4}x^2} e^{\Re\mathfrak{e} F(x)} |A(x)| \frac{|p||x|}{2} \, dx \, dp \\ &\leq C_A \frac{P^2}{M^{\text{Pek}}} \, \langle |x|^4 \rangle \, \left(\int \frac{|v(p)|^2 |p|^3}{\epsilon(p)^2} dp \right) \left(1 + C\frac{P^2}{\alpha^3} \right) \leq C \frac{P^2}{\alpha^2}. \end{aligned} \tag{3.158}$$

Combining all the estimates, we conclude that in the regime of large α and small $|P|/\alpha$ we have

$$\sqrt{\alpha} \frac{\langle \phi_P | \mathbb{V} | \phi_P \rangle}{\langle \phi_P | \phi_P \rangle} \leq -2\alpha \int \frac{|v(p)|^2}{\epsilon(p)} dp + \frac{d\omega}{4} + \frac{m\omega^2}{8} \langle x^2 \rangle + C \frac{|P|}{\alpha}. \tag{3.159}$$

Bound on the kinetic energy: By plugging (3.116) into (3.111), we see that the first term in

(3.103) is given by

$$\frac{1}{2m} \frac{\langle \phi_P | (P - P_f)^2 | \phi_P \rangle}{\langle \phi_P | \phi_P \rangle} = \frac{d\omega}{4} - \frac{m\omega^2}{8} \frac{\langle x^2 \cos A(x) \rangle}{\langle \cos A(x) \rangle}, \tag{3.160}$$

where $\langle \phi_P | \phi_P \rangle = G_{\psi,\varphi}(P) = I \langle \cos A(x) \rangle$ and, in particular, $0 < \langle \cos A(x) \rangle \leq 1$. We have, by (3.142),

$$\langle x^2 \cos A(x) \rangle \geq \langle x^2 \rangle - CP^2 \langle |x|^8 \rangle, \tag{3.161}$$

and thus

$$\frac{\langle x^2 \cos A(x) \rangle}{\langle \cos A(x) \rangle} \geq \langle x^2 \rangle - CP^2 \langle x^8 \rangle \geq \langle x^2 \rangle - CP^2 \alpha^{-4} \tag{3.162}$$

using (3.138). In particular,

$$\frac{1}{2m} \frac{\langle \phi_P | (P - P_f)^2 | \phi_P \rangle}{\langle \phi_P | \phi_P \rangle} \leq \frac{d\omega}{4} - \frac{m\omega^2 \langle x^2 \rangle}{8} + C \frac{P^2}{\alpha^3}. \tag{3.163}$$

Upon adding (3.163), (3.159), and (3.147), we arrive at the claimed upper bound. □

CHAPTER 4

The ground state energy of the strongly coupled polaron in free space - lower bound, revisited

This chapter contains the unpublished note

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Abstract
We provide a better error estimate for the Lieb and Thomas lower bound to the ground state energy of the Fröhlich polaron in the limit of strong coupling, directly adapting a method recently used in the proof of the ground state asymptotics of the confined model.

4.1 The Fröhlich Hamiltonian

When an electron is moving through a polarizable crystal, it starts to interact with the emerging instanteneous dipoles. In the classical picture, this creates a cloud of screening charge which is dragged along with the electron. In the quantum point of view, this cloud gives rise to a quasi-particle called the polaron, and the actual dipoles themselves amount to a phonon field with a dispersion relation corresponding to the optical branch. This heuristic picture leads to the model of a single quantum particle interacting with a scalar boson field. Because the electrostatic potential from a dipole scales as the square inverse distance from the dipole, in the simplest case of a linear electron-phonon coupling, we have the following (formal) Hamiltonian

$$\mathbb{H} = p^2 + \mathbb{N} - \sqrt{\alpha}\int_{\mathbb{R}^3} dy \frac{1}{2\pi^2|x-y|^2} a_y^\dagger + h.c., \tag{4.1}$$

acting on $L^2(\mathbb{R}^3) \otimes \mathcal{F}$, where $\mathcal{F}$ is the bosonic Fock space over $L^2(\mathbb{R}^3)$. Here $x \in \mathbb{R}^3$ is the electon's coordinate, p^2 is the electron's kinetic energy operator, $\mathbb{N}$ is the number operator on $\mathcal{F}$, and the $a_y^\dagger$ are the bosonic creation operators (operator-valued distributions) on $\mathcal{F}$ creating a dipole at $y \in \mathbb{R}^3$, and $\alpha > 0$ is the coupling constant. Typically in the literature one passes to the Fourier space, in which the *Fröhlich Hamiltonian* arises

$$\mathbb{H} = p^2 + \mathbb{N} - \frac{\sqrt{\alpha}}{(2\pi)^3}\int_{\mathbb{R}^3} dk \frac{1}{|k|} e^{ikx} a_k + h.c., \tag{4.2}$$

with $[a_k, a_{k'}^\dagger] = \delta(k-k')$, and the k's label the momentum modes of the phonon field.
In this work, we will be concerned with the question of the ground state energy of (4.2), $E(\alpha)$, in the case of the strong coupling limit, i.e. $\alpha \gg 1$. Despite the fact that (4.2) has been proposed almost a century ago, the question of the ground state energy asymptotics is still an object of intensive studies when it comes to proving rigorous statements. It has been first suggested in calculations by Pekar and Feynman [9, 4] and then proven by Donsker and Varadhan [58] that $\lim_{\alpha\to\infty} E(\alpha)/\alpha^2 = e^{\mathrm{Pek}}$, where $e^{\mathrm{Pek}} \approx -0.109/(16\pi^2)$ is the *Pekar constant*, which arises if the semiclassical approximation is applied to the problem, wherein the creation and annihilation operators are treated as complex numbers. In 1997 Lieb and Thomas [2] have given a very nice proof of a lower bound to the ground state energy in this form, which came along with the first known error estimate, which scales as $\alpha^{9/5}$. This estimate is far away from the conjectured behaviour of the first order correction to the ground state energy, which should reflect the effects of quantum fluctuations of the phonon field on the energy and is believed to be smaller than the leading term by a factor of α^{-2}. This has recently been proven rigorously by Frank and Seiringer [66] for the case of the confined model, that is, for the case when the electron and the field are confined to move in a set Ω being an open, bounded subset of $\mathbb{R}^3$ with a sufficiently regular boundary, and under some natural assumptions on the *Pekar functional*, an object which naturally appears in the discussion. These assumptions have been recently verified for the case of Ω being a ball in $\mathbb{R}^3$ by Feliciangeli and Seiringer [60].
The proof of the conjecture about the next order term in the functional form of the ground state energy in the case of $\Omega = \mathbb{R}^3$ remains an open problem, however. While in our work are still far away from providing that proof, we at least slightly improve the error bound of Lieb and Thomas, using some techniques that were developed by Frank and Seiringer for the confined case, but which can be (in contrast, however, to some of their results which do rely on the boundedness of Ω) easily adapted to $\Omega = \mathbb{R}^3$.

4.1.1 Notation and units

We mentioned that the problem is physically linked to *quantum fluctuations of the phonon field* because the Pekar calculation, and also the Lieb and Thomas proof relies on a c-number substitution in place of the non-commuting creation and annihilation operators. The subleading term should hence reflect the effect of the $a, a^\dagger$ being actually non-commuting objects. This fact of itself motivates our choice of units, in which the α is incorporated into the length scale of the problem, and then into the creation and annihilation operators [64] These new operators, for $f, g \in L^2$, commute to

$$[a_f, a_g^\dagger] = \frac{(f,g)}{\alpha^2}, \tag{4.3}$$

explicitly displaying the relation between the semi-classical and strong coupling limits. The Hamiltonian is therefore unitarily equivalent to $\alpha^2\mathbb{H}$ with

$$\mathbb{H} = p^2 + \mathbb{N} - (2\pi)^{-3}\int_{\mathbb{R}^3} dk \frac{1}{|k|} e^{ikx} a_k + h.c; \tag{4.4}$$

with $p^2 = -\triangle_{\mathbb{R}^3}$ being the Laplace operator acting on the electronic coordinates. For some orthonormal basis of $L^2(\mathbb{R}^3)$, $\mathbb{N} = \int_{\mathbb{R}^3} a_k^\dagger a_k dk = \sum_i a^\dagger(\phi_i) a(\phi_i)$ with spectrum $\{\frac{i}{\alpha^2}\}_{i=0}^\infty$.

It is understood that in general k stands for the phonon momentum variable and x for the electron's position. We denote the characteristic function of a subset $A \subset \mathbb{R}^3$ by χ_A. For $h(\cdot)$ being an L^2-function of the phonon variables, we denote $h_x(k) = h(k)e^{ikx}$ and $a(f_x) = (2\pi)^{-\frac{3}{2}} \int dk f(k) e^{ikx} a_k$ and similarly for $a^\dagger(f_x)$. Even though

$$v := |k|^{-1} \tag{4.5}$$

and

$$w_x := v_x \chi_{|k| \geq K} \tag{4.6}$$

for any $K > 0$ are not in L^2, we will continue to use this notation for the corresponding operators which appear in the definition of $\mathbb{H}$. Actually, the fact that $v_x \notin L^2(\mathbb{R}^3)$ causes concern about the domain of $\mathbb{H}$, in particular whether it is densely defined ot not. This question was tackled by Griesemer and Wünsch in 2016 [74] and some ideas used in this work were first developed there. Finally, we use the notation that $a \lesssim b$ means that $a \leqslant Cb$ for some constant $C > 0$ independent on the parameters on which b or a possibly depend. Having established the notation and conventions, we are now free to pass to the section containing the main ideas and results.

4.2 Auxiliary considerations, main result and proof strategy

For $K > 0$, write the Hamiltonian as

$$\mathbb{H} = p^2 + \mathbb{N}_- + \mathbb{N}_+ - V_+ - V_- \tag{4.7}$$

with $\mathbb{N}_- = \int_{|k|<K} a_k^\dagger a_k dk$, $\mathbb{N}_+ = \mathbb{N} - \mathbb{N}_-$, $V_+ = a(w_x) + a^\dagger(w_x)$ and $V_- = a(v_x - w_x) + h.c.$. Denote then

$$\mathbb{H}_K := p^2 + N_- - V_-. \tag{4.8}$$

Since we are interested in the lower bound, we can drop the $\mathbb{N}_+$ due to its positivity. The paper of Lieb and Thomas [2] (in fact, only sections II-IV) can be applied to provide an estimate on $\mathbb{H}_K$, which we will state in the form of a theorem.

Theorem 6. *For any $E > 0, P > 0$ and $K > 0$ and $\delta > 0$ sufficiently small, we have*

$$\inf \operatorname{spec} \mathbb{H}_K - e^{\text{Pek}} \geqslant c_1 \delta - E + c_2 \frac{P^2 K}{\delta E} + c_3 \frac{K^3}{\alpha^2 P^3} \tag{4.9}$$

where the c_i's are negative constants independent of α.

The method used in the proof consists of the following steps:

1. First, one localizes the electron in a cube of side length $\sim E^{-1/2}$. By the IMS localization formula, this gives rise to an error of order E, as given above.

2. The phonon modes are already localized into a ball of radius K, which is later divided into cubes of side length P, called *blocks*, and labelled by B_i. Within each block, one chooses some arbitrary point k_B. Using $|e^{ikx} - e^{ik_Bx}| \leqslant |(k - k_B)x| \lesssim PE^{-1/2}$ and the obvious positivity of $(\sqrt{\delta} a_k^\dagger - \delta^{-1/2}|k|^{-1}(e^{ikx} - e^{ik_Bx}))$(h.c.) for any δ, one replaces $\mathbb{H}_K$ with $H'_K = p^2 + \sum_i \int_{B_i} dk (1-\delta) a_k^\dagger a_k + \frac{a_k e^{ik_Bx}}{|k|} + hc.)$ at the energy penalty $\sim \frac{P^2K}{\delta E}$.

3. One introduces $A_{B_i} = \int_{B_i} dk a_k |k|^{-1} / \sqrt{\int_{B_i} dk|k|^{-1}}$ with $A^\dagger_{B_i} A_{B_i} \leqslant \int_{B_i} a^\dagger_k a_k dk$. Then by replacing a_k with A_B in the Hamiltonian, one can apply a coherent-state Ansatz and choose k_B optimally in each block. This directly leads to the Pekar functional (with coefficients altered by $\sim \delta$), whose minimization leads to e^{Pek}, as desired. The $-\frac{K^3}{\alpha^2 P^3}$ term stems from the application of the coherent state ansatz, which replaces $A^\dagger_B A_B$ with $|A|^2 - 1/\alpha^2$, where A is the corresponding $c-$number substitute, and the α^{-2} term is rooted in the commutator. This $-\alpha^{-2}$ term appears one per block, and the total number of blocks is of order K^3/P^3. In this way, we arrive at the statement of the Theorem.

We are therefore left with the interaction term V_+, which describes the interaction of the electron with high-momentum modes of the phonon field. Giving an estimate to this part of the energy is essential both from the physical and mathematical perspective. In fact, it is the V_+ which contains the part of v_x not in L^2, raising problems concerning the domain of $\mathbb{H}$. On the other hand, physically, one expects that the electron has to be localized on the lengthscale of the wavelength of the phonon mode to effectively interact with it. This localization increases the kinetic energy, which, by the uncertainty principle, becomes larger with the localization accuracy. It is therefore expected that the high momentum modes contribute only negligibly to the ground state energy.
Assuming that the effect of the interaction with high-momentum phonon modes decays according to a power-law decay in the cut-off parameter K, we have now the simple

Theorem 7. *Assume that* $\inf \mathrm{spec}\ \mathbb{H} \geqslant \inf \mathrm{spec} \mathbb{H}_K - \frac{c}{K^\beta}$ *holds for some* $\beta > 0$ *and* $c > 0$. *Then*

$$\inf \mathrm{spec}\ \mathbb{H} - e^{\mathrm{Pek}} \gtrsim -\alpha^\epsilon \tag{4.10}$$

with $\epsilon = \frac{-4\beta}{11\beta+9}$ *and* α *sufficiently large.*

Proof. The proof is elementary. Invoking Theorem 2.1, we get for any $E > 0, P > 0, K > 0$ and $\delta > 0$ sufficiently small,

$$\inf \mathrm{spec} \mathbb{H} - e^{\mathrm{Pek}} \geqslant c_1 \delta - E + c_2 \frac{P^2 K}{\delta E} + c_3 \frac{K^3}{\alpha^2 P^3} - cK^{-\beta}. \tag{4.11}$$

Now, we optimize over E, P, K and δ, assuming that $K \sim \alpha^\kappa, P \sim \alpha^p, E \sim \alpha^\epsilon$ and $\delta \sim \alpha^d$. Since the function in question behaves like $-y^a - y^{-b}$ for $y \in \{E, \delta, K, P\}$ for the relevant exponents $a > 0, b > 0$, at the optimum we have that $y^{a-1} \sim y^{-b-1}$. We conclude that at the optimum, every term is of the same order. After imposing this condition, we get a set of linear equations on the exponents

$$-\beta\kappa = -2 - 3\kappa - 3p = d = \kappa + 2p - d - \epsilon = \epsilon.$$

It yields $\epsilon = \frac{-4\beta}{11\beta+9}$, and, consistently, that $\delta \ll 1$ and $K \gg 1$ if $\alpha \gg 1$. □

Remark 7.1. The original method of Lieb and Thomas, based on the Lieb–Yamazaki estimate, leads to $\beta = 1$, which gives $\epsilon = -1/5$. We will improve the ultraviolet regularization scaling law to $\beta = 5/2$, yielding $\epsilon = -20/73$, which is slightly better, although still by a factor $\alpha^{126/73}$ larger than expected.

Remark 7.2. In the limit where β becomes arbitrarily large, the best estimate we can get is $-4/11$, effectively squaring the Lieb and Thomas correction but still being off the mark by

$\alpha^{18/11}$. This is the best one can do by using a power-like estimate on the interaction with high-momentum modes and combining it with the Lieb and Thomas method. To attack the ground state energy asymptotics in full space, we need additional ideas.

Remark 7.3. In the case of the confined model, the IMS localization error disappears as the electron is localized in a fixed volume Ω from the very beginning. Then repeating the remaining steps, we have

$$\inf \mathrm{spec}\, \mathbb{H} - e^{\mathrm{Pek}} \geqslant c_1\delta + c_2|\Omega|^{2/3}\frac{P^2K}{\delta} + c_3\frac{K^3}{\alpha^2P^3} - cK^{-\beta}. \tag{4.12}$$

Performing the optimizing procedure now, we get that the error term scales as α^{ϵ_Ω} with $\epsilon_\Omega = \frac{-4\beta}{8\beta+9}$. This gives asymptotically an error of order $\alpha^{-1/2}$; the original LT ultraviolet regularization leads to $\alpha^{-4/17}$ whereas $\beta = 5/2$ yields $\alpha^{-20/58}$. Confining the electron makes the LT result closer to the expectations, but is still not sufficient.

As announced, we shall improve the (unconfined) error bound by proving that one can take β larger than unity. The essential technical result is hence the following.

Theorem 8. *For any $K > 0$ and $\alpha \gg 1$, we have*

$$\inf \mathrm{spec}\, \mathbb{H} \geq \inf \mathrm{spec}\, \mathbb{H}_K - \mathrm{const.}(K^{-5/2} + \alpha^{-1}K^{-3/2} + \alpha^{-2}K^{-1}). \tag{4.13}$$

Taking now $K \sim \alpha^\kappa$ with $0 < \kappa < 1$, which is consistent with the statement and proof of Theorem 7, we see that the leading term is $K^{-5/2}$. Therefore, given the above considerations, it directly leads to the main result:

Corollary 4.2.1. *For the Fröhlich Hamiltonian in free space, we have the following lower bound for the ground state energy asymptotics*

$$\inf \mathrm{spec}\, \mathbb{H} \geqslant e^{\mathrm{Pek}} - const.\alpha^{-20/73} \tag{4.14}$$

for $\alpha \gg 1$.

4.2.1 Overview of the proof

As we see, the main point is to provide a power-like ultraviolet regularization estimate. Recall that the ultraviolet cutoff problem in the original proof of Lieb and Thomas was handled using the identity

$$-V_+ = \sum_j \left[p_j, a\left(\frac{k_j}{|k|^2}w_x\right) - h.c.\right]. \tag{4.15}$$

Using this, one readily applies the Cauchy-Schwarz inequality to get the bound

$$-V_+ \gtrsim -\frac{\tilde{c}_1}{K}p^2 - \mathbb{N}_+ - \frac{3}{2\alpha^2} \tag{4.16}$$

for $\tilde{c}_1 > 0$. The cutoff thus gives rise to an error of order K^{-1}, which effectively sets the scale of the entire error estimate. The method of Frank and Seiringer, which essentially amounts to replacing $\frac{1}{k}v_x \to \frac{1}{k^3}v_x$ and differentiating it *three times*, enables one to replace the above bound by

$$-V_+ \gtrsim -\left(p^2 + \mathbb{N} + 1\right)^2 K^{-5/2}; \tag{4.17}$$

which goes along with a better error in the cutoff parameter $\sim K^{-5/2}$, but one is faced with the appeareance of the square of the non-interacting Hamiltonian. This can be handled, however, by an appropriate unitary transformation. It effectively replaces (4.17) with

$$V_+ \gtrsim -(\mathbb{H}^2 + C^2)K^{-5/2} \tag{4.18}$$

for some $C > 0$, which can be chosen to be independent of α. Now, if Ψ is a state in the domain of $\mathbb{H}$ such that $(\Psi, \mathbb{H}\Psi)$ is sufficiently close to $\inf \operatorname{spec} \mathbb{H}$, then $(\Psi, \mathbb{H}^2\Psi)$ can be chosen to be of order $(e^{\text{Pek}})^2$, independently of α. This observation immediately leads to

$$\inf \operatorname{spec} \mathbb{H} \geqslant \inf \operatorname{spec} \mathbb{H}_K - \text{const.} K^{-5/2}, \tag{4.19}$$

and the way towards the final estimate is now cleared: we can apply the remaining steps of the Lieb and Thomas proof to $\mathbb{H}_K$, now equipped with a better error estimate for the UV cut-off, which scales as $K^{-5/2}$ and not as K^{-1} as before.
The remaining sections are devoted to the proof of Theorem 2.3. We directly adapt the results of Frank and Seiringer, which were originally obtained for the confined model, to the case of $\Omega = \mathbb{R}^3$. This actually requires only minor modifications, which in many cases amount merely to notational adjustments. In fact, most of the material is actually easier to handle in the unconfined case. However, we work it out here in detail to make the presentation self-contained. The section is split into two parts: first, we demonstrate the triple commutator method and a subsequent proof of (4.17). Secondly, we apply the Gross transformation to the original Hamiltonian, estimate the additional terms which arise, and finally prove (4.18). As already pointed out, this immediately yields the main result, Corollary 2.1, thus establishing a new error estimate on the subleading term in the lower bound to the ground state energy of the strongly-coupled polaron in free space.

4.3 The ultraviolet cutoff

4.3.1 The triple Lieb–Yamazaki bound

As announced, this section gives rise to the following

Proposition 4.3.1. *For any $K > 0$ and α large enough, we have*

$$-V_+ \gtrsim -\left(p^2 + \mathbb{N} + 1\right)^2 \left(K^{-5/2} + \alpha^{-1}K^{-3/2}\right). \tag{4.20}$$

Proof. Clearly, with $p = -\mathrm{i}\nabla_x$,

$$V_+ = \sum_{rst} \left[p_r, \left[p_s, \left[p_t, a^\dagger\left(\frac{k_s k_r k_t}{|k|^6} w_x\right) - a\left(\frac{k_s k_r k_t}{|k|^6} w_x\right)\right]\right]\right]. \tag{4.21}$$

It is convenient to rewrite the above commutator as a multi(anti)linear expression in the p's and $B_{rst} \equiv a^\dagger\left(\frac{k_s k_r k_t}{|k|^6} w_x\right) - a\left(\frac{k_s k_r k_t}{|k|^6} w_x\right)$, which makes it ready for a direct application of the Cauchy-Schwarz inequality in the form

$$AC + C^\dagger A^\dagger \leqslant \epsilon A A^\dagger + \frac{1}{\epsilon} C^\dagger C \tag{4.22}$$

for any A, C and arbitrary $\epsilon > 0$. We get

$$V_+ = \sum_{rst} \left(p_r p_s [p_t, B_{rst}] + [p_t, B_{rst}] p_r p_s\right) - 2\left(p_r p_s B_{rst} p_t + p_t B_{rst}^\dagger p_r p_s\right). \tag{4.23}$$

The second term is obtained by renaming the indices, which is possible by the invariance of B_{rst} under this operation. This term is bounded by

$$-\left(p_r p_s B_{rst} p_t + p_t B^\dagger_{rst} p_r p_s\right) \leqslant \epsilon p_r^2 p_s^2 + \frac{1}{\epsilon} p_t B^\dagger_{rst} B_{rst} p_t \tag{4.24}$$

for any $\epsilon > 0$. On the other hand, for any $\Psi \in \mathcal{F}$, $f \in L^2$ and $B = a^\dagger(f) - a(f)$,

$$(\Psi, B^\dagger B \Psi) = ||B\Psi||^2 \leqslant 2(||a(f)\Psi||^2 + ||a^\dagger(f)\Psi||^2)$$
$$\leq 4(\Psi, a^\dagger(f)a(f)\Psi) + 2(\Psi, [a(f), a^\dagger(f)]\Psi) \leqslant ||f||_2^2(\Psi, 4\mathbb{N} + \frac{2}{\alpha^2}, \Psi).$$

Using this, we obtain

$$B^\dagger_{rst} B_{rst} \lesssim K^{-5}(4\mathbb{N} + \frac{2}{\alpha^2}). \tag{4.25}$$

In exactly the same way one can handle the first term; by defining $\sum_t [p_t, B_{rst}] \equiv C_{rs}$ we get for any $\mu > 0$ that this term is bounded by $\mu p_s^2 p_r^2 + \frac{1}{\mu} C_{rs}^2$, and

$$C_{rs}^2 \leqslant 4a^\dagger \left(\frac{k_r k_s}{|k|^4} w_x\right) a \left(\frac{k_r k_s}{|k|^4} w_x\right) + \frac{2}{\alpha^2} || \frac{k_r k_s}{|k|^4} w_x ||^2. \tag{4.26}$$

However, here the norm scales as $K^{-3/2}$, which is not dangerous in the term stemming from the commutator, as it gets multiplied by α^{-2}. The *bare* term has to be improved, however, if we wish to maintain the better $K^{-5/2}$ decay rate. This can be done using the following lemma, which will be useful also afterwards.

Lemma 4.3.2. *Let* $f \in (L^2 \cap L^\infty)(\mathbb{R}^3)$. *Then* $a^\dagger(f_x)a(f_x) \leqslant (3(2\pi)^{2/3} \|f\|_\infty^{4/3} \|f\|_2^{2/3}) p^2 \mathbb{N}$.

Proof. It is enough to restrict ourselves to the one-particle sector of the Fock space $\mathbb{C} \otimes L^2(\mathbb{R}^3) \simeq L^2(\mathbb{R}^3)$. Then for all $\Psi \in L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)$,

$$||a(f)\Psi||^2 = \int dp | \int dk f(k) \Phi(p-k, k)|^2; \tag{4.27}$$

here, we have written down the integral in the $x-$space, absorbed the e^{ikx} factor into the Ψ, and used the Parseval's identity (Φ stands for the Fourier transform of $\Psi(x,k)$ regarded as a function of x). Now we use the CS inequality to bound the above by

$$||a(f)\Psi||^2 \leqslant \int dp \left(\int dk \frac{|f(k)|^2}{|k-p|^2}\right) \left(\int dk |k-p|^2 |\Phi(p-k,k)|^2\right) \leqslant$$
$$\leqslant \left(\sup_q \int dk \frac{|f(k)|^2}{|k-q|^2}\right) (\Psi, p^2 \mathbb{N} \Psi). \tag{4.28}$$

The prefactor is now estimated directly:

$$\int dk |f(k)|^2 |k-q|^{-2} = \int_{B(q,R)} dk |f(k)|^2 |k-p|^{-2} + \int_{B^c(q,R)} dk |f(k)|^2 |p-k|^{-2}$$
$$\leq ||f^2||_\infty 4\pi R + \frac{||f||_2^2}{R}; \tag{4.29}$$

where $B(x,R)$ is the ball of radius R centered at $x \in \mathbb{R}^3$. Optimizing over R, we arrive at the statement of the Lemma. □

Using the lemma for $f_x = \frac{k_r k_s}{|k|^4} w_x$ we get $a^\dagger\left(\frac{k_r k_s}{|k|^4} w_x\right) a\left(\frac{k_r k_s}{|k|^4} w_x\right) \lesssim K^{-5} p^2 \mathbb{N}$ since in this case $\|f\|_\infty \sim K^{-3}$ and $\|f\|_2 \sim K^{-3/2}$. We have thus gained an additional power in the decay rate at the cost of the electron's kinetic energy. This conforms with the physical interpretation of the cutoff decay rate given in the introduction.
Finally, after taking $\epsilon = 2K^{-5/2}$, $\mu = 6(K^{-5/2} + 2\alpha^{-1}K^{-3/2})$, summing over the indices, and combining the above inequalities we get

$$V_+ \lesssim K^{-5/2}(|p|^4 + 3p^2(\mathbb{N} + 2\alpha^{-2})) + (K^{-5/2} + \alpha^{-1}K^{-3/2})(|p|^4 + p^2\mathbb{N} + 1/2). \quad (4.30)$$

Since p^2 and $\mathbb{N}$ commute, are positive and self-adjoint, we can treat the above operator term as an ordinary polynomial, which can be bounded by the one given in the statement of the proposition for α sufficiently large. □

4.3.2 The Gross transformation

The operator inequality given in Proposition 3.1 is not sufficient for our purpose, as in principle $(\Psi, (p^2 + \mathbb{N})^2\Psi)$ is infinite if Ψ is in the domain of $\mathbb{H}$. Our goal will be to replace the non-interacting Hamiltonian there by $\mathbb{H}$. Then also (4.19) will be true. We will achieve this result by (4.18). To get there, we need

Proposition 4.3.3. *Let Ψ be in the domain of $p^2 + \mathbb{N}$, being a dense subset of $L^2(\mathbb{R}^3) \otimes \mathcal{F}$. Then for any $\epsilon > 0$ there exist constants $K' > 0, C > 0$ and a unitary transformation $U_{K',\alpha}$, parametrized by K' and α, such that*

$$(1+\epsilon)||(p^2 + \mathbb{N})\Psi|| + C||\Psi|| \geqslant ||U^\dagger_{K',\alpha}\mathbb{H}U_{K',\alpha}\Psi|| \geqslant (1-\epsilon)||(p^2 + \mathbb{N})\Psi|| - C||\Psi||, \quad (4.31)$$

assuming that α is sufficiently large.

Proof. Consider some function of the phonon variables, f, such that $f_x \in L^2(\mathbb{R}^3)$ and $(f_x, pf_x) = \int k|f(k)|^2 dk = 0$. Take

$$U = e^{\alpha^2(a(f_x) - a^\dagger(f_x))}. \quad (4.32)$$

Using the easy to prove formulae, valid for any h s.t. $(h, f_x) < \infty$,

$$Ua_hU^\dagger = a_h + (h, f_x) \quad Ua_h^\dagger U^\dagger = a_h^\dagger + (f_x, h), \quad (4.33)$$

as well as

$$[p, U] = (-i\nabla_x U), \quad (-i\nabla_x a)(f_x) = -a(pf_x), \quad (-i\nabla_x a^\dagger)(f_x) = a^\dagger(pf_x) \quad (4.34)$$

and the formula

$$\frac{de^{A(x)}}{dx} = \int_0^1 e^{tA(x)}A'(x)e^{(1-t)A(x)}dt \quad (4.35)$$

one finds

$$UHU^\dagger = p^2 + \mathbb{N} + \alpha^4(a^\dagger(pf_x) + a(pf_x))^2 + 2\alpha^2 pa(pf_x) + 2\alpha^2 a^\dagger(pf_x)p +$$
$$+ a(\alpha^2 p^2 f_x + f_x - v_x) + a^\dagger(\alpha^2 p^2 f_x + f_x - v_x) + ||f_x||_2^2 - 2\mathrm{Re}(v_x, f_x) \equiv p^2 + \mathbb{N} + \tilde{V},$$

we see that the proposition will be true if we find f_x and C such that

$$||\tilde{V}\Psi|| \leqslant \epsilon||(p^2 + \mathbb{N})\Psi|| + C||\Psi||$$

for all $\Psi \in D(p^2+\mathbb{N})$. Take any $K'>0$ and consider $f_x = \frac{\chi_{|k|>K'}e^{ikx}}{|k|(\alpha^2|k|^2+1)}$ with

$$\alpha^2 p^2 f_x + f_x - v_x = -\frac{\chi_{k\leqslant K'}e^{ikx}}{|k|} \equiv g_x.$$

Writing down the relevant integrals, we readily have the following estimates:

$$||g_x||_2^2 \lesssim K', \quad ||f_x||_2^2 \lesssim \alpha^{-4}K'^{-3} \tag{4.36}$$

and

$$(v_x, f_x) \lesssim \alpha^{-2}K'^{-1}, \quad ||pf_x||_2^2 \lesssim \alpha^{-4}K'^{-1}. \tag{4.37}$$

We are now able to estimate every term in $\tilde{V}$. We have, by similar computations as in Proposition 3.1

$$||(a(g_x)+a^\dagger(g_x))\Psi|| \leqslant ||g_x||_2 \left|\left|\sqrt{(\mathbb{N}+\alpha^{-2})}\Psi\right|\right| \lesssim \delta||(\mathbb{N}+\alpha^{-2})\Psi|| + \delta^{-1}K'||\Psi|| \tag{4.38}$$

for any $\delta>0$. Similarly,

$$\alpha^4||(a^\dagger(pf_x)+a(pf_x))^2\Psi|| \lesssim K'^{-1}||(\mathbb{N}+\alpha^{-2})\Psi||. \tag{4.39}$$

The cross-terms give, by $pa_f a_f^\dagger p \lesssim p^2(\mathbb{N}+\alpha^{-2})||f||_2^2 \lesssim (p^2+\mathbb{N}+\alpha^{-2})^2||f||_2^2$,

$$\alpha^2||a^\dagger(pf_x)p\Psi|| \lesssim K'^{-1/2}||(p^2+\mathbb{N}+\alpha^{-2})\Psi||. \tag{4.40}$$

The term $\alpha^2 pa(pf_x)$ requires a bit more work. "Commuting the p through", we get that it can be bounded using the former estimate, and an estimate on $\alpha^2 a(p^2 f_x)$. $p^2 f_x \notin L^2$, however, so we split it as

$$\alpha^2 p^2 f_x = g_x - f_x + e^{ikx}\left(\frac{1}{|k|} - \frac{1}{\sqrt{K'^2+|k|^2}}\right) + \frac{e^{ikx}}{\sqrt{K'^2+|k|^2}}. \tag{4.41}$$

Then we estimate term by term. The g_x and f_x estimates are exactly as above, the operator estimates included. Clearly, $j_x := |k|^{-1} - (K'^2+|k|^2)^{-1/2} \leqslant K'|k|^{-1}(K'^2+|k|^2)^{-1/2}$ with the square of the L^2 norm of the latter bounded by $\sim K'$. We are left with an estimate of the last term. We can use the Cauchy-Schwarz inequality in the same way as in Lemma 3.1 and estimate

$$||a((K'^2+|k|^2)^{-1/2}e^{ikx})\Psi|| \leqslant \sqrt{\left(\sup_p \int dk \frac{1}{(K'^2+|k|^2)|k-p|^2}\right)(\Psi, \mathbb{N}p^2\Psi)}. \tag{4.42}$$

The integral can be shown to be bounded by $\sim \int dk (K'^2+|k|^2)^{-1}|k|^{-2} \sim K'^{-1}$. Indeed, we split it into an integral over the set $A_p := \{k : |k-p|^2 \geq |k|^2\}$ and its complement. On A_p, the bound holds clearly; on the complement, we bound it by $\int dk(K'^2+|k-p|^2)^{-1}|k-p|^{-2}$ and translate the coordinate system. Consequently,

$$||a((K'^2+|k|^2)^{-1/2}e^{ikx})\Psi|| \lesssim K'^{-1/2}||(p^2+\mathbb{N})\Psi||. \tag{4.43}$$

The remaining estimates are

$$||a(g_x)\Psi|| \lesssim K'^{1/2}||\mathbb{N}^{1/2}\Psi|| \leqslant \delta||\mathbb{N}\Psi|| + \delta^{-1}K'||\Psi||, \tag{4.44}$$

$$||a(f_x)\Psi|| \lesssim \alpha^{-2}K'^{-3/2}||\sqrt{\mathbb{N}}\Psi|| \leqslant \delta||\mathbb{N}\Psi|| + \delta^{-1}\alpha^{-4}K'^{-3}||\Psi|| \tag{4.45}$$

and

$$||a(j_x)\Psi|| \lesssim \delta||\mathbb{N}\Psi|| + \delta^{-1}K'||\Psi|| \tag{4.46}$$

so that remaining part of $a(p^2 f_x)$ is bounded by $\delta||\mathbb{N}\Psi|| + \delta^{-1}K'(1+\frac{1}{K'^4\alpha^2})||\Psi||$. Putting it all together we see that the $p^2+\mathbb{N}$ terms are multiplied by $\delta, K'^{-1/2}, K'^{-1}$, and the bare Ψ terms -by $\delta^{-1}K'(2+K'^{-4}\alpha^{-2})$. It therefore suffices, assuming $\alpha \gg 1$, to take $\delta \sim \epsilon$ and $K' \sim \epsilon^{-2}$, and hence also $C \sim \epsilon^{-1}$. □

Equipped with the last statement, which establishes a link between the domains of the interacting and non-interacting Hamiltonians, we now use the obvious fact that $A \leqslant 0 \implies BAB^\dagger \leqslant 0$ for any B . Then from Proposition 3.1. we have

$$-UV_+U^\dagger \gtrsim -U(p^2+\mathbb{N})^2U^\dagger\left(K^{-5/2}+\alpha^{-1}K^{-3/2}\right). \tag{4.47}$$

For the choice of f_x as in Proposition 3.3, we have $U^\dagger V_+ U = V_+ + (w_x, f_x)$ as the inner product is finite. Now, it is easy to see that $(w_x, f_x) \lesssim \alpha^{-2}K^{-1}$ for the chosen K' and any $K > 0$. Combining this with Proposition 3.3 by taking $\Psi = U^\dagger\Psi'$ for Ψ' in the domain of $\mathbb{H}$, as well as some $\epsilon \in (0,1)$, we conclude $U(p^2+\mathbb{N})^2U^\dagger \leqslant \frac{2}{(1-\epsilon)^2}(\mathbb{H}^2+C^2)$ and hence

$$-V_+ \gtrsim -(\mathbb{H}^2+C^2)\left(K^{-5/2}+\alpha^{-1}K^{-3/2}\right) - \alpha^{-2}K^{-1}. \tag{4.48}$$

We can now always choose Ψ' such that both $(\Psi', \mathbb{H}, \Psi')$ is arbitrarily close to $\inf\operatorname{spec}\mathbb{H}$ and $(\Psi', \mathbb{H}^2\Psi')$ can be bounded by a constant independent of Ψ' and α. Choosing such Ψ', we have finally

$$\inf\operatorname{spec}\mathbb{H} \geqslant \inf\operatorname{spec}\mathbb{H}_K - \text{const.}(K^{-5/2}+\alpha^{-1}K^{-3/2}+\alpha^{-2}K^{-1}) \tag{4.49}$$

This is precisely the result that has been claimed.

CHAPTER 5

Optimal upper bound for the energy-momentum relation of a strongly coupled polaron

This chapter contains the submitted paper

- D. Mitrouskas, K. Myśliwy and R. Seiringer, *Optimal parabolic upped bound for the energy-momentum relation of a strongly-coupled polaron*, arXiv:2203.02454.

Abstract. We consider the large polaron described by the Fröhlich Hamiltonian and study its energy-momentum relation defined as the lowest possible energy as a function of the total momentum. Using a suitable family of trial states, we derive an optimal parabolic upper bound for the energy-momentum relation in the limit of strong coupling. The upper bound consists of a momentum independent term that agrees with the predicted two-term expansion for the ground state energy of the strongly coupled polaron at rest, and a term that is quadratic in the momentum with coefficient given by the inverse of twice the classical effective mass introduced by Landau and Pekar.

5.1 Introduction

5.1.1 The Model

The large polaron provides an idealized description for the motion of a slow band electron through a polarizable crystal. The analysis of the polaron is a classic problem in solid state physics that first appeared in 1933 when Landau introduced the idea of self-trapping of an electron in a polarizable environment [77]. Since it provides a simple model for a particle interacting with a nonrelativistic quantum field, the polaron has been of interest also in field theory and mathematical physics. In particular the strong coupling theory of the polaron and Pekar's adiabatic approximation have been the source of interesting and challenging mathematical problems.

Following H. Fröhlich [68] the Hamiltonian of the model acts on the Hilbert space

$$\mathscr{H} = L^2(\mathbb{R}^3, \mathrm{d}x) \otimes \mathcal{F}, \tag{5.1}$$

with $\mathcal{F}$ the bosonic Fock space over $L^2(\mathbb{R}^3)$, and is given by

$$H_\alpha = -\Delta_x + \alpha^{-2}\mathbb{N} + \alpha^{-1}\phi(h_x). \tag{5.2}$$

Here $x \in \mathbb{R}^3$ is the coordinate of the electron, $\mathbb{N}$ denotes the number operator on Fock space, and the field operator $\phi(h_x) = a^\dagger(h_x) + a(h_x)$ with coupling function

$$h_x(y) = -\frac{1}{2\pi^2|x-y|^2} \tag{5.3}$$

accounts for the interaction between the electron and the quantum field. The creation and annihilation operators satisfy the usual canonical commutation relations

$$\left[a(f), a^\dagger(g)\right] = \left\langle f|g\right\rangle_{L^2}, \quad \left[a(f), a(g)\right] = 0. \tag{5.4}$$

Since we set $\hbar = 1$ and the mass of the electron equal to $1/2$, the only free parameter is the coupling constant $\alpha > 0$.

By rescaling all lengths by a factor $1/\alpha$, one can show that $\alpha^2 H_\alpha$ is unitarily equivalent to the Hamiltonian

$$H_\alpha^{\mathrm{Polaron}} = -\Delta_x + \mathbb{N} + \sqrt{\alpha}\phi(h_x), \tag{5.5}$$

which is more common in the polaron literature and also explains why $\alpha \to \infty$ is called the strong coupling limit.

The Fröhlich Hamiltonian defines a translation invariant model, i.e., it commutes with the total momentum operator,

$$[H_\alpha, -i\nabla_x + P_f] = 0 \tag{5.6}$$

where $P_f = \mathrm{d}\Gamma(-i\nabla)$ denotes the momentum operator of the phonons. This allows the definition of the energy-momentum relation $E_\alpha(P)$ as the lowest possible energy of H_α when restricted to states with total momentum $P \in \mathbb{R}^3$. To this end, it is convenient to switch to the Lee–Low–Pines representation

$$H_\alpha(P) = (P_f - P)^2 + \alpha^{-2}\mathbb{N} + \alpha^{-1}\phi(h_0), \tag{5.7}$$

where $H_\alpha(P)$ acts on the Fock space only [79]. The Fröhlich Hamiltonian H_α is unitarily equivalent to the fiber decomposition $\int_{\mathbb{R}^3}^{\oplus} H_\alpha(P)\mathrm{d}P$, which follows easily from transforming H_α with $e^{iP_f x}$ and diagonalizing the obtained operator in the electron coordinate. The energy-momentum relation is then defined as the ground state energy of the fiber Hamiltonian,

$$E_\alpha(P) = \inf \sigma(H_\alpha(P)), \tag{5.8}$$

which by construction satisfies $E_\alpha(RP) = E_\alpha(P)$ for all rotations $R \in \mathsf{SO}(3)$. It is known that $E_\alpha(0) \leq E_\alpha(P)$ and hence $E_\alpha(0) = \inf\sigma(H_\alpha)$ (in fact it is expected that $E_\alpha(0) < E_\alpha(P)$ for all $P \neq 0$ [59]). Further properties, such as the domain of analyticity, existence of ground states and the value of the bottom of the continuous spectrum, were analyzed in [69, 97, 90, 71, 57].

The aim of this work is to analyze the quantitative behavior of the energy-momentum relation for large coupling $\alpha \to \infty$. Our main result provides an upper bound for $E_\alpha(P)$. The upper bound consists of a momentum independent part coinciding with the optimal upper bound for the ground state energy of the strongly coupled polaron at rest, and a momentum dependent part. In more detail, the momentum independent part is given by the classical Pekar energy and the corresponding quantum fluctuations that are described by the energy of a system of harmonic oscillators with frequencies determined by the Hessian of the corresponding classical field functional. This part agrees with the expected asymptotic form of $E_\alpha(0)$, see (5.25). The momentum dependent part, on the other hand, describes the energy of a free particle with mass $M(\alpha) = \frac{2\alpha^4}{3} \int |\nabla\varphi|^2$, where φ denotes the self-consistent polarization field, which coincides with the classical polaron mass introduced by Landau and Pekar [78], see (5.24). As will be explained in Section 5.1.3, our result confirms the heuristic picture of the polaron (the electron and the accompanying classical field) as a free quasi-particle with largely enhanced mass. To our best knowledge, the upper bound we present in this work is the first rigorous result about the connection between the energy-momentum relation $E_\alpha(P)$ and the classical polaron mass $M(\alpha)$.

Starting from the works in the 30's and 40's [77, 78, 67] there has been a large number of publications in the physics literature that studied the ground state energy $E_\alpha(0)$ and the effective mass, that is, the inverse curvature of $E_\alpha(P)$ at $P = 0$. For a comprehensive summary of the earlier results, we refer to [87]. More recent developments are reviewed in [50]. Mathematically rigorous results for the leading order asymptotics of $E_\alpha(0)$, for α large, were obtained by Lieb and Yamazaki [86] (with non-matching upper and lower bounds) and by Donsker and Varadhan [58] as well as Lieb and Thomas [2]. The effective mass has been studied in [96, 59, 62, 85, 84, 53]. Further improvements have been obtained for confined polarons or polaron models with more regular interaction [66, 63, 93]. For completeness, let us also mention recent progress in the understanding of the polaron path measure [92, 52] as well as the increased interest in the analysis of the Schrödinger time evolution of strongly coupled polarons [73, 81, 82, 88, 61, 64, 65].

5.1.2 Pekar functionals

The semiclassical theory of the polaron has been introduced by Pekar [94]. It arises naturally in the context of strong coupling, based on the expectation that the electron and the phonons are adiabatically decoupled, similarly as the electrons are adiabatically decoupled from the heavy nuclei in the famous Born–Oppenheimer theory [55, 54]. With this in mind, one can minimize the Fröhlich Hamiltonian over product states of the form

$$\Psi_{u,v} = u \otimes e^{a^\dagger(\alpha v)}\Omega \tag{5.9}$$

where $u \in H^1(\mathbb{R}^3)$ is a normalized electron wave function, $\Omega = (1, 0, 0, \ldots)$ the Fock space vacuum and $e^{a^\dagger(\alpha v)}\Omega$ the coherent state, up to normalization, that is associated with a classical field $\alpha v \in L^2(\mathbb{R}^3)$. A simple computation leads to the Pekar energy functional

$$\mathcal{G}(u, v) = \frac{\left\langle \Psi_{u,v} | H_\alpha \Psi_{u,v} \right\rangle_{\mathscr{H}}}{\left\langle \Psi_{u,v} | \Psi_{u,v} \right\rangle_{\mathscr{H}}} = \left\langle u | (-\Delta + V^v) u \right\rangle_{L^2} + \|v\|_{L^2}^2 \tag{5.10}$$

with polarization potential

$$V^v(x) = -2 \operatorname{Re} \left\langle v | h_x \right\rangle_{L^2} = -\operatorname{Re} \int \frac{v(y)}{\pi^2 |x-y|^2} \mathrm{d}y. \tag{5.11}$$

By completing the square, one can further remove the field variable and obtain the energy functional for the electron wave function,

$$\mathcal{E}(u) = \inf_{v \in L^2} \mathcal{G}(u, v) = \int |u(x)|^2 \mathrm{d}x - \frac{1}{4\pi} \iint \frac{|u(x)|^2 |u(y)|^2}{|x-y|} \mathrm{d}x \mathrm{d}y, \tag{5.12}$$

which is known [83] to admit a unique rotational invariant minimizer $\psi > 0$ (the minimizing property is unique only up to translations and multiplications by a constant phase). Alternatively, one can minimize the Pekar energy functional w.r.t. the electron wave function first. This leads to the classical field functional

$$\mathcal{F}(v) \;=\; \inf_{\|u\|_{L^2}=1} \mathcal{G}(u,v) \;=\; \inf \mathsf{spec}\left(-\Delta + V^v\right) + \|v\|_{L^2}^2 \tag{5.13}$$

whose unique rotational invariant minimizer is readily shown to be

$$\varphi(z) \;=\; -\left\langle \psi \middle| h.(z)\psi \right\rangle_{L^2} \;=\; \int \frac{|\psi(y)|^2}{2\pi^2|z-y|^2}\mathsf{d}y. \tag{5.14}$$

The corresponding classical ground state energy is called the Pekar energy

$$e^{\mathrm{Pek}} \;=\; \mathcal{E}(\psi) \;=\; \mathcal{F}(\varphi), \quad e^{\mathrm{Pek}} < 0, \tag{5.15}$$

and by the variational principle it provides an upper bound for $\inf \sigma(H_\alpha)$. The validity of Pekar's ansatz was rigorously verified by Donsker and Varadhan [58] who proved that $\lim_{\alpha\to\infty} \inf \sigma(H_\alpha) = e^{\mathrm{Pek}}$ and subsequently by Lieb and Thomas [2] who added a quantitative bound for the error by showing that

$$\inf \sigma(H_\alpha^{\mathrm{F}}) \;\geq\; e^{\mathrm{Pek}} + O(\alpha^{-1/5}). \tag{5.16}$$

Given the potential V^φ for the field φ, one can define the Schrödinger operator

$$h^{\mathrm{Pek}} \;=\; -\Delta + V^\varphi(x) - \lambda^{\mathrm{pek}}, \quad \lambda^{\mathrm{Pek}} \;=\; e^{\mathrm{Pek}} - \|\varphi\|_{L^2}^2 \tag{5.17}$$

with $\lambda^{\mathrm{Pek}} = \inf \sigma(-\Delta + V^\varphi(x)) < 0$ and ψ the corresponding unique ground state. It follows from general arguments for Schrödinger operators that h^{Pek} has a finite spectral gap above zero, and thus the reduced resolvent

$$R \;=\; Q_\psi (h^{\mathrm{Pek}})^{-1} Q_\psi \quad \text{with} \quad Q_\psi \;=\; 1 - P_\psi, \quad P_\psi \;=\; |\psi\rangle\langle\psi|, \tag{5.18}$$

defines a bounded operator (P_ψ denotes the orthogonal projection onto the state ψ).

The last object to be introduced in this section is the Hessian H^{Pek} of the energy functional $\mathcal{F}$ at its minimizer φ, defined by

$$\left\langle v \middle| H^{\mathrm{Pek}} v \right\rangle_{L^2} \;=\; \lim_{\varepsilon\to 0} \frac{1}{\varepsilon^2}\Big(\mathcal{F}(\varphi + \varepsilon v) - \mathcal{F}(\varphi)\Big) \quad \forall v \in L^2(\mathbb{R}^3). \tag{5.19}$$

In the following lemma we collect some important properties of H^{Pek}.

Lemma 5.1.1. *The operator H^{Pek} has integral kernel*

$$H^{\mathrm{Pek}}(y,z) \;=\; \delta(y-z) - 4\,\mathrm{Re}\left\langle \psi \middle| h.(y) R h.(z)\psi \right\rangle_{L^2} \tag{5.20}$$

and satisfies the following properties.

(i) $0 \leq H^{\mathrm{Pek}} \leq 1$

(ii) $\mathsf{Ker} H^{\mathrm{Pek}} = \mathsf{Span}\{\partial_i \varphi \,:\, i = 1,2,3\}$

(iii) $H^{\mathrm{Pek}} \geq \tau > 0$ *when restricted to* $(\mathsf{Ker} H^{\mathrm{Pek}})^\perp$

(iv) $\mathrm{Tr}_{L^2}(1 - \sqrt{H^{\mathrm{Pek}}}) < \infty.$

The proof of the lemma, in particular Item (ii), is based on the analysis of the Hessian of the energy functional $\mathcal{E}$ [80]. The details are given in Section 5.4.

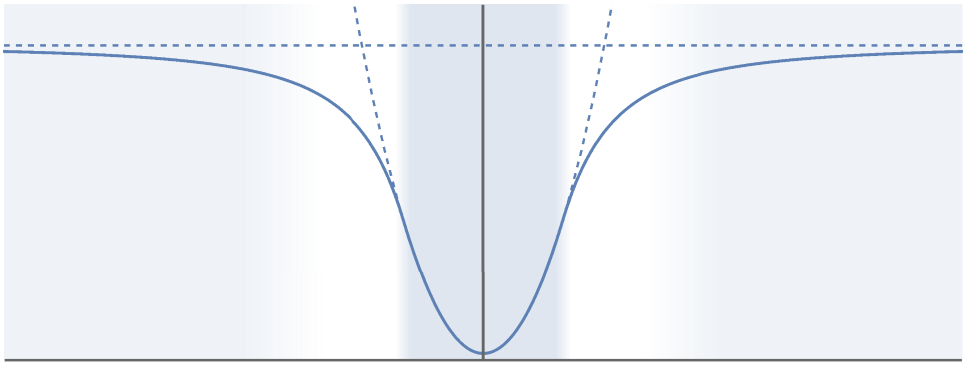

Figure 5.1: The energy-momentum relation $E_\alpha(P)$ is expected to have two characteristic regimes: The parabolic quasi-particle regime for small momenta (dark area) and the radiative regime for large momenta (light area). For the transition between the two there is no concrete prediction. The dashed lines denote the quasi-particle energy (5.21) and the bottom of the continuous spectrum (5.23). Their intersection defines the momentum scale $P_c(\alpha)$ that is proportional to α for large coupling.

5.1.3 Motivation and goal of this work

In this work, we are interested in the behavior of the energy-momentum relation $E_\alpha(P)$ for large values of the coupling α. In general, $E_\alpha(P)$ is expected to interpolate between two distinct regimes (see for instance [72, 70, 99, 97]): The *quasi-particle regime* and the *radiative regime*. The former corresponds to small momenta, and the expectation is that the system behaves effectively like a free particle with energy

$$E_\alpha^{\mathrm{eff}}(P) = E_\alpha(0) + \frac{P^2}{2M^{\mathrm{eff}}(\alpha)} \tag{5.21}$$

where the effective mass is determined by the inverse curvature of $E_\alpha(P)$ at $P = 0$ (which is known to be well-defined),

$$M^{\mathrm{eff}}(\alpha) := \frac{1}{2} \lim_{P\to 0} \left(\frac{E_\alpha(P) - E_\alpha(0)}{P^2} \right)^{-1}. \tag{5.22}$$

It is easy to verify that $M^{\mathrm{eff}}(\alpha) \geq 1/2$ (the mass of the electron in our units), and one can further show that the inequality is strict if $\alpha > 0$, so that the emerging quasi-particle is heavier than the bare electron. The heuristic idea is that the electron drags along a cloud of phonons when it moves through the crystal and thus appears to be heavier than it would be without the interaction. The radiative regime, on the other hand, describes a polaron at rest and an unbound/radiative phonon carrying the total momentum P. It is expected to be valid for large momenta and it is characterized by a flat energy-momentum relation that equals or approaches the bottom of the continuous spectrum [90],

$$\inf \sigma_{\mathrm{cont}}(H_\alpha(P)) = E_\alpha(0) + \alpha^{-2}. \tag{5.23}$$

The two regimes cross at $|P| = P_{\mathrm{c}}(\alpha) := \sqrt{2M^{\mathrm{eff}}(\alpha)}/\alpha$ which marks a characteristic momentum scale of the polaron. While the quasi-particle picture is expected to be accurate for $|P| \ll P_{\mathrm{c}}(\alpha)$, the radiative regime should hold for $|P| \gtrsim P_{\mathrm{c}}(\alpha)$ (see also Remark 2 below). Between the two regimes there is no concrete prediction for the behavior of $E_\alpha(P)$. A schematic plot is provided in Figure 5.1.

One aspect of this work is to show that the quasi-particle picture is mathematically rigorous, insofar as it provides a parabolic upper bound on $E_\alpha(P)$ that coincides with the expected form of the quasi-particle energy in the limit of large coupling. Since the quasi-particle energy (5.21) is determined by the values of $E_\alpha(0)$ and $M^{\mathrm{eff}}(\alpha)$, it is instructive to recall two long-standing open conjectures concerning their behavior for $\alpha \to \infty$. As explained in the previous section, the phonon field behaves classically for large coupling, and thus it is expected that $M^{\mathrm{eff}}(\alpha)$ should asymptotically tend to the expression that follows from the corresponding semiclassical counterpart of the problem. This semiclassical theory of the effective mass was introduced by Landau and Pekar in 1948 [78], and, based on this work (see also [96, 62]), it is conjectured that

$$\lim_{\alpha\to\infty} \frac{M^{\mathrm{eff}}(\alpha)}{\alpha^4} = M^{\mathrm{LP}} \quad \text{with} \quad M^{\mathrm{LP}} = \frac{2}{3}\|\nabla\varphi\|_{L^2}^2. \tag{5.24}$$

Although this problem is many decades old, the best available rigorous result is that $M^{\mathrm{eff}}(\alpha)$ is divergent [85], with a recent proof that it diverges at least as fast as $\alpha^{2/5}$ [53]. Regarding the ground state energy $E_\alpha(0)$ the prediction from the physics literature (see e.g. [51, 89, 98, 75]) is that

$$E_\alpha(0) = e^{\mathrm{Pek}} + \frac{1}{2\alpha^2}\mathrm{Tr}_{L^2}(\sqrt{H^{\mathrm{Pek}}} - 1) + O(\alpha^{-2-\delta}) \quad \text{as} \quad \alpha \to \infty \tag{5.25}$$

for some $\delta > 0$ (in fact it is predicted that $\delta = 2$ [75]). Compared to the semiclassical expansion this includes a subleading correction of order α^{-2}, which we call the *Bogoliubov energy*, and which arises from quantum fluctuations of the field around its classical value. For a nice heuristic derivation of this correction, we recommend the study of [89]. Now inserting (5.24) and (5.25) into (5.21), and based on the expectation that the quasi-particle regime is restricted to $|P| \ll \sqrt{2M^{\mathrm{eff}}(\alpha)}/\alpha \sim \alpha$, it is clear that the Bogoliubov energy needs to be taken into account in order to see the quasi-particle energy shift given by $P^2/(2\alpha^4 M^{\mathrm{LP}}) \ll \alpha^{-2}$. Mathematically, the validity of (5.25) has been established only for confined polaron models [66, 63]. The corresponding upper bound for the unconfined model is a corollary of our main result.

As a summary of the above we arrive at the following claim.

Conjecture. *Let M^{LP} be the Landau–Pekar mass defined in* (5.24). *There exists a continuous function $f : [0,\infty) \to [0,\infty)$, satisfying $f(s) \to 1$ as $s \to \infty$ and*

$$f(s) = \frac{s}{2M^{\mathrm{LP}}} + O(s^2) \quad \text{as} \quad s \to 0, \tag{5.26}$$

such that for all $P \in \mathbb{R}^3$

$$\lim_{\alpha\to\infty} \alpha^2 \left(E_\alpha(\alpha P) - e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}_{L^2}\left(\sqrt{H^{\mathrm{Pek}}} - 1\right)\right) = f(P^2). \tag{5.27}$$

Our main result, Theorem 5.2.1 below, provides an upper bound for $E_\alpha(\alpha P)$ that is compatible with the conjecture in the quasi-particle regime. To be more precise, our result implies that the left side of (5.27), with the limit replaced by the $\limsup$, is bounded from above by $P^2/(2M^{\mathrm{LP}})$ for all $P \in \mathbb{R}^3$. This shows that the corrections to the quasi-particle energy are always negative, a conclusion that is not entirely obvious a priori.

Remark 1. An immediate consequence of the conjecture would be that

$$\frac{1}{2}\lim_{P\to 0}\lim_{\alpha\to\infty} \alpha^2 \left(\frac{E_\alpha(\alpha P) - E_\alpha(0)}{P^2}\right)^{-1} = M^{\mathrm{LP}} \tag{5.28}$$

which is to be compared with (5.24) where the limits are taken in reversed order.

Remark 2. Even though our analysis is focused on the quasi-particle regime, let us mention an interesting problem concerning the radiative regime. The question is whether $E_\alpha(P)$ enters the continuous part of the spectrum, i.e. whether the spectral gap closes at some finite momentum, or not. The answer may in fact depend on the dimension and possibly also on the value of α. It is known that in two dimensions $E_\alpha(P)$ remains an isolated eigenvalue for all P, meaning that the curve approaches $\inf \sigma_{\text{cont}}(H_\alpha(P))$ only in the limit $|P| \to \infty$ [97]. To our knowledge in three dimensions the question is not completely settled. While for small momenta it is known that $E_\alpha(P)$ corresponds to a simple eigenvalue [97], there is indication from results obtained for weak coupling that $E_\alpha(P)$ agrees with the bottom of the continuous spectrum when $|P|$ is sufficiently large [57].

5.2 Main Result

We are now ready to state the main result.

Theorem 5.2.1. *Let $E_\alpha(P) = \inf \sigma(H_\alpha(P))$, $M^{\text{LP}} = \frac{2}{3}\|\nabla\varphi\|_{L^2}^2$ with φ defined in* (5.14) *and choose $c > 0$. For every $\varepsilon > 0$ there exists a constant $C_{c,\varepsilon} > 0$ such that*

$$E_\alpha(P) \leq e^{\text{Pek}} + \frac{\text{Tr}_{L^2}(\sqrt{H^{\text{Pek}}} - 1)}{2\alpha^2} + \frac{P^2}{2\alpha^4 M^{\text{LP}}} + C_{c,\varepsilon}\, \alpha^{-\frac{5}{2}+\varepsilon} \tag{5.29}$$

for all $|P|/\alpha \leq c$ and all α large enough.

Since the operator $\sqrt{H^{\text{Pek}}} - 1$ is trace class, non-zero and non-positive (see Lemma 5.1.1), the second term on the right side is finite and lowers the energy. It corresponds to the predicted quantum corrections of the ground state energy of the Fröhlich Hamiltonian [51, 89, 98, 75]. Since $E_\alpha(0) = \inf \sigma(H_\alpha)$, our theorem implies a two-term upper bound for the ground state energy of the Fröhlich Hamiltonian that agrees with this prediction. For momenta in the range $\alpha^{-\frac{1}{4}+\frac{\varepsilon}{2}} \ll |P|/\alpha \leq c$, the last term in (5.29) is subleading for large α when compared to the momentum dependent term. In this region the upper bound describes a quadratic dispersion relation for a free quasi-particle with mass $\alpha^4 M^{\text{LP}}$. The upper restriction on the range of $|P|$ is natural, since for $|P|/\alpha \geq \sqrt{2M^{\text{LP}}}$ the right side of (5.29) would be larger than the value of the bottom of the continuous spectrum (5.23). The lower restriction $|P|/\alpha \gg \alpha^{-\frac{1}{4}+\frac{\varepsilon}{2}}$, on the other hand, could in principle be improved by deriving a better error term in (5.29).

The derivation of a matching lower bound is, of course, more involved. To our knowledge the best known parabolic lower bound is still the one obtained by Lieb and Yamazaki [86] in 1958 stating that $E_\alpha(P) \geq c_1 e^{\text{Pek}} + c_2 P^2/(2\alpha^4 M^{\text{LP}})$ with $c_1 \approx 3.07$ and $c_2 \approx 0.11$. Even for $P = 0$ it remains a challenging problem to improve the Lieb–Thomas bound (5.15) such that it includes the quantum corrections of order α^{-2}. Progress in this direction has been achieved in [66, 63] for simplified polaron models in which the electron and the quantum field are confined to suitable finite size regions.

In the next two sections we provide the definition of our trial state and formulate our main statement as a variational estimate. The remainder of the paper is devoted to the proof of the variational estimate. A sketch of the strategy of the proof is given in Section 5.3.2.

5.2.1 Bogoliubov Hamiltonian

In this section we introduce and discuss a quadratic Hamiltonian defined on the Fock space. For its definition we set Π_0 and Π_1 to be the orthogonal projectors onto KerH^{Pek} = Span$\{\partial_i\varphi :$

$i = 1, 2, 3\}$ and $(\mathsf{Ker} H^{\mathrm{Pek}})^{\perp}$, that is

$$\mathsf{Ran}(\Pi_0) = \mathsf{Ker} H^{\mathrm{Pek}}, \quad \mathsf{Ran}(\Pi_1) = (\mathsf{Ker} H^{\mathrm{Pek}})^{\perp}. \tag{5.30}$$

Even though we will not make explicit use of it, it is convenient to keep in mind that the decomposition $L^2(\mathbb{R}^3) = \mathsf{Ran}(\Pi_0) \oplus \mathsf{Ran}(\Pi_1)$ implies the factorization

$$\mathcal{F} = \mathcal{F}_0 \otimes \mathcal{F}_1 \quad \text{with} \quad \mathcal{F}_0 = \mathcal{F}(\mathsf{Ran}(\Pi_0)) \quad \text{and} \quad \mathcal{F}_1 = \mathcal{F}(\mathsf{Ran}(\Pi_1)). \tag{5.31}$$

For technical reasons, which are explained in Section 5.3.4, we introduce the Bogoliubov Hamiltonian $\mathbb{H}_K$ with a momentum cutoff $K \in (0, \infty]$. Setting $\mathbb{N}_1 = \mathsf{d}\Gamma(\Pi_1)$ (the number operator on $\mathcal{F}_1$) we define

$$\mathbb{H}_K = \mathbb{N}_1 - \left\langle \psi \middle| \phi(h^1_{K,\cdot}) R \phi(h^1_{K,\cdot}) \psi \right\rangle_{L^2}, \tag{5.32}$$

where the new coupling function

$$h^1_{K,x}(y) = \int \mathsf{d}z\, \Pi_1(y,z) h_{K,x}(z) \quad \text{with} \quad h_{K,x}(y) = \frac{1}{(2\pi)^3} \int_{|k| \leq K} \frac{e^{ik(x-y)}}{|k|} \mathsf{d}k \tag{5.33}$$

results from the coupling function h_x by removing all momenta larger than K and then projecting to $\mathsf{Ran}(\Pi_1)$. The second term in (5.32) defines the quadratic operator given by

$$\begin{aligned} &\left\langle \psi \middle| \phi(h^1_{K,\cdot}) R \phi(h^1_{K,\cdot}) \psi \right\rangle_{L^2} \\ &\quad = \iint \mathsf{d}y \mathsf{d}z \left\langle \psi \middle| (h^1_{K,\cdot})(y) R (h^1_{K,\cdot})(z) \psi \right\rangle_{L^2} (a^\dagger_y + a_y)(a^\dagger_z + a_z). \end{aligned} \tag{5.34}$$

By definition $\mathbb{H}_K$ acts non-trivially only on the tensor component $\mathcal{F}_1$. Below we will show that $\mathbb{H}_K$ is bounded from below and diagonalizable by a unitary Bogoliubov transformation. For the precise statement, we need some further preparations.

For $K \in (0, \infty]$ we introduce H^{Pek}_K as the operator on $L^2(\mathbb{R}^3)$ defined by

$$H^{\mathrm{Pek}}_K \restriction \mathsf{Ran}(\Pi_1) = \Pi_1 - 4T_K \tag{5.35a}$$

$$H^{\mathrm{Pek}}_K \restriction \mathsf{Ran}(\Pi_0) = 0 \tag{5.35b}$$

where T_K is defined by the integral kernel

$$T_K(y,z) = \mathrm{Re} \left\langle \psi \middle| h^1_{K,\cdot}(y) R h^1_{K,\cdot}(z) \psi \right\rangle_{L^2}. \tag{5.36}$$

By definition $H^{\mathrm{Pek}}_\infty = H^{\mathrm{Pek}}$, see (5.20). Moreover we set $\Theta_K = (H^{\mathrm{Pek}}_K)^{1/4}$ and

$$A_K \restriction \mathsf{Ran}(\Pi_1) = \frac{\Theta_K^{-1} + \Theta_K}{2} \qquad B_K \restriction \mathsf{Ran}(\Pi_1) = \frac{\Theta_K^{-1} - \Theta_K}{2} \tag{5.37a}$$

$$A_K \restriction \mathsf{Ran}(\Pi_0) = \Pi_0 \qquad B_K \restriction \mathsf{Ran}(\Pi_0) = 0. \tag{5.37b}$$

The next lemma, whose proof can be found in Section 5.4, implies some useful properties of these operators, among others, that there is a constant $C > 0$ such that

$$\sup_{K \geq K_0} \left(\|A_K\|_{\mathrm{op}} + \|B_K\|_{\mathrm{HS}} \right) \leq C \tag{5.38}$$

for some K_0 large enough.

Lemma 5.2.2. *For K_0 large enough there exist constants $\beta \in (0,1)$ and $C > 0$ such that*

(i) $0 \leq H_K^{\mathrm{Pek}} \leq 1$ *and* $(H_K^{\mathrm{Pek}} - \beta) \restriction \mathsf{Ran}(\Pi_1) \geq 0$

(ii) $(B_K)^2 \leq C(1 - H_K^{\mathrm{Pek}})$

(iii) $\mathrm{Tr}_{L^2}(1 - H_K^{\mathrm{Pek}}) \leq C$

for all $K \in (K_0, \infty]$*. Moreover for all* $K \in (K_0, \infty)$

(iv) $\mathrm{Tr}_{L^2}((-i\nabla)(1 - H_K^{\mathrm{Pek}})(-i\nabla)) \leq CK$*.*

Up to normal ordering the Hamiltonian $\mathbb{H}_K$ corresponds to the second quantization of H_K^{Pek}. From the properties of the latter we can deduce that $\mathbb{H}_K$ is diagonizable by a unitary Bogoliubov transformation. To this end we introduce the transformation

$$\mathbb{U}_K a(f) \mathbb{U}_K^\dagger \, = \, a(A_K f) + a^\dagger(B_K \overline{f}) \quad \text{for all } f \in L^2(\mathbb{R}^3). \tag{5.39}$$

That this transformation defines a unitary operator $\mathbb{U}_K$ for all $K \in (K_0, \infty]$ is a consequence of (5.38). This is known as the Shale-Stinespring condition and we refer to [95] for more details. Also note that $\mathbb{U}_K$ does not mix the two components in $\mathcal{F} = \mathcal{F}_0 \otimes \mathcal{F}_1$.

Lemma 5.2.3. *For* $K \in (K_0, \infty]$ *with* K_0 *large enough and* $\mathbb{U}_K$ *the unitary operator defined by* (5.39)*, we have*

$$\mathbb{U}_K \mathbb{H}_K \mathbb{U}_K^\dagger \, = \, \mathsf{d}\Gamma\left(\sqrt{H_K^{\mathrm{Pek}}}\right) + \frac{1}{2} \mathsf{Tr}_{L^2}\left(\sqrt{H_K^{\mathrm{Pek}}} - \Pi_1\right) \tag{5.40}$$

with H_K^{Pek} *defined by* (5.35a) *and* (5.35b)*.*

The proof is obtained by an explicit computation and postponed to Section 5.4. From this lemma, we can infer that the ground state energy of $\mathbb{H}_K$ is given by

$$\inf \sigma(\mathbb{H}_K) \, = \, \frac{1}{2} \mathsf{Tr}_{L^2}\Big(\sqrt{H_K^{\mathrm{Pek}}} - \Pi_1\Big) \, = \, \frac{1}{2} \mathsf{Tr}_{L^2}\Big(\sqrt{H_K^{\mathrm{Pek}}} - 1\Big) + \frac{3}{2}, \tag{5.41}$$

where we also used $\Pi_1 = 1 - \Pi_0$ and $\mathsf{Tr}_{L^2}(\Pi_0) = 3$. Moreover, since $H_K^{\mathrm{Pek}} \leq \Pi_1$ we have $\inf \sigma(\mathbb{H}_K) < 0$ and from Item (iv) of Lemma 5.2.2 we find that $\inf \sigma(\mathbb{H}_K) > -\infty$ uniformly in $K \to \infty$.

For the ground state of $\mathbb{H}_K$ we shall use the notation

$$\Upsilon_K \, = \, \mathbb{U}_K^\dagger \Omega, \tag{5.42}$$

where it is important to keep in mind that the state Υ_K has excitations only in $\mathcal{F}_1$ (i.e., no zero-mode excitations) since $\mathbb{U}_K^\dagger$ acts as the identity on $\mathcal{F}_0$, see (5.37b).

5.2.2 Trial state and variational estimate

As starting point for the definition of our trial state consider the Fock space wave function obtained from the fiber decomposition of the classical Pekar product state $\Psi_{\psi,\varphi}$, that is

$$\Psi_\alpha^{\mathrm{Pek}}(P) = \int \mathrm{d}x\, e^{i(P_f - P)x}\psi(x)e^{a^\dagger(\alpha\varphi)}\Omega. \tag{5.43}$$

Testing the energy of $H_\alpha(P)$ with $\Psi_\alpha^{\mathrm{Pek}}(P)$, one would in fact obtain that $E_\alpha(P)$ is bounded from above by

$$e^{\mathrm{Pek}} - \frac{3}{2\alpha^2} + \frac{P^2}{\alpha^4 M^{\mathrm{LP}}} + o(\alpha^{-2}). \tag{5.44}$$

For $E_\alpha(0)$ this provides already a better bound compared to the semiclassical approximation for $\inf\sigma(H_\alpha)$. The improvement comes from taking into account the translational symmetry and can be interpreted as the missing zero-point energy of three quantum oscillators (that turned into translational degrees of freedom). As a side remark, we find it somewhat surprising that fiber decompositions of this form have been employed very rarely in the polaron literature, exceptions being [76] and [11]. We think they could be of interest also for other translation-invariant polaron type models.

To obtain the desired bound for $E_\alpha(P)$, we need to add several modifications to the integrand in (5.43). On the one hand, we have to replace the classical field φ by a suitably shifted φ_P in order to get the correct momentum dependent term (note that (5.44) is missing a factor $\frac{1}{2}$ in the quadratic term). The missing part of the rest energy (compare with (5.41)), on the other hand, is caused by two types of correlations that need to be added to the Pekar product state. First, we include correlations between the electron and the phonons. This is done in the spirit of first-order adiabatic perturbation theory. Second, we rotate the vacuum by the unitary transformation (5.39) that diagonalizes the Bogoliubov Hamiltonian (5.32). As discussed, the latter describes the quantum fluctuations of the phonons around the classical field. For technical reasons, briefly explained in Section 5.3.2, we also need to introduce suitable momentum and space cutoffs in the trial state.

Explicitly, we consider the family of Fock space wave functions $\Psi_{K,\alpha}(P) \in \mathcal{F}$, depending on the coupling α, the total momentum $P \in \mathbb{R}^3$ and the cutoff $K \in (K_0, \infty)$, given by

$$\Psi_{K,\alpha}(P) = \int \mathrm{d}x\, e^{i(P_f - P)x}\, e^{a^\dagger(\alpha\varphi_P) - a(\alpha\varphi_P)}\Big(G^0_{K,x} - \alpha^{-1}G^1_{K,x}\Big) \tag{5.45}$$

where

$$\varphi_P = \varphi + i\xi_P \quad \text{with} \quad \xi_P = \frac{1}{\alpha^2 M^{\mathrm{LP}}}(P\nabla)\varphi, \quad M^{\mathrm{LP}} = \frac{2}{3}\|\nabla\varphi\|^2_{L^2}, \tag{5.46}$$

and

$$G^0_{K,x} = \psi(x)\Upsilon_K, \quad G^1_{K,x} = u_\alpha(x)(R\phi(h^1_{K,\cdot})\psi)(x)\Upsilon_K \quad \text{and} \quad \Upsilon_K = \mathbb{U}_K^\dagger\Omega. \tag{5.47}$$

Here $u_\alpha : \mathbb{R}^3 \to [0,1]$ is a radial function, satisfying

$$u_\alpha(x) = \begin{cases} 1 & \forall\, |x| \le \alpha \\ 0 & \forall\, |x| \ge 2\alpha \end{cases} \quad \text{and} \quad \|\nabla u_\alpha\|_{L^\infty} + \|\Delta u_\alpha\|_{L^\infty} \le C\alpha^{-1} \tag{5.48}$$

for some $C > 0$. For completeness, we recall that $\psi > 0$ and φ are the unique rotational invariant minimizers of the Pekar functionals (5.12) and (5.13).

Remark 3. Writing $G^i_{K,x}$ we think of these states as elements in $L^2(\mathbb{R}^3, \mathcal{F})$ and of

$$(R\phi(h^1_{K,\cdot})\psi)(x) \;=\; \iint \mathrm{d}z\mathrm{d}y\, R(x,y)h^1_{K,y}(z)\psi(y)\left(a^\dagger_z + a_z\right) \tag{5.49}$$

as an x-dependent Fock space operator. Via the isomorphism $L^2(\mathbb{R}^3, \mathcal{F}) \simeq \mathscr{H}$, we can view $G^i_{K,x}$ also as a wave function in $\mathscr{H}$. In this case we shall write

$$G^0_K \;=\; \psi \otimes \Upsilon_K, \quad G^1_K \;=\; u_\alpha R\phi(h^1_{K,\cdot})\psi \otimes \Upsilon_K. \tag{5.50}$$

For the introduced trial states, we prove the following variational estimate, where $\mathbb{H}_\infty$ denotes the Bogoliubov Hamiltonian (5.32) for $K = \infty$.

Proposition 5.2.4. *Let $\Psi_{K,\alpha}(P) \in \mathcal{F}$ as in* (5.45)*, choose $c, \tilde{c} > 0$ and set $r(K,\alpha) = K^{-1/2}\alpha^{-2} + \sqrt{K}\alpha^{-3}$. For every $\varepsilon > 0$ there exists a constant $C_\varepsilon > 0$* (*we omit the dependence on c and $\tilde{c}$*) *such that*

$$\frac{\left\langle \Psi_{K,\alpha}(P) | H_\alpha(P)\Psi_{K,\alpha}(P)\right\rangle_{\mathcal{F}}}{\left\langle \Psi_{K,\alpha}(P)|\Psi_{K,\alpha}(P)\right\rangle_{\mathcal{F}}} \;\le\; e^{\mathrm{Pek}} + \frac{\inf\sigma(\mathbb{H}_\infty) - \frac{3}{2}}{\alpha^2} + \frac{P^2}{2\alpha^4 M^{\mathrm{LP}}} + C_\varepsilon \alpha^\varepsilon r(K,\alpha) \tag{5.51}$$

for all $|P|/\alpha \le c$ and all K, α large enough with $K/\alpha \le \tilde{c}$.

With (5.41) and $H^{\mathrm{Pek}}_\infty = H^{\mathrm{Pek}}$ we can rewrite the term of order α^{-2} as

$$\inf\sigma(\mathbb{H}_\infty) - \frac{3}{2} \;=\; \frac{1}{2}\mathrm{Tr}_{L^2}\left(\sqrt{H^{\mathrm{Pek}}} - 1\right). \tag{5.52}$$

Choosing K now proportional to α optimizes the asymptotics of the error in (5.51) and proves Theorem 5.2.1.

5.3 Proof of Proposition 5.2.4

We recall the definition of the field operators

$$\phi(f) = a^\dagger(f) + a(f), \quad \pi(f) = \phi(if) \tag{5.53}$$

and the Weyl operator

$$W(f) \;=\; e^{-i\pi(f)} \;=\; e^{a^\dagger(f) - a(f)} \;=\; e^{a^\dagger(f)}e^{-a(f)}e^{-\frac{1}{2}\|f\|^2_{L^2}}. \tag{5.54}$$

The Weyl operator is unitary and satisfies

$$W^\dagger(f) \;=\; W(-f), \quad W(f)W(g) \;=\; W(g)W(f)e^{2i\,\mathrm{Im}\langle g|f\rangle_{L^2}} \;=\; W(f+g)e^{i\,\mathrm{Im}\langle g|f\rangle_{L^2}}. \tag{5.55}$$

5.3.1 The total energy

The proof of Proposition 5.2.4 starts with a convenient formula for the energy evaluated in the trial state. For the precise statement, we introduce the y-dependent function in $L^2(\mathbb{R}^3)$,

$$w_{P,y} \;=\; (1-e^{-y\nabla})\varphi_P, \tag{5.56}$$

and the y-dependent Fock space operator

$$A_{P,y} \;=\; iP_f y + i g_P(y), \quad g_P(y) \;=\; -\frac{2}{M^{\mathrm{LP}}}\int_0^1 \mathrm{d}s\, \langle \varphi | e^{-sy\nabla}(y\nabla)^3(P\nabla)\varphi\rangle_{L^2}. \tag{5.57}$$

Since $g_P(y)$ is real-valued we have $(A_{P,y})^\dagger = -A_{P,y}$. We further consider the Weyl-transformed Fröhlich Hamiltonian,

$$\widetilde{H}_{\alpha,P} \;=\; W(\alpha\varphi_P)^\dagger\Big(H_\alpha - e^{\mathrm{Pek}}\Big)W(\alpha\varphi_P) \;=\; h^{\mathrm{Pek}} + \alpha^{-2}\mathbb{N} + \alpha^{-1}\phi(h_x+\varphi_P), \tag{5.58}$$

where we recall $h^{\mathrm{Pek}} = -\Delta + V^\varphi - \lambda^{\mathrm{Pek}}$, and denote the shift operator acting on $L^2(\mathbb{R}^3)$ by $T_y = e^{y\nabla}$ with $y\in\mathbb{R}^3$.

Lemma 5.3.1. *For $\Psi_{K,\alpha}(P)$ defined in* (5.45) *we have*

$$\Big\langle \Psi_{K,\alpha}(P) | H_\alpha(P)\Psi_{K,\alpha}(P)\Big\rangle_{\mathcal{F}} \;=\; \Big(e^{\mathrm{Pek}} + \frac{P^2}{2\alpha^4 M^{\mathrm{LP}}}\Big)\mathcal{N} + \mathcal{E} + \mathcal{G} + \mathcal{K} \tag{5.59}$$

where $\mathcal{N} = \|\Psi_{K,\alpha}(P)\|^2_{\mathcal{F}}$ and

$$\mathcal{E} \;=\; \int \mathrm{d}y\, \Big\langle G_K^0 | \widetilde{H}_{\alpha,P} T_y e^{A_{P,y}} W(\alpha w_{P,y}) G_K^0\Big\rangle_{\mathscr{H}} \tag{5.60a}$$

$$\mathcal{G} \;=\; -\frac{2}{\alpha}\int \mathrm{d}y\, \mathrm{Re}\Big\langle G_K^0 | \widetilde{H}_{\alpha,P} T_y e^{A_{P,y}} W(\alpha w_{P,y}) G_K^1\Big\rangle_{\mathscr{H}} \tag{5.60b}$$

$$\mathcal{K} \;=\; \frac{1}{\alpha^2}\int \mathrm{d}y\, \Big\langle G_K^1 | \widetilde{H}_{\alpha,P} T_y e^{A_{P,y}} W(\alpha w_{P,y}) G_K^1\Big\rangle_{\mathscr{H}}. \tag{5.60c}$$

For the proof we recall that the Weyl operator shifts the creation and annihilation operators by complex numbers,

$$W(g)^\dagger a^\dagger(f) W(g) \;=\; a^\dagger(f) + \langle g|f\rangle_{L^2}, \quad W(g)^\dagger a(f) W(g) \;=\; a(f) + \overline{\langle g|f\rangle_{L^2}}, \tag{5.61}$$

and, as a simple consequence,

$$W(g)^\dagger \phi(f) W(g) \;=\; \phi(f) + 2\,\mathrm{Re}\Big\langle f|g\Big\rangle_{L^2}, \tag{5.62a}$$

$$W(g)^\dagger \mathbb{N} W(g) \;=\; \mathbb{N} + \phi(g) + \|g\|^2_{L^2}, \tag{5.62b}$$

$$W(g)^\dagger P_f W(g) \;=\; P_f - a^\dagger(i\nabla g) - a(i\nabla g) - \Big\langle g|i\nabla g\Big\rangle_{L^2}. \tag{5.62c}$$

Moreover we need the following identity.

Lemma 5.3.2. *Let $\varphi_P = \varphi + i\xi_P$ with ξ_P defined by* (5.46)*. Then*

$$W^\dagger(\alpha\varphi_P) e^{i(P_f - P)y} W(\alpha\varphi_P) \;=\; e^{A_{P,y}} W(\alpha w_{P,y}). \tag{5.63}$$

Proof of Lemma 5.3.2. We first observe that

$$e^{-iP_f y} a^\dagger(f) e^{iP_f y} \;=\; a^\dagger(e^{-y\nabla} f) \tag{5.64}$$

which follows from $\frac{d}{ds} e^{-isP_f y} a^\dagger(e^{(s-1)y\nabla} f) e^{isP_f y} = 0$. In combination with (5.55) this leads to

$$W^\dagger(\alpha\varphi_P) e^{iP_f y} W(\alpha\varphi_P) \;=\; e^{iP_f y} W(\alpha(1-e^{-y\nabla})\varphi_P) \exp\Big(i\alpha^2 \operatorname{Im}\langle\varphi_P| e^{-y\nabla}\varphi_P\rangle_{L^2}\Big). \tag{5.65}$$

Recalling $\varphi_P = \varphi + i\frac{1}{\alpha^2 M^{\mathrm{LP}}}(P\nabla)\varphi$, we compute

$$\begin{aligned}\alpha^2 \operatorname{Im}\langle\varphi_P|e^{-y\nabla}\varphi_P\rangle_{L^2} \;&=\; \frac{2}{M^{\mathrm{LP}}}\langle\varphi|e^{-y\nabla}(P\nabla)\varphi\rangle_{L^2}\\ &=\; -\frac{2}{M^{\mathrm{LP}}}\langle\varphi|(y\nabla)(P\nabla)\varphi\rangle_{L^2} - \frac{2}{M^{\mathrm{LP}}}\int_0^1 \mathsf{d}s\,\langle\varphi|e^{-sy\nabla}(y\nabla)^3(P\nabla)\varphi\rangle_{L^2}\end{aligned} \tag{5.66}$$

where we inserted $e^{-y\nabla} = 1-(y\nabla)+\frac{1}{2}(y\nabla)^2 - \int_0^1 \mathsf{d}s\, e^{-sy\nabla}(y\nabla)^3$ and used that, due to rotational invariance of φ, $\langle\varphi|(P\nabla)\varphi\rangle_{L^2} = 0 = \langle\varphi|(y\nabla)^2(P\nabla)\varphi\rangle_{L^2}$. Also because of rotational invariance,

$$\langle\varphi|(y\nabla)(P\nabla)\varphi\rangle_{L^2} \;=\; -\frac{(Py)}{3}\|\nabla\varphi\|_{L^2}^2 \;=\; -\frac{(Py)}{2}M^{\mathrm{LP}}, \tag{5.67}$$

and thus, $\alpha^2\operatorname{Im}\langle\varphi_P|e^{-y\nabla}\varphi_P\rangle_{L^2} = Py + g_P(y)$. □

Proof of Lemma 5.3.1. The norm squared is given by

$$\begin{aligned}\mathcal{N} &= \Big\| \int \mathsf{d}x\, e^{i(P_f-P)x} W(\alpha\varphi_P)\Big(G^0_{K,x} - \alpha^{-1}G^1_{K,x}\Big)\Big\|^2_{\mathcal{F}}\\ &= \sum_{i\in\{0,1\}} \alpha^{-2i} \iint \mathsf{d}y\mathsf{d}x\,\Big\langle G^i_{K,x}|W(\alpha\varphi_P)^\dagger e^{i(P_f-P)(y-x)} W(\alpha\varphi_P) G^i_{K,y}\Big\rangle_{\mathcal{F}}\\ &\quad - 2\alpha^{-1}\operatorname{Re}\iint \mathsf{d}y\mathsf{d}x\,\Big\langle G^0_{K,x}|W(\alpha\varphi_P)^\dagger e^{i(P_f-P)(y-x)} W(\alpha\varphi_P) G^1_{K,y}\Big\rangle_{\mathcal{F}}.\end{aligned} \tag{5.68}$$

Shifting $y \to y+x$ and writing the x-integration as an inner product in the electron coordinate, cf. Remark 3, we can proceed for $i,j\in\{0,1\}$ with

$$\begin{aligned}&\iint \mathsf{d}y\mathsf{d}x\,\Big\langle G^i_{K,x}|W(\alpha\varphi_P)^\dagger e^{i(P_f-P)(y-x)} W(\alpha\varphi_P) G^j_{K,y}\Big\rangle_{\mathcal{F}}\\ &\quad= \iint \mathsf{d}y\mathsf{d}x\,\Big\langle G^i_{K,x}|W(\alpha\varphi_P)^\dagger e^{i(P_f-P)y} W(\alpha\varphi_P) G^j_{K,y+x}\Big\rangle_{\mathcal{F}}\\ &\quad= \int \mathsf{d}y\,\Big\langle G^i_K|W(\alpha\varphi_P)^\dagger e^{i(P_f-P)y} W(\alpha\varphi_P) T_y G^j_K\Big\rangle_{\mathscr{H}}\\ &\quad= \int \mathsf{d}y\,\Big\langle G^i_K|e^{A_{P,y}} W(\alpha w_{P,y}) T_y G^j_K\Big\rangle_{\mathscr{H}},\end{aligned} \tag{5.69}$$

where we applied Lemma 5.3.2 in the last step. Similarly for the energy

$$\begin{aligned}&\Big\langle \Psi_{K,\alpha}(P)|H_\alpha(P)\Psi_{K,\alpha}(P)\Big\rangle_{\mathcal{F}}\\ &= \sum_{i\in\{0,1\}} \alpha^{-2i}\iint \mathsf{d}y\mathsf{d}x\,\Big\langle G^i_{K,x}|W(\alpha\varphi_P)^\dagger e^{-i(P_f-P)x} H_\alpha(P) e^{i(P_f-P)y} W(\alpha\varphi_P) G^i_{K,y}\Big\rangle_{\mathcal{F}}\\ &- 2\alpha^{-1}\operatorname{Re}\iint \mathsf{d}y\mathsf{d}x\Big\langle G^0_{K,x}|W(\alpha\varphi_P)^\dagger e^{-i(P_f-P)x} H_\alpha(P) e^{i(P_f-P)y} W(\alpha\varphi_P) G^1_{K,y}\Big\rangle_{\mathcal{F}}\end{aligned} \tag{5.70}$$

where we also used self-adjointness of $H_\alpha(P)$. Next we invoke

$$e^{-i(P_f-P)x}H_\alpha(P) = \Big(-\Delta_x + \alpha^{-2}\mathbb{N} + \alpha^{-1}\phi(h_x)\Big)e^{-i(P_f-P)x} \tag{5.71}$$

to proceed for $i,j \in \{0,1\}$ with

$$\begin{aligned}
&\iint \mathrm{d}y\mathrm{d}x \left\langle G^i_{K,x}|W(\alpha\varphi_P)^\dagger\Big(-\Delta_x + \alpha^{-2}\mathbb{N} + \alpha^{-1}\phi(h_x)\Big)e^{i(P_f-P)(y-x)}W(\alpha\varphi_P)G^j_{K,y}\right\rangle_{\mathcal{F}} \\
&= \int \mathrm{d}y \left\langle G^i_K|W(\alpha\varphi_P)^\dagger H_\alpha e^{i(P_f-P)y}W(\alpha\varphi_P)T_yG^j_K\right\rangle_{\mathscr{H}} \\
&= \int \mathrm{d}y \left\langle G^i_K|W(\alpha\varphi_P)^\dagger H_\alpha W(\alpha\varphi_P)e^{A_{P,y}}W(\alpha w_{P,y})T_yG^j_K\right\rangle_{\mathscr{H}}.
\end{aligned} \tag{5.72}$$

Using (5.62a), (5.62b) and $-2\,\mathrm{Re}\langle\varphi_P|h_x\rangle_{L^2} = -2\,\mathrm{Re}\langle\varphi|h_x\rangle_{L^2} = V^\varphi(x)$ we have

$$\begin{aligned}
W(\alpha\varphi_P)^\dagger H_\alpha W(\alpha\varphi_P) &= -\Delta_x + V^\varphi(x) + \alpha^{-2}\mathbb{N} + \alpha^{-1}\phi(h_x+\varphi_P) + \|\varphi_P\|^2_{L^2} \\
&= \widetilde{H}_{\alpha,P} + e^{\mathrm{Pek}} + \|\varphi_P\|^2_{L^2} - \|\varphi\|^2_{L^2}
\end{aligned} \tag{5.73}$$

where we added and subtracted $e^{\mathrm{Pek}} = \lambda^{\mathrm{Pek}} + \|\varphi\|^2_{L^2}$. It remains to compute

$$\|\varphi_P\|^2_{L^2} - \|\varphi\|^2_{L^2} \;=\; \frac{1}{\alpha^4(M^{\mathrm{LP}})^2}\|(P\nabla)\varphi\|^2_{L^2} \;=\; \frac{P^2}{2\alpha^4 M^{\mathrm{LP}}} \tag{5.74}$$

since $\|(P\nabla)\varphi\|^2_{L^2} = \frac{P^2}{3}\|\nabla\varphi\|^2_{L^2} = \frac{P^2}{2}M^{\mathrm{LP}}$ because of rotational invariance of φ. With (5.73) inserted into (5.72), the stated formula for the energy follows from (5.68) and (5.70). □

5.3.2 A short guide to the proof

Heuristic picture

Given Lemma 5.3.1, the remaining task is to show that $(\mathcal{E}+\mathcal{G}+\mathcal{K})/\mathcal{N}$ coincides, up to small errors, with the energy contribution of order α^{-2} in (5.51). Although our proof is somewhat technical, the main idea is a simple one, and we explain the corresponding heuristics here in order to facilitate the reading. The main point is that the integrals appearing in the terms given in Lemma 5.3.1 turn out to be, as $\alpha \to \infty$ and $|P|/\alpha \le c$, sharply localized around zero at the length scale of order α^{-1}. In this regime, as formally $w_{P,y}(z) \approx y\nabla\varphi(z)$ for y small, the Weyl operator $W(\alpha w_{P,y})$ effectively acts non-trivially only on the $\mathcal{F}_0$ part of the Fock space (at this point it is convenient to recall the factorization (5.31)). Moreover, we shall show that $e^{A_{P,y}}$ can be effectively replaced by the identity operator and it suffices to consider $T_y \approx 1 + y\nabla$. Since our trial state coincides with the vacuum on $\mathcal{F}_0$, we thus expect for $|y|$ small that

$$T_y e^{A_{P,y}}W(\alpha w_{P,y})G^i_K \approx e^{-\lambda\alpha^2y^2}\,(1+y\nabla)\,e^{a^\dagger(\alpha y\nabla\varphi)}G^i_K, \quad i=0,1 \tag{5.75}$$

with $\lambda = \frac{1}{6}\|\nabla\varphi\|^2_{L^2}$. (Since T_y acts on the electron coordinate, it commutes with $e^{A_{P,y}}$ and $W(\alpha w_{P,y})$). Taking this approximation for granted, and considering only the term with $i=j=0$ in (5.69), would lead to

$$\mathcal{N} \;\approx\; \int \mathrm{d}y \left\langle G^0_K|T_ye^{A_{P,y}}W(\alpha w_{P,y})G^0_K\right\rangle_{\mathscr{H}} \;=\; \int \mathrm{d}y\, e^{-\lambda\alpha^2y^2} \;+\; \text{Errors}. \tag{5.76}$$

With the above replacement, and keeping only the terms of order α^{-2} (relative to the factor from the norm), the energy terms are found to be given by

$$\mathcal{E} = \frac{1}{\alpha^2}\big\langle\psi\otimes\Upsilon_K|\mathbb{N}_1\psi\otimes\Upsilon_K\big\rangle_{\mathscr{H}}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2} \;+\; \text{Errors} \tag{5.77a}$$

$$+\frac{1}{\alpha}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2}\big\langle\psi\otimes\Upsilon_K|\big(\phi(h_\cdot+\varphi)(1+(y\nabla)a^\dagger(\alpha y\nabla\varphi))\big)\psi\otimes\Upsilon_K\big\rangle_{\mathscr{H}} \tag{5.77b}$$

$$\mathcal{G} = -\frac{2}{\alpha^2}\operatorname{Re}\big\langle\psi\otimes\Upsilon_K|\phi(h_\cdot^1)u_\alpha R\phi(h_{K,\cdot}^1)\psi\otimes\Upsilon_K\big\rangle_{\mathscr{H}}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2} \;+\; \text{Errors} \tag{5.77c}$$

$$\mathcal{K} = \frac{1}{\alpha^2}\big\langle\psi\otimes\Upsilon_K|\phi(h_\cdot^1)Ru_\alpha h^{\mathrm{Pek}}u_\alpha R\phi(h_{K,\cdot}^1)\psi\otimes\Upsilon_K\big\rangle_{\mathscr{H}}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2} \;+\; \text{Errors.} \tag{5.77d}$$

From here the Bogoliubov energy is obtained by setting $u_\alpha = 1$ and $K = \infty$ in the leading-order terms, and using $Rh^{\mathrm{Pek}}R = R$, since this would imply (omitting the errors)

$$\begin{aligned}(5.77\text{a}) + (5.77\text{c}) + (5.77\text{d}) &= \big\langle\psi\otimes\Upsilon_\infty|(\mathbb{N}_1-\phi(h_\cdot^1)R\phi(h_{\infty,\cdot}^1))\psi\otimes\Upsilon_\infty\big\rangle_{\mathscr{H}}\frac{1}{\alpha^2}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2}\\ &= \frac{\inf\sigma(\mathbb{H}_\infty)}{\alpha^2}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2}.\end{aligned} \tag{5.78}$$

The remaining $-\frac{3}{2\alpha^2}$ term stems from the part of the interaction involving the zero modes. In (5.77b), the term not involving $y\nabla$ vanishes due to $\langle\psi|h_\cdot\psi\rangle_{L^2} = -\varphi$. Moreover, $\langle\psi|h_\cdot\nabla\psi\rangle_{L^2} = -\frac{1}{2}\nabla\varphi$ using $\nabla h_\cdot = -(\nabla h)_\cdot$ via integration by parts (in the sense of distributions). Thus, since $[a^\dagger(y\nabla\varphi), \mathbb{U}_\infty^\dagger] = 0$,

$$\begin{aligned}(5.77\text{b}) &= \int \mathrm{d}y\, e^{-\lambda\alpha^2y^2}\big\langle\Omega|\phi(\langle\psi|h_\cdot y\nabla\psi\rangle)a^\dagger(y\nabla\varphi)\Omega\big\rangle_{\mathcal{F}}\\ &= -\frac{1}{2}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2}\|y\nabla\varphi\|_{L^2}^2 = -\frac{3}{2\alpha^2}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2}.\end{aligned} \tag{5.79}$$

Equations (5.78) and (5.79) now add up to the desired energy of order α^{-2}, see (5.52). Note that for estimating the error induced by replacing $e^{A_{P,y}}$ by unity we require the momentum cutoff K in the definition of the trial state, see Lemma 5.3.14.

The main issue in (5.75) is that while for small enough y one can use the first-order approximation $W(\alpha w_{P,y}) \approx W(\alpha y\nabla\varphi)$, for y large, on the other hand, the higher-order terms in $w_{P,y}$ begin to play an important part, ultimately killing the Gaussian factor. Writing

$$\begin{aligned}&\big\langle G_K^i|\widetilde{H}_\alpha(P)e^{A_{P,y}}W(\alpha w_{P,y})T_yG_K^j\big\rangle_{\mathscr{H}}\\ &= e^{-\frac{\alpha^2}{2}\|w_{P,y}\|_{L^2}^2}\big\langle G_K^i|\widetilde{H}_\alpha(P)e^{A_{P,y}}e^{a^\dagger(\alpha w_{P,y})}e^{-a(\alpha w_{P,y})}T_yG_K^j\big\rangle_{\mathscr{H}}, \quad i,j=0,1,\end{aligned} \tag{5.80}$$

we notice that, since

$$\|w_{P,y}\|_{L^2}^2 = 2\int \mathrm{d}k\,|\hat{\varphi}_P(k)|^2(1-\cos(ky)) \to 2\|\varphi_P\|_{L^2}^2 \quad \text{for} \quad |y|\to\infty, \tag{5.81}$$

the prefactor should lead to a y-independent, exponentially small constant. In order to make use of this exponential decay in α, however, we need to ensure that

$$\Big|\big\langle G_K^i|\widetilde{H}_\alpha(P)e^{A_{P,y}}e^{a^\dagger(\alpha w_{P,y})}e^{-a(\alpha w_{P,y})}T_yG_K^j\big\rangle_{\mathscr{H}}\Big| \leq C\alpha^n g(y) \tag{5.82}$$

is polynomially bounded in α with some integrable function $g(y)$, which heuristically can be expected to be true since the average number of particles in the state $\widetilde{H}_\alpha(P)G_K^i$ is of order one w.r.t. α. To obtain the required integrability in y is also the reason for introducing the cutoff function u_α in the definition of G_K^1.

Outline of the proof

Although the replacement (5.75) illustrates the main idea behind extracting the leading order terms, in our proof we do not directly perform this replacement and estimate the resulting error. Instead, when taking inner products, we commute the exponential operators $e^{a^\dagger(\alpha w_P)}$ and $e^{-a(\alpha w_P)}$ in $W(\alpha w_{P,y})$ to the left resp. to the right until they hit the vacuum state in G_K^i. This involves the Bogoliubov transformation, cf. Lemma 5.3.10, and gives rise to a slight modification of $w_{P,y}$, which we denote by $\widetilde{w}_{P,y}$. These manipulations naturally lead to a multiplicative factor $\exp(-\frac{\alpha^2}{2}\|\widetilde{w}_{P,y}\|_{L^2}^2)$ which, as we shall see, indeed behaves like the Gaussian function in (5.75) for $|y|$ small and tends to a constant exponentially small in α as $|y| \to \infty$. In Lemma 5.3.4 we prove the large α asymptotics of integrals of the type $\int g(y)\exp(-\frac{\alpha^2}{2}\|\widetilde{w}_{P,y}\|_{L^2}^2)\mathrm{d}y$ for a suitable class of functions g. The major part of the proof, apart from extracting the leading order terms, is to establish that the resulting error terms in the integrands are, in fact, functions in this class. This is, for the most part, achieved by use of elementary estimates combined with the commutator method by Lieb and Yamazaki [86] in the form stated in Lemma 5.3.8. As already mentioned, for certain terms this makes the introduction of the space cutoff u_α and the momentum cutoff K necessary, while for others, it is enough to use the well-known regularity properties of ψ, the relevant consequences of which are summarized in Lemma 5.3.6.

In the next two sections, we state the remaining necessary lemmas. The main proof is then carried out in Sections 5.3.5–5.3.9.

Throughout the remainder of the proof we will abbreviate constants by the letter C and write C_τ whenever we want to specify that it depends on a parameter τ. As usual, the value of a constant may change from one line to the next.

5.3.3 The Gaussian lemma

We recall that $w_{P,y} = (1 - e^{-y\nabla})\varphi_P$ and $\Theta_K = (H_K^{\mathrm{Pek}})^{1/4}$ and set

$$w_{P,y}^0 = \Pi_0 w_{P,y} \in \mathrm{Ker} H^{\mathrm{Pek}} \tag{5.83a}$$

$$w_{P,y}^1 = \Pi_1 w_{P,y} \in (\mathrm{Ker} H^{\mathrm{Pek}})^\perp \tag{5.83b}$$

$$\widetilde{w}_{P,y} = w_{P,y}^0 + \Theta_K \operatorname{Re}(w_{P,y}^1) + i\Theta_K^{-1}\operatorname{Im}(w_{P,y}^1). \tag{5.83c}$$

Remark 4. Note that $(y,z) \mapsto \operatorname{Re}(w_{P,y})(z)$ is even as a function on $\mathbb{R}^6$, while $\operatorname{Im}(w_{P,y})(z)$ is odd on the same space. Since Π_0 and Θ_K have real-valued kernels that are even as functions on $\mathbb{R}^6$, they preserve the parity properties just mentioned. That Π_0 has the desired properties follows directly from its explicit form. To see this for Θ_K, it is enough to check this for H_K^{Pek}, which can be easily done using the fact that the resolvent R commutes with the reflection operator, which, on the other hand, follows from the invariance of h^{Pek} and Π_i under parity. Thus $(y,z) \mapsto \operatorname{Re}(w_{P,y}^i)(z)$ is even as a function on $\mathbb{R}^6$ for $i = 0, 1$ while the corresponding imaginary parts are odd on the same space. These facts will be of relevance below where they lead to the vanishing of several integrals.

The following lemma is proven in Section 5.4.

Lemma 5.3.3. *Let $\lambda = \frac{1}{6}\|\nabla\varphi\|_{L^2}^2$ and $K_0 > 0$ large enough. For every $c > 0$ there exists a constant $C > 0$ such that*

$$\|w^1_{P,y}\|^2_{L^2} + \|\widetilde{w}^1_{P,y}\|^2_{L^2} \;\le\; C\Big(\alpha^{-2}y^2 + y^4\Big) \tag{5.84a}$$

$$\Big|\|w^0_{P,y}\|^2_{L^2} - 2\lambda y^2\Big| \;\le\; C\Big(\alpha^{-2}y^2 + y^4 + y^6\Big) \tag{5.84b}$$

$$\Big|\|\widetilde{w}_{P,y}\|^2_{L^2} - 2\lambda y^2\Big| \;\le\; C\Big(\alpha^{-2}y^2 + y^4 + y^6\Big) \tag{5.84c}$$

for all $y \in \mathbb{R}^3$, $|P|/\alpha \le c$, $K \in (K_0, \infty]$ and $\alpha > 0$.

For $0 \le \delta < 1$ and $\eta > 0$ we introduce the weight function

$$n_{\delta,\eta}(y) \;=\; \exp\left(-\frac{\eta\alpha^{2(1-\delta)}\|\widetilde{w}_{P,y}\|^2_{L^2}}{2}\right) \tag{5.85}$$

where, for ease of notation, the dependence on α, P and K is omitted. Using the arguments laid down in Remark 4, it is easy to see that $n_{\delta,\eta}(y)$ is even as a function of y. Moreover in the limit of large α the dominant part of the weight function when integrated against suitably decaying functions comes from the term in the exponent that is quadratic in y, cf. (5.84c). This is a crucial ingredient in our proofs and the content of the next lemma.

Lemma 5.3.4. *Let $\eta_0 > 0$, $c > 0$, $\lambda = \frac{1}{6}\|\nabla\varphi\|^2_{L^2}$ and $n_{\delta,\eta}(y)$ defined in (5.85). For every $n \in \mathbb{N}_0$ there exist constants $d, C_n > 0$ such that*

$$\int |y|^n g(y)\left|n_{\delta,\eta}(y) - e^{-\eta\lambda\alpha^{2(1-\delta)}y^2}\right|\mathrm{d}y \;\le\; C_n\frac{\|g\|_{L^\infty}}{\alpha^{(4+n)(1-\delta)+\delta}} + e^{-d\alpha^{-2\delta+1}}\||\cdot|^n g\|_{L^1} \tag{5.86}$$

for all non-negative functions $g \in L^\infty(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$, $\eta \ge \eta_0$, $\delta \in [0,1)$, $|P|/\alpha \le c$ and all K, α large enough.

At first reading, one should think of $n = 0$, $\delta = 0$, $\eta = 1$ and g a suitable α-independent non-negative function. In this case the integral involving the Gaussian is of order α^{-3} whereas the term on the right hand side is of order α^{-4} and thus contributing a subleading error. The proof of the lemma is given in Section 5.4. As a direct consequence that will be useful to estimate error terms, we find

Corollary 5.3.5. *Given the same assumptions as in Lemma 5.3.4, for every $n \in \mathbb{N}_0$ there exist constants $d, C_n > 0$ such that*

$$\int |y|^n g(y) n_{\delta,\eta}(y)\mathrm{d}y \;\le\; C_n\frac{\|g\|_{L^\infty}}{\alpha^{(3+n)(1-\delta)}} + e^{-d\alpha^{-2\delta+1}}\||\cdot|^n g\|_{L^1} \tag{5.87}$$

for all non-negative functions $g \in L^\infty(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$, $\eta \ge \eta_0$, $\delta \in [0,1)$, $|P|/\alpha \le c$ and all K, α large enough.

Proof of Corollary 5.3.5. Since

$$\int \mathrm{d}y\, |y|^n e^{-\eta\lambda\alpha^{2(1-\delta)}y^2} \;=\; (\eta\lambda\alpha^{2(1-\delta)})^{-\frac{3+n}{2}}\int \mathrm{d}y\,|y|^n e^{-y^2} \;=\; C_n\alpha^{-(3+n)(1-\delta)}, \tag{5.88}$$

the statement follows immediately from Lemma 5.3.4. ☐

5.3.4 Further preliminaries

Estimates involving the Pekar minimizers

Lemma 5.3.6. *Let $\psi > 0$ be the rotational invariant unique minimizer of the Pekar functional* (5.12)*, and let*

$$H(x) := \left\langle \psi | T_x \psi \right\rangle_{L^2} = (\psi * \psi)(x). \tag{5.89}$$

We have that ψ, $|\nabla\psi|$ and H are $L^p(\mathbb{R}^3, (1+|x|^n)\mathrm{d}x)$ functions for all $1 \le p \le \infty$ and all $n \ge 0$. Moreover, there exists a constant $C > 0$ such that for all x we have

$$|H(x) - 1| \le Cx^2. \tag{5.90}$$

Proof. As follows from [83], $\psi(x)$ is monotone decreasing in $|x|$; moreover, it is smooth and bounded and vanishes exponentially at infinity, i.e. there exists a constant $C0$ such that $\psi(x) \le Ce^{-|x|/C}$ for all $|x|$ large enough (for the precise asymptotics see [91]). This clearly implies the statement for ψ. It further implies that all the derivatives of ψ are bounded. Hence, in order to show the desired result for $|\nabla\psi|$, it suffices to show that $\int \mathrm{d}x |x|^n |\nabla\psi(x)|$ is finite for all $n \ge 0$. Since ψ is radial, i.e. there is a function $\psi^{\mathrm{rad}} : [0,\infty) \to (0,\infty)$ such that $\psi(x) = \psi^{\mathrm{rad}}(|x|)$, and monotone decreasing, we have

$$\begin{aligned} \int \mathrm{d}x\, |x|^n |\nabla\psi(x)| &= -4\pi \int_0^\infty \frac{\mathrm{d}\psi^{\mathrm{rad}}(r)}{\mathrm{d}r} r^{n+2} \mathrm{d}r = (n+2) \int \frac{|\psi(x)|}{|x|} |x|^n \mathrm{d}x \\ &\le 4\pi \left(R_0^{n+2} \|\psi\|_{L^\infty} + \frac{n+2}{R_0} \||\cdot|^n \psi\|_{L^1} \right) \end{aligned} \tag{5.91}$$

for all $R_0 > 0$. Clearly H is bounded, and hence, by $|x+y|^n \le 2^{1-n}(|x|^n + |y|^n)$, we can easily bound

$$\int |x|^n H(x) \mathrm{d}x \le 2^{2-n} \|\psi\|_{L^1} \||\cdot|^n \psi\|_{L^1} \tag{5.92}$$

from which the statement follows also for H. To show (5.90), use the Fourier representation

$$H(x) = \int |\widehat{\psi}(k)|^2 \cos(kx) \mathrm{d}k, \tag{5.93}$$

together with $H(x) \le 1$, $\cos(kx) \ge 1 - \frac{(kx)^2}{2}$ and $\nabla\psi \in L^2$. □

The next lemma contains suitable bounds for the potential V^φ and the resolvent R introduced in (5.11), (5.14) and (5.18).

Lemma 5.3.7. *There is a constant $C > 0$ such that*

$$(V^\varphi)^2 \le C(1-\Delta), \quad \pm V^\varphi \le \frac{1}{2}(-\Delta) + C \quad \textit{and} \quad \|\nabla R^{1/2}\|_{\mathrm{op}} \le C. \tag{5.94}$$

Proof. For the proof of the first two inequalities, we refer to [82, Lemma III.2]. The bound for the resolvent is obtained through

$$0 \le R^{\frac12}(-\Delta)R^{\frac12} \le R^{\frac12} h^{\mathrm{Pek}} R^{\frac12} - R^{\frac12}(V^\varphi - \lambda^{\mathrm{Pek}})R^{\frac12} \le CR + \frac{1}{2} R^{\frac12}(-\Delta)R^{\frac12}, \tag{5.95}$$

where we made use of the second inequality in (5.94). □

The commutator method

In the course of the proof we are frequently faced with bounding field operators like $\phi(h_x)$. From the standard estimates for creation and annihilation operators, we would obtain

$$\|a(f)\Psi\|_{\mathscr{H}} \leq \|f\|_{L^2}\|\mathbb{N}^{1/2}\Psi\|_{\mathscr{H}}, \ \|a^\dagger(f)\Psi\|_{\mathscr{H}} \leq \|f\|_{L^2}\|(\mathbb{N}+1)^{1/2}\Psi\|_{\mathscr{H}}, \ \Psi\in\mathscr{H}, \quad (5.96)$$

which is not sufficient since $h_0(y)$ is not square-integrable. With the aid of the commutator method introduced by Lieb and Yamazaki [86] one obtains suitable upper bounds by using in addition some regularity in the electron variable of the wave function Ψ. For our purpose, the version summarized in the following lemma will be sufficient.

Lemma 5.3.8. *Let $h_{K,\cdot}$ for $K\in(1,\infty]$ as defined in* (5.33)*, let A denote a bounded operator in $L^2(\mathbb{R}^3)$* (*acting on the field variable*) *and $a^\bullet\in\{a,a^\dagger\}$. Further let X,Y be bounded symmetric operators in $L^2(\mathbb{R}^3)$* (*acting on the electron variable*) *that satisfy $D_0 := \|X\|_{\text{op}}\|Y\|_{\text{op}} + \|\nabla X\|_{\text{op}}\|Y\|_{\text{op}} + \|X\|_{\text{op}}\|\nabla Y\|_{\text{op}} < \infty$. There exists a constant $C>0$ such that*

$$\|Xa^\bullet(Ah_{K,\cdot+y})Y\Psi\|_{\mathscr{H}} \leq CD_0\|(\mathbb{N}+1)^{1/2}\Psi\|_{\mathscr{H}} \quad (5.97a)$$

$$\|Xa^\bullet(Ah_{\Lambda,\cdot+y} - Ah_{K,\cdot+y})Y\Psi\|_{\mathscr{H}} \leq \frac{CD_0}{\sqrt{K}}\|(\mathbb{N}+1)^{1/2}\Psi\|_{\mathscr{H}} \quad (5.97b)$$

for all $y\in\mathbb{R}^3$, $\Psi\in\mathscr{H}$ and $\Lambda>K>1$.

Remark 5. Note that $Ah_{K,\cdot+y} = T_y(Ah_{K,\cdot})$ and in case that A has an integral kernel,

$$(Ah_{K,x})(z) = \int \mathrm{d}u\, A(z,u)h_{K,x}(u). \quad (5.98)$$

Proof of Lemma 5.3.8. To obtain the first inequality, write $h_{K,\cdot} = (h_{K,\cdot} - h_{1,\cdot}) + h_{1,\cdot}$ and apply the second inequality (with Λ and K interchanged) to the term in parenthesis. The bound for the term involving $h_{1,\cdot}$ follows from (5.96), as

$$\|a^\bullet(Ah_{1,\cdot+y})Y\Psi\|^2_{\mathscr{H}} = \int \mathrm{d}x\, \|a^\bullet(Ah_{1,x+y})(Y\Psi)(x)\|^2_{\mathcal{F}} \quad (5.99)$$
$$\leq \int \mathrm{d}x \|Ah_{1,x+y}\|^2_{L^2}\, \|(\mathbb{N}+1)^{1/2}(Y\Psi)(x)\|^2_{\mathcal{F}} \leq \|A\|^2_{\text{op}}\|h_{1,0}\|^2_{L^2}\|Y\|^2_{\text{op}}\|(\mathbb{N}+1)^{1/2}\Psi\|^2_{\mathscr{H}}.$$

To verify the second inequality, write the difference as a commutator

$$h_{\Lambda,x}(z) - h_{K,x}(z) = [-i\nabla_x, j_{K,\Lambda,x}(z)], \quad j_{K,\Lambda,x}(z) = \frac{1}{(2\pi)^3}\int_{K\leq|k|\leq\Lambda} \mathrm{d}k\frac{ke^{ik(x-z)}}{|k|^3} \quad (5.100)$$

and use that ∇ and A commute (they act on different variables). Then similarly as in (5.99) we obtain

$$\|Xa^\bullet([\nabla, Aj_{K,\Lambda,\cdot+y}])Y\Psi\|_{\mathscr{H}} \leq \|X\nabla a^\bullet(Aj_{K,\Lambda,\cdot+y})Y\Psi\|_{\mathscr{H}} + \|Xa^\bullet(Aj_{K,\Lambda,\cdot+y})\nabla Y\Psi\|_{\mathscr{H}}$$
$$\leq \|X\nabla\|_{\text{op}}\|a^\bullet(Aj_{K,\Lambda,\cdot+y})Y\Psi\|_{\mathscr{H}} + \|X\|_{\text{op}}\|a^\bullet(Aj_{K,\Lambda,\cdot+y})\nabla Y\Psi\|_{\mathscr{H}}$$
$$\leq \|A\|_{\text{op}}\Big(\|X\nabla\|_{\text{op}}\|Y\|_{\text{op}} + \|X\|_{\text{op}}\|\nabla Y\|_{\text{op}}\Big)\,\|j_{K,\Lambda,0}\|_{L^2}\,\|(\mathbb{N}+1)^{1/2}\Psi\|_{\mathscr{H}}. \quad (5.101)$$

The desired bound now follows from $\sup_{\Lambda>K}\|j_{K,\Lambda,0}\|^2_{L^2}\leq C/K$. □

A simple but useful corollary is given by

Corollary 5.3.9. *Under the same conditions as in Lemma 5.3.8, with the additional assumption that Y is a rank-one operator, there exists a constant $C > 0$ such that*

$$\int \mathrm{d}z \, \|X(Ah_{K,\cdot+y})(z)Y\|_{\mathrm{op}}^2 \le CD_0^2 \tag{5.102a}$$

$$\int \mathrm{d}z \, \|X\Big((Ah_{K,\cdot+y})(z) - (Ah_{\Lambda,\cdot+y})(z)\Big)Y\|_{\mathrm{op}}^2 \le \frac{CD_0^2}{\Lambda} \tag{5.102b}$$

for all $y \in \mathbb{R}^3$ and $\Lambda > K > 1$.

Proof. Since Y has rank one, we can use

$$\int \mathrm{d}z \, \|X(Ah_{K,\cdot+y})(z)w\|_{L^2}^2 = \|Xa^\dagger(Ah_{K,\cdot+y})w \otimes \Omega\|_{\mathscr{H}}^2, \tag{5.103}$$

for any $w \in L^2(\mathbb{R}^3)$, and similarly for (5.102b), and apply Lemma 5.3.8. □

Transformation properties of $\mathbb{U}_K$

The next lemma collects relations for the Bogoliubov transformation $\mathbb{U}_K$ defined in (5.39). Its proof follows directly from this definition and the fact that $\Theta_K = (H^{\mathrm{Pek}})^{1/4}$ is real-valued. We omit the details.

Lemma 5.3.10. *Let $f \in L^2(\mathbb{R}^3)$, $f^0 = \Pi_0 f$, $f^1 = \Pi_1 f$ with Π_i defined in* (5.30) *and set*

$$\underline{f} = f^0 + \Theta_K^{-1} \operatorname{Re}(f^1) + i\Theta_K \operatorname{Im}(f^1) \tag{5.104a}$$

$$\widetilde{f} = f^0 + \Theta_K \operatorname{Re}(f^1) + i\Theta_K^{-1} \operatorname{Im}(f^1). \tag{5.104b}$$

The unitary operator $\mathbb{U}_K$ defined in (5.39) *satisfies the relations*

$$\mathbb{U}_K a(f) \mathbb{U}_K^\dagger = a(f^0) + a(A_K f^1) + a^\dagger(B_K \overline{f^1}) \tag{5.105a}$$

$$\mathbb{U}_K^\dagger a(f) \mathbb{U}_K = a(f^0) + a(A_K f^1) - a^\dagger(B_K \overline{f^1}) \tag{5.105b}$$

$$\mathbb{U}_K \phi(f) \mathbb{U}_K^\dagger = \phi(\underline{f}), \quad \mathbb{U}_K \pi(f) \mathbb{U}_K^\dagger = \pi(\widetilde{f}) \tag{5.105c}$$

$$\mathbb{U}_K W(f) \mathbb{U}_K^\dagger = W(\widetilde{f}). \tag{5.105d}$$

The following statements provide helpful bounds involving the number operator when transformed with the Bogoliubov transformation.

Lemma 5.3.11. *There exists a constant $b > 0$ such that*

$$\mathbb{U}_K(\mathbb{N}+1)^n \mathbb{U}_K^\dagger \le b^n n^n (\mathbb{N}+1)^n, \quad \mathbb{U}_K^\dagger(\mathbb{N}+1)^n \mathbb{U}_K \le b^n n^n (\mathbb{N}+1)^n \tag{5.106}$$

for all $n \in \mathbb{N}$ and $K \in (K_0, \infty]$ with K_0 large enough.

Proof. With b replaced by $b_K = 2\|B_K\|_{\mathrm{HS}}^2 + \|A_K\|_{\mathrm{op}}^2 + 1$, both estimates follow from [56, Lemma 4.4] together with (5.105a) and (5.105b). That $b_K \le b$ for some K-independent $b > 0$ is inferred from Lemma 5.2.2. □

In the next two statements we denote by $1(\mathbb{N} > c)$ (resp. $1(\mathbb{N} \leq c)$) the orthogonal projector in $\mathcal{F}$ to all states with phonon number larger than (resp. less or equal to) c.

Corollary 5.3.12. *Let $\Upsilon_K = \mathbb{U}_K^\dagger \Omega$ and $\Upsilon_K^> := 1(\mathbb{N} > \alpha^\delta)\Upsilon_K$ for $\delta > 0$. There exist constants $b, C_{\delta,n} > 0$ such that*

$$\left\langle \Upsilon_K | (\mathbb{N}+1)^n \Upsilon_K \right\rangle_{\mathcal{F}} \leq b^n n^n \tag{5.107a}$$

$$\left\langle \Upsilon_K^> | (\mathbb{N}+1)^n \Upsilon_K^> \right\rangle_{\mathcal{F}} \leq C_{\delta,n}\, \alpha^{-20}. \tag{5.107b}$$

for all $n \in \mathbb{N}_0$ and all $K \in (K_0, \infty]$ with K_0 large enough.

Proof. The first bound follows directly from Lemma 5.3.11. The second one is obtained from

$$\begin{aligned} \left\langle \Upsilon_K^> | (\mathbb{N}+1)^n \Upsilon_K^> \right\rangle_{\mathcal{F}} &\leq \|\mathbb{N}^m (\mathbb{N}+1)^n \Upsilon_K^>\|_{\mathcal{F}} \, \|\mathbb{N}^{-m} \Upsilon_K^>\|_{\mathcal{F}} \\ &\leq \|(\mathbb{N}+1)^{n+m} \Upsilon_K\|_{\mathcal{F}}\, \alpha^{-m\delta} \leq (2(n+m)b)^{n+m} \alpha^{-m\delta} \end{aligned} \tag{5.108}$$

with $m \geq 20/\delta$. □

Lemma 5.3.13. *For $\delta > 0$ and $\kappa = 1/(16eb\alpha^\delta)$ with $b > 0$ the constant from Lemma 5.3.11, the operator inequality*

$$1(\mathbb{N} \leq 2\alpha^\delta) \mathbb{U}_K^\dagger \exp(2\kappa \mathbb{N}) \mathbb{U}_K 1(\mathbb{N} \leq 2\alpha^\delta) \leq 2 \tag{5.109}$$

holds for all K, α large enough.

Proof. We write out the Taylor series for the exponential and invoke Lemma 5.3.11,

$$\begin{aligned} 1(\mathbb{N} \leq 2\alpha^\delta) \mathbb{U}_K^\dagger e^{2\kappa\mathbb{N}} \mathbb{U}_K 1(\mathbb{N} \leq 2\alpha^\delta) &= \sum_{n=0}^{\infty} \frac{(2\kappa)^n}{n!} 1(\mathbb{N} \leq 2\alpha^\delta) \mathbb{U}_K^\dagger (\mathbb{N}+1)^n \mathbb{U}_K 1(\mathbb{N} \leq 2\alpha^\delta) \\ &\leq \sum_{n=0}^{\infty} \frac{(2\kappa b n)^n}{n!} 1(\mathbb{N} \leq 2\alpha^\delta)(\mathbb{N}+1)^n 1(\mathbb{N} \leq 2\alpha^\delta) \\ &\leq \sum_{n=0}^{\infty} \frac{(8\alpha^\delta \kappa b n)^n}{n!} \end{aligned} \tag{5.110}$$

where we used $1 \leq 2\alpha^\delta$ in the last step. The stated bound now follows from the elementary inequality $n! \geq (\frac{n}{e})^n$. □

The reason for introducing the momentum cutoff in $\mathbb{H}_K$ is to obtain a finite upper bound for the norm of the state $P_f|\Upsilon_K\rangle$. This is the content of the next lemma, whose proof is given in Section 5.4.

Lemma 5.3.14. *Let $P_f = \int \mathrm{d}k\, k\, a_k^\dagger a_k$ and K_0 large enough. There is a $C > 0$ such that*

$$\left\langle \Omega | \mathbb{U}_K (P_f)^2 \mathbb{U}_K^\dagger \Omega \right\rangle_{\mathcal{F}} \leq CK \tag{5.111}$$

for all $K \in (K_0, \infty)$.

5.3.5 The norm

In this section we provide the computation of the norm $\mathcal{N} = \|\Psi_{K,\alpha}(P)\|^2_{\mathcal{F}}$.

Proposition 5.3.15. *Let $\lambda = \frac{1}{6}\|\nabla\varphi\|^2_{L^2}$ and $c > 0$. For every $\varepsilon > 0$ there exist a constant $C_\varepsilon > 0$ (we omit the dependence on c) such that*

$$\left| \mathcal{N} - \left(\frac{\pi}{\lambda\alpha^2}\right)^{3/2} \right| \leq C_\varepsilon \sqrt{K} \alpha^{-4+\varepsilon} \tag{5.112}$$

for all $|P|/\alpha \leq c$ and all K, α large enough.

Proof. It follows from (5.68) and (5.69) that $\mathcal{N} = \mathcal{N}_0 + \mathcal{N}_1 + \mathcal{N}_2$ with

$$\mathcal{N}_0 = \int \mathrm{d}y \left\langle G^0_K \middle| T_y e^{A_{P,y}} W(\alpha w_{P,y}) G^0_K \right\rangle_{\mathscr{H}} \tag{5.113a}$$

$$\mathcal{N}_1 = -\frac{2}{\alpha} \int \mathrm{d}y \ \mathrm{Re} \left\langle G^0_K \middle| T_y e^{A_{P,y}} W(\alpha w_{P,y}) G^1_K \right\rangle_{\mathscr{H}} \tag{5.113b}$$

$$\mathcal{N}_2 = \frac{1}{\alpha^2} \int \mathrm{d}y \left\langle G^1_K \middle| T_y e^{A_{P,y}} W(\alpha w_{P,y}) G^1_K \right\rangle_{\mathscr{H}}. \tag{5.113c}$$

Term $\mathcal{N}_0$. This part contains the leading order contribution $(\frac{\pi}{\lambda\alpha^2})^{3/2}$. With H defined in (5.89), let us write

$$\begin{aligned} \mathcal{N}_0 &= \int \mathrm{d}y\, H(y) \left\langle \Upsilon_K \middle| W(\alpha w_{P,y}) \Upsilon_K \right\rangle_{\mathcal{F}} \\ &\quad + \int \mathrm{d}y\, H(y) \left\langle \Upsilon_K \middle| (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \right\rangle_{\mathcal{F}} = \mathcal{N}_{01} + \mathcal{N}_{02}. \end{aligned} \tag{5.114}$$

In the first term we use $|\Upsilon_K\rangle = \mathbb{U}^\dagger_K |\Omega\rangle$ and apply (5.105d) to transform the Weyl operator with the Bogoliubov transformation. This gives

$$\mathbb{U}_K W(\alpha w_{P,y}) \mathbb{U}^\dagger_K = W(\alpha \widetilde{w}_{P,y}) \tag{5.115}$$

with $\widetilde{w}_{P,y}$ defined in (5.83c). From (5.54) and (5.85), we thus obtain

$$\mathcal{N}_{01} = \int \mathrm{d}y\, H(y) \left\langle \Omega \middle| W(\alpha \widetilde{w}_{P,y}) \Omega \right\rangle_{\mathcal{F}} = \int \mathrm{d}y\, H(y) n_{0,1}(y). \tag{5.116}$$

Since $\|H\|_{L^1} + \|H\|_{L^\infty} \leq C$, cf. Lemma 5.3.6, we can apply Lemma 5.3.4 in order to replace the weight function $n_{0,1}(y)$ by the Gaussian $e^{-\lambda\alpha^2 y^2}$. More precisely,

$$\left| \int \mathrm{d}y\, H(y) n_{0,1}(y) - \int \mathrm{d}y\, H(y) e^{-\lambda\alpha^2 y^2} \right| \leq C\alpha^{-4} \tag{5.117}$$

for all $|P|/\alpha \leq c$ and all K, α large enough. Then we use $|H(y) - 1| \leq Cy^2$ in order to obtain

$$\left| \mathcal{N}_{01} - \left(\frac{\pi}{\lambda\alpha^2}\right)^{3/2} \right| \leq C\alpha^{-4}. \tag{5.118}$$

To treat $\mathcal{N}_{02}$ it is convenient to decompose the state Υ_K into a part with bounded particle number and a remainder. To this end, we choose a small $\delta > 0$ and write

$$\Upsilon_K = \Upsilon^<_K + \Upsilon^>_K = 1(\mathbb{N} \leq \alpha^\delta)\Upsilon_K + 1(\mathbb{N} > \alpha^\delta)\Upsilon_K. \tag{5.119}$$

Inserting this into $\mathcal{N}_{02}$ and using unitarity of $e^{A_{P,y}}$ and $\|H\|_{L^1} \le C$, we can estimate

$$|\mathcal{N}_{02}| \le \int \mathrm{d}y\, H(y) \Big| \Big\langle \Upsilon_K^{<} \Big| (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \Big\rangle_{\mathcal{F}} \Big| + C \|\Upsilon_K^{>}\|_{\mathcal{F}}. \tag{5.120}$$

By Corollary 5.3.12 for $n = 0$, $\|\Upsilon_K^{>}\| \le C_\delta\, \alpha^{-10}$. In the remaining expression we use (5.115),

$$\Big\langle \Upsilon_K^{<} \Big| (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \Big\rangle_{\mathcal{F}} = \Big\langle \Upsilon_K^{<} \Big| (e^{A_{P,y}} - 1) \mathbb{U}_K^\dagger W(\alpha \widetilde{w}_{P,y}) \Omega \Big\rangle_{\mathcal{F}}, \tag{5.121}$$

and insert the identity

$$1 = e^{\kappa \mathbb{N}} e^{-\kappa \mathbb{N}} \quad \text{with} \quad \kappa = \frac{1}{16 e b \alpha^\delta} \tag{5.122}$$

on the left of the Weyl operator (where $b > 0$ is the constant from Lemma 5.3.11). After applying the Cauchy–Schwarz inequality, this leads to

$$\begin{aligned} &\Big| \Big\langle \Upsilon_K^{<} \Big| (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \Big\rangle_{\mathcal{F}} \Big| \\ &\qquad \le \|e^{\kappa \mathbb{N}} \mathbb{U}_K (e^{-A_{P,y}} - 1) \Upsilon_K^{<}\|_{\mathcal{F}} \|e^{-\kappa \mathbb{N}} W(\alpha \widetilde{w}_{P,y}) \Omega\|_{\mathcal{F}}. \end{aligned} \tag{5.123}$$

In the second factor we then employ

$$\|e^{-\kappa \mathbb{N}} W(\alpha \widetilde{w}_{P,y}) \Omega\|_{\mathcal{F}} = e^{-\frac{\alpha^2}{2} \|\widetilde{w}_{P,y}\|_{L^2}^2} \|e^{-\kappa \mathbb{N}} e^{a^\dagger(\alpha \widetilde{w}_{P,y})} e^{\kappa \mathbb{N}} \Omega\|_{\mathcal{F}} \tag{5.124}$$

and use $e^{-\kappa \mathbb{N}} a^\dagger(f) e^{\kappa \mathbb{N}} = a^\dagger(e^{-\kappa} f)$ to write

$$e^{-\kappa \mathbb{N}} e^{a^\dagger(\alpha \widetilde{w}_{P,y})} e^{\kappa \mathbb{N}} \Omega = e^{a^\dagger(e^{-\kappa} \alpha \widetilde{w}_{P,y})} \Omega = e^{\frac{\alpha^2 e^{-2\kappa}}{2} \|\widetilde{w}_{P,y}\|_{L^2}^2} W(e^{-\kappa} \alpha \widetilde{w}_{P,y}) \Omega. \tag{5.125}$$

Combining the previous two lines we obtain

$$\|e^{-\kappa \mathbb{N}} W(\alpha \widetilde{w}_{P,y}) \Omega\|_{\mathcal{F}} = \exp\Big(-\frac{\alpha^2}{2} (1 - e^{-2\kappa}) \|\widetilde{w}_{P,y}\|_{L^2}^2 \Big) \le n_{\delta,\eta}(y) \tag{5.126}$$

for some α-independent $\eta > 0$ and α large enough. To estimate the first factor in (5.123), we apply Lemma 5.3.13 (note that $(e^{A_{P,y}} - 1)\Upsilon_K^{<} \in \mathrm{Ran}(1(\mathbb{N} \le 2\alpha^\delta))$)

$$\|e^{\kappa \mathbb{N}} \mathbb{U}_K (e^{-A_{P,y}} - 1) \Upsilon_K^{<}\|_{\mathcal{F}} \le \sqrt{2} \|(e^{-A_{P,y}} - 1) \Upsilon_K\|_{\mathcal{F}}. \tag{5.127}$$

On the right side we use the functional calculus for self-adjoint operators

$$\|(e^{-A_{P,y}} - 1) \Upsilon_K\|_{\mathcal{F}} \le \|A_{P,y} \Upsilon_K\|_{\mathcal{F}} \le \|(y P_f) \Upsilon_K\|_{\mathcal{F}} + |g_P(y)| \le C\Big(\sqrt{K} |y| + \alpha |y|^3 \Big), \tag{5.128}$$

where in the last step we applied Lemma 5.3.14 and used

$$|g_P(y)| \le C \alpha |y|^3, \tag{5.129}$$

which is inferred from (5.57) using $\|\Delta \varphi\|_{L^2} < \infty$. Returning to (5.123) we have shown that

$$|\mathcal{N}_{02}| \le C \int \mathrm{d}y\, H(y) \Big(\sqrt{K} |y| + \alpha |y|^3 \Big) n_{\delta,\eta}(y) + C_\delta\, \alpha^{-10}, \tag{5.130}$$

and hence we are in a position to apply Corollary 5.3.5. This implies for all K, α large

$$|\mathcal{N}_{02}| \le C\Big(\sqrt{K} \alpha^{-4(1-\delta)} + \alpha^{-6(1-\delta)+1} \Big) + C_\delta\, \alpha^{-10} \le C_\delta \sqrt{K} \alpha^{-4(1-\delta)}. \tag{5.131}$$

Term $\mathcal{N}_1$. We start by inserting (5.50) for G_K^1 in expression (5.113b). Since the Weyl operator commutes with u_α, R and $P_\psi = |\psi\rangle\langle\psi|$, we can apply (5.62a) to obtain

$$W(\alpha w_{P,y})G_K^1 \;=\; u_\alpha R\Big(\phi(h_{K,\cdot}^1) + 2\alpha\langle h_{K,\cdot}|\,\mathrm{Re}(w_{P,y}^1)\rangle_{L^2}\Big)P_\psi W(\alpha w_{P,y})G_K^0, \tag{5.132}$$

where we used that $h_{K,x}$ is real-valued. Note that $\langle h_{K,\cdot}|\,\mathrm{Re}(w_{P,y}^1)\rangle_{L^2}$ is a y-dependent multiplication operator in the electron variable. With $(T_y e^{A_{P,y}})^\dagger = T_{-y}e^{-A_{P,y}}$ and (5.119), we can thus write

$$\mathcal{N}_1 \;=\; -\frac{2}{\alpha}\int \mathsf{d}y\ \mathrm{Re}\Big\langle R_{1,y}\psi\otimes\Big(\Upsilon_K^< + \Upsilon_K^>\Big)\Big|W(\alpha w_{P,y})G_K^0\Big\rangle_{\mathscr{H}} = \mathcal{N}_1^< + \mathcal{N}_1^>, \tag{5.133}$$

where we introduced the operator $R_{1,y} = R_{1,y}^1 + R_{1,y}^2$ with

$$R_{1,y}^1 \;=\; P_\psi\phi(h_{K,\cdot}^1)Ru_\alpha T_{-y}P_\psi e^{-A_{P,y}}, \tag{5.134a}$$

$$R_{1,y}^2 \;=\; 2\alpha P_\psi\Big\langle h_{K,\cdot}|\,\mathrm{Re}(w_{P,y}^1)\Big\rangle_{L^2}Ru_\alpha T_{-y}P_\psi e^{-A_{P,y}}. \tag{5.134b}$$

Using Lemma 5.3.8 in combination with $\|\nabla P_\psi\|_{\mathrm{op}} + \|\nabla R^{1/2}\|_{\mathrm{op}} < \infty$, see Lemmas 5.3.6 and 5.3.7, we can bound the first operator, for any $\Psi\in\mathscr{H}$, by

$$\|R_{1,y}^1\Psi\|_{\mathscr{H}} \le C\|(\mathbb{N}+1)^{1/2}u_\alpha T_{-y}P_\psi e^{-A_{P,y}}\Psi\|_{\mathscr{H}} \le C\|u_\alpha T_{-y}P_\psi\|_{\mathrm{op}}\|(\mathbb{N}+1)^{1/2}\Psi\|_{\mathscr{H}}. \tag{5.135}$$

To estimate the second operator, we write out the inner product, use Cauchy–Schwarz twice, apply Corollary 5.3.9 (with $A=1$, $X=R$ and $Y=P_\psi$) and use (5.84a),

$$\begin{aligned}\|R_{1,y}^2\Psi\|_{\mathscr{H}}^2 \;&=\; 4\alpha^2\|\int \mathsf{d}z\ \mathrm{Re}(w_{P,y}^1(z))P_\psi h_{K,\cdot}(z)Ru_\alpha T_{-y}P_\psi e^{-A_{P,y}}\Psi\|_{\mathscr{H}}^2\\ &\le\; 4\alpha^2\int \mathsf{d}u\,|w_{P,y}^1(u)|^2\int \mathsf{d}z\,\|P_\psi h_{K,\cdot}(z)R\|_{\mathrm{op}}^2\,\|u_\alpha T_{-y}P_\psi e^{-A_{P,y}}\Psi\|_{\mathscr{H}}^2\\ &\le\; C\alpha^2\|w_{P,y}^1\|_{L^2}^2\|u_\alpha T_{-y}P_\psi e^{-A_{P,y}}\Psi\|_{\mathscr{H}}^2\\ &\le\; C\alpha^2(y^4+\alpha^{-4})\|u_\alpha T_{-y}P_\psi\|_{\mathrm{op}}^2\|\Psi\|_{\mathscr{H}}^2.\end{aligned} \tag{5.136}$$

Combining the above estimates we arrive at

$$\|R_{1,y}\Psi\|_{\mathscr{H}} \;\le\; C\|u_\alpha T_{-y}P_\psi\|_{\mathrm{op}}(1+\alpha y^2)\|(\mathbb{N}+1)^{1/2}\Psi\|_{\mathscr{H}}. \tag{5.137}$$

Since $\psi(x)$ decays exponentially for large $|x|$, the function $f_\alpha(y) := \|u_\alpha T_{-y}P_\psi\|_{\mathrm{op}}$ satisfies

$$\||\cdot|^n f_\alpha\|_{L^1} \;\le\; \int \mathsf{d}y\,|y|^n\bigg(\int \mathsf{d}x\,\psi(x+y)^2u_\alpha(x)^2\bigg)^{1/2} \;\le\; C_n\alpha^{3+n}\quad\text{for all } n\in\mathbb{N}_0. \tag{5.138}$$

With this at hand we can estimate the part containing the tail. Invoking Corollary 5.3.12

$$|\mathcal{N}_1^>| \;\le\; \frac{C}{\alpha}\|(\mathbb{N}+1)^{1/2}\Upsilon_K^>\|_{\mathcal{F}}\int \mathsf{d}y\,f_\alpha(y)(1+\alpha y^2) \;\le\; C_\delta\,\alpha^{-5}. \tag{5.139}$$

To estimate the first term in (5.133), we proceed similarly as in the bound for $\mathcal{N}_{02}$. We insert the identity (5.122), apply Cauchy–Schwarz and employ (5.126). This leads to

$$\begin{aligned}|\mathcal{N}_1^<| \;&\le\; \frac{2}{\alpha}\int \mathsf{d}y\,\|e^{\kappa\mathbb{N}}\mathbb{U}_K(e^{-A_{P,y}}R_{1,y}\psi\otimes\Upsilon_K^<)\|_{\mathcal{F}}\,\|e^{-\kappa\mathbb{N}}W(\alpha\widetilde{w}_{P,y})\Omega\|_{\mathcal{F}}\\ &\le\; \frac{2}{\alpha}\int \mathsf{d}y\,\|e^{\kappa\mathbb{N}}\mathbb{U}_K(e^{-A_{P,y}}R_{1,y}\psi\otimes\Upsilon_K^<)\|_{\mathcal{F}}\,n_{\delta,\eta}(y).\end{aligned} \tag{5.140}$$

In the remaining norm we use the fact that $R_{1,y}$ changes the number of phonons at most by one, and thus we can apply Lemma 5.3.13 and (5.137), together with (5.107a), to get

$$\|e^{\kappa\mathbb{N}}\mathbb{U}_K(e^{-A_{P,y}}R_{1,y}\psi\otimes\Upsilon_K^<)\|_{\mathcal{F}} \le \sqrt{2}\|R_{1,y}\psi\otimes\Upsilon_K^<\|_{\mathcal{F}} \le Cf_\alpha(y)\Big(1+\alpha y^2\Big). \tag{5.141}$$

With Corollary 5.3.5, (5.138) and $\|f_\alpha\|_{L^\infty}\le 1$, this leads to

$$|\mathcal{N}_1^<| \le \frac{C}{\alpha}\int \mathrm{d}y\, f_\alpha(y)\Big(1+\alpha y^2\Big)\,n_{\delta,\eta}(y) \le C\alpha^{-1-3(1-\delta)}. \tag{5.142}$$

Term $\mathcal{N}_2$. The strategy for estimating this term is similar to the one for $\mathcal{N}_1$. Proceeding as described before (5.133), one obtains

$$\mathcal{N}_2 = \frac{1}{\alpha^2}\int \mathrm{d}y\,\Big\langle R_{2,y}\psi\otimes\Big(\Upsilon_K^<+\Upsilon_K^>\Big)\Big|W(\alpha w_{P,y})G_K^0\Big\rangle_{\mathscr{H}} = \mathcal{N}_2^<+\mathcal{N}_2^> \tag{5.143}$$

with $R_{2,y}=R_{2,y}^1+R_{2,y}^2$ and

$$R_{2,y}^1 = P_\psi\phi(h_{K,\cdot}^1)Re^{-A_{P,y}}u_\alpha T_{-y}u_\alpha R\phi(h_{K,\cdot}^1)P_\psi, \tag{5.144a}$$
$$R_{2,y}^2 = 2\alpha P_\psi\langle h_{K,\cdot}|\,\mathrm{Re}(w_{P,y}^1)\rangle_{L^2}Re^{-A_{P,y}}u_\alpha T_{-y}u_\alpha R\phi(h_{K,\cdot}^1)P_\psi. \tag{5.144b}$$

It follows in close analogy as for $R_{1,y}$ in (5.134a)–(5.134b) that given any $\Psi\in\mathscr{H}$,

$$\|R_{2,y}\Psi\|_{\mathscr{H}} \le C\|u_\alpha T_{-y}u_\alpha\|_{\mathrm{op}}(1+\alpha y^2)\|(\mathbb{N}+1)\Psi\|_{\mathscr{H}}, \tag{5.145}$$

and since $\|u_\alpha T_{-y}u_\alpha\|_{\mathrm{op}}\le 1(|y|\le 4\alpha)$, we can use Corollary 5.3.12 to estimate

$$|\mathcal{N}_2^>| \le \frac{C}{\alpha^2}\|(\mathbb{N}+1)\Upsilon_K^>\|_{\mathcal{F}}\int \mathrm{d}y\,1(|y|\le 4\alpha)(1+\alpha y^2) \le C_\delta\,\alpha^{-6}. \tag{5.146}$$

To bound the first term in (5.143) we proceed similarly as for $\mathcal{N}_{01}$,

$$\begin{aligned}|\mathcal{N}_2^<| &\le \alpha^{-2}\int \mathrm{d}y\,\|e^{\kappa\mathbb{N}}\mathbb{U}_K(R_{2,y}\psi\otimes\Upsilon_K^<)\|_{\mathcal{F}}\,\|e^{-\kappa\mathbb{N}}W(\alpha\widetilde{w}_{P,y})\Omega\|_{\mathcal{F}}\\ &\le \frac{\sqrt{2}}{\alpha^2}\int \mathrm{d}y\,\|R_{2,y}\psi\otimes\Upsilon_K^<\|_{\mathscr{H}}\,n_{\delta,\eta}(y) \le \frac{C}{\alpha^2}\int \mathrm{d}y\,1(|y|\le 4\alpha)(1+\alpha y^2)\,n_{\delta,\eta}(y).\end{aligned} \tag{5.147}$$

The last integral is estimated again via Corollary 5.3.5, and thus $|\mathcal{N}_2^<|\le C\alpha^{-5+3\delta}$.

Collecting all relevant estimates and choosing $\delta>0$ small enough completes the proof of the proposition. □

5.3.6 Energy contribution $\mathcal{E}$

In this section we prove the following estimate for the energy contribution $\mathcal{E}$ defined in (5.60a).

Proposition 5.3.16. *Let* $\mathbb{N}_1=\mathrm{d}\Gamma(\Pi_1)$ *and choose* $c>0$*. For every* $\varepsilon>0$ *there is a constant* $C_\varepsilon>0$ (*we omit the dependence on* c) *such that*

$$\left|\mathcal{E}-\frac{1}{\alpha^2}\bigg(\Big\langle\Upsilon_K|\mathbb{N}_1\Upsilon_K\Big\rangle_{\mathcal{F}}-\frac{3}{2}\bigg)\mathcal{N}\right| \le C_\varepsilon\sqrt{K}\alpha^{-6+\varepsilon} \tag{5.148}$$

for all $|P|/\alpha\le c$ *and* K,α *large enough.*

Proof. Since $G_K^0 = \psi \otimes \Upsilon_K$, $h^{\mathrm{Pek}}\psi = 0$ and $\mathbb{N}\Upsilon_K = \mathbb{N}_1\Upsilon_K$, one has

$$\mathcal{E} = \int \mathrm{d}y \left\langle G_K^0 \middle| \left(\alpha^{-2}\mathbb{N}_1 + \alpha^{-1}\phi(h_\cdot + \varphi_P)\right) T_y e^{A_{P,y}} W(\alpha w_{P,y}) \middle| G_K^0 \right\rangle_{\mathscr{H}} = \mathcal{E}_1 + \mathcal{E}_2, \quad (5.149)$$

where both terms provide contributions to the energy of order α^{-2}.

Term $\mathcal{E}_1$. Recall that $H(y) = \langle \psi | T_y \psi \rangle_{L^2}$ and use this to write

$$\begin{aligned}\mathcal{E}_1 &= \frac{1}{\alpha^2}\int \mathrm{d}y\, H(y) \left\langle \Upsilon_K \middle| \mathbb{N}_1 W(\alpha w_{P,y}) \Upsilon_K \right\rangle_{\mathcal{F}} \\ &\quad + \frac{1}{\alpha^2}\int \mathrm{d}y\, H(y) \left\langle \Upsilon_K \middle| \mathbb{N}_1 (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \right\rangle_{\mathcal{F}} = \mathcal{E}_{11} + \mathcal{E}_{12}. \end{aligned} \quad (5.150)$$

With (5.115), (5.55) and (5.85) it follows that

$$W(\alpha w_{P,y})\Upsilon_K = \mathbb{U}_K^\dagger W(\alpha \widetilde{w}_{P,y})\Omega = n_{0,1}(y) \mathbb{U}_K^\dagger\, e^{a^\dagger(\alpha w_{P,y}^0)} e^{a^\dagger(\alpha \widetilde{w}_{P,y}^1)} \Omega, \quad (5.151)$$

and since $e^{a^\dagger(\alpha w^0_{P,y})}$ commutes with $\mathbb{U}_K \mathbb{N}_1 \mathbb{U}_K^\dagger$ and $e^{a(\alpha w^0_{P,y})}\Upsilon_K = \Upsilon_K$ (we use $\mathbb{U}_K a^\dagger(f^0)\mathbb{U}_K^\dagger = a^\dagger(f^0)$ for $f^0 \in \mathrm{Ran}(\Pi_0)$), this leads to

$$\mathcal{E}_{11} = \frac{1}{\alpha^2}\int \mathrm{d}y\, H(y) n_{0,1}(y) \left\langle \Omega \middle| \mathbb{U}_K \mathbb{N}_1 \mathbb{U}_K^\dagger e^{a^\dagger(\alpha \widetilde{w}^1_{P,y})} \Omega \right\rangle_{\mathcal{F}}. \quad (5.152)$$

Because $\mathbb{U}_K \mathbb{N}_1 \mathbb{U}_K^\dagger$ is quadratic in creation and annihilation operators, we can expand the exponential in the inner product and use that only the zeroth and second order terms give a non-vanishing contribution,

$$\begin{aligned}\mathcal{E}_{11} &= \frac{1}{\alpha^2}\int \mathrm{d}y\, H(y) n_{0,1}(y) \left\langle \Upsilon_K \middle| \mathbb{N}_1 \Upsilon_K \right\rangle_{\mathcal{F}} \\ &\quad + \frac{1}{2\alpha^2}\int \mathrm{d}y\, H(y) n_{0,1}(y) \left\langle \Upsilon_K \middle| \mathbb{N}_1 \mathbb{U}_K^\dagger a^\dagger(\alpha \widetilde{w}^1_{P,y}) a^\dagger(\alpha \widetilde{w}^1_{P,y}) \Omega \right\rangle_{\mathcal{F}} = \mathcal{E}_{111} + \mathcal{E}_{112}. \end{aligned} \quad (5.153)$$

Next we add and subtract the Gaussian to separate the leading-order term,

$$\begin{aligned}\mathcal{E}_{111} &= \frac{1}{\alpha^2}\int \mathrm{d}y\, H(y)\, e^{-\lambda\alpha^2 y^2} \left\langle \Upsilon_K \middle| \mathbb{N}_1 \Upsilon_K \right\rangle_{\mathcal{F}} \\ &\quad + \frac{1}{\alpha^2}\int \mathrm{d}y\, H(y) \left(n_{0,1}(y) - e^{-\lambda\alpha^2 y^2}\right) \left\langle \Upsilon_K \middle| \mathbb{N}_1 \Upsilon_K \right\rangle_{\mathcal{F}} = \mathcal{E}_{111}^{\mathrm{lo}} + \mathcal{E}_{111}^{\mathrm{err}}. \end{aligned} \quad (5.154)$$

In $\mathcal{E}_{111}^{\mathrm{lo}}$ we use $|H(y) - 1| \le Cy^2$ and Corollary 5.3.12 to replace $H(y)$ by unity at the cost of an error of order α^{-7}. In the term where $H(y)$ is replaced by unity, we perform the Gaussian integral and use Proposition 5.3.15 and again Corollary 5.3.12. This leads to

$$\left| \mathcal{E}_{111}^{\mathrm{lo}} - \mathcal{N}\frac{1}{\alpha^2}\left\langle \Upsilon_K \middle| \mathbb{N}_1 \Upsilon_K \right\rangle_{\mathcal{F}} \right| \le C_\varepsilon \sqrt{K} \alpha^{-6+\varepsilon}. \quad (5.155)$$

The error in (5.154) is bounded with the help of Lemma 5.3.4,

$$|\mathcal{E}_{111}^{\mathrm{err}}| \le \frac{C}{\alpha^2}\int \mathrm{d}y\, H(y) |n_{0,1}(y) - e^{-\lambda\alpha^2 y^2}| \le C\alpha^{-6}. \quad (5.156)$$

In $\mathcal{E}_{112}$ we use the Cauchy–Schwarz inequality, Corollary 5.3.12 and Lemma 5.3.3, to obtain

$$\begin{aligned}&\left| \left\langle \Upsilon_K \middle| \mathbb{N}_1 \mathbb{U}_K^\dagger a^\dagger(\alpha \widetilde{w}^1_{P,y}) a^\dagger(\alpha \widetilde{w}^1_{P,y}) \Omega \right\rangle_{\mathcal{F}} \right| \\ &\quad \le \|\mathbb{N}_1 \Upsilon_K\|_{\mathcal{F}} \, \|a^\dagger(\alpha \widetilde{w}^1_{P,y}) a^\dagger(\alpha \widetilde{w}^1_{P,y})\Omega\|_{\mathcal{F}} \le 2\alpha^2 \|\widetilde{w}^1_{P,y}\|^2_{L^2} \le C\alpha^2(y^4 + \alpha^{-4}). \end{aligned} \quad (5.157)$$

With $\| |\cdot|^n H\|_{L^1} \le C_n$ we can now apply Corollary 5.3.5 to obtain

$$|\mathcal{E}_{112}| \le C \int \mathrm{d}y\, H(y)(y^4 + \alpha^{-4}) n_{0,1}(y) \le C\alpha^{-7}. \tag{5.158}$$

In order to bound $\mathcal{E}_{12}$ in (5.150), we decompose $\Upsilon_K = \Upsilon_K^< + \Upsilon_K^>$ for some $\delta > 0$, see (5.119), and then follows similar steps as described below (5.121). This way we can estimate

$$|\mathcal{E}_{12}| \le \frac{1}{\alpha^2} \int \mathrm{d}y\, H(y) \|e^{\kappa \mathbb{N}} \mathbb{U}_K (e^{-A_{P,y}} - 1) \mathbb{N}_1 \Upsilon_K^< \|_{\mathcal{F}}\, n_{\delta,\eta}(y) + \frac{2}{\alpha^2} \|\mathbb{N}_1 \Upsilon_K^>\|_{\mathcal{F}} \int \mathrm{d}y\, H(y). \tag{5.159}$$

While the second term is bounded via (5.107b) by $C_\delta\, \alpha^{-12}$, in the first term we apply Lemma 5.3.13 and use the functional calculus for self-adjoint operators,

$$\begin{aligned} \|e^{\kappa \mathbb{N}} \mathbb{U}_K (e^{-A_{P,y}} - 1) \mathbb{N}_1 \Upsilon_K^< \|_{\mathcal{F}} &\le \sqrt{2} \|(e^{-A_{P,y}} - 1) \mathbb{N}_1 \Upsilon_K^< \|_{\mathcal{F}} \\ &\le \sqrt{2} \|(P_f y + g_P(y)) \mathbb{N}_1 \Upsilon_K^< \|_{\mathcal{F}}. \end{aligned} \tag{5.160}$$

Since P_f changes the number of phonons in $\mathcal{F}_1$ at most by one, we can proceed by

$$\|(P_f y + g_P(y)) \mathbb{N}_1 \Upsilon_K^< \|_{\mathcal{F}} \le (\alpha^\delta + 1) \|(P_f y + g_P(y)) \Upsilon_K \|_{\mathcal{F}} \le C\alpha^\delta (\sqrt{K}|y| + \alpha |y|^3), \tag{5.161}$$

where we used $1 \le \alpha^\delta$, Lemma 5.3.14 and (5.129) in the second step. We conclude via Corollary 5.3.5 that

$$|\mathcal{E}_{12}| \le \frac{C}{\alpha^2} \int \mathrm{d}y\, H(y)(\sqrt{K}|y| + \alpha|y|^3) n_{\delta,\eta}(y) + C_\delta\, \alpha^{-12} \le C_\delta \sqrt{K} \alpha^{-6+4\delta}. \tag{5.162}$$

Term $\mathcal{E}_2$. Here we start with

$$\begin{aligned} \mathcal{E}_2 &= \alpha^{-1} \int \mathrm{d}y \left\langle \Upsilon_K | L_{1,y} W(\alpha w_{P,y}) \Upsilon_K \right\rangle_{\mathcal{F}} \\ &\quad + \alpha^{-1} \int \mathrm{d}y \left\langle \Upsilon_K | L_{1,y} (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \right\rangle_{\mathcal{F}} = \mathcal{E}_{21} + \mathcal{E}_{22}, \end{aligned} \tag{5.163}$$

where

$$L_{1,y} = \left\langle \psi | \phi(h_\cdot + \varphi_P) T_y \psi \right\rangle_{L^2} = \phi(l_y) + \pi(j_y) \tag{5.164}$$

with

$$l_y = H(y)\varphi + \left\langle \psi | h_\cdot T_y \psi \right\rangle_{L^2}, \quad j_y = H(y)\xi_P, \tag{5.165}$$

and ξ_P defined in (5.46). We record the following properties of l_y and its derivative. The proof of the lemma is postponed until the end of the present section.

Lemma 5.3.17. *For $k = 0, 1$ and for all $n \in \mathbb{N}_0$,*

$$\sup_y \|\nabla^k l_y\|_{L^2} < \infty, \quad \int |y|^n \|\nabla^k l_y\|_{L^2}\, \mathrm{d}y < \infty. \tag{5.166}$$

Note that, by Lemma 5.3.6, j_y clearly has these properties as well. We proceed by writing $\mathcal{E}_{21} = \mathcal{E}_{21}^0 + \mathcal{E}_{21}^P$ with

$$\mathcal{E}_{21}^0 = \alpha^{-1} \int \mathrm{d}y \left\langle \Upsilon_K | \phi(l_y) W(\alpha w_{P,y}) \Upsilon_K \right\rangle_{\mathcal{F}} \tag{5.167a}$$

$$\mathcal{E}_{21}^P = \alpha^{-1} \int \mathrm{d}y \left\langle \Upsilon_K | \pi(j_y) W(\alpha w_{P,y}) \Upsilon_K \right\rangle_{\mathcal{F}}, \tag{5.167b}$$

and estimate the two parts separately. Using the canonical commutation relations and (5.105c), we evaluate

$$\begin{aligned} \mathcal{E}_{21}^0 &= \int \left\langle \underline{l_y} | \widetilde{w}_{P,y} \right\rangle_{L^2} n_{0,1}(y) \mathrm{d}y \\ &= \int \left(\left\langle l_y^0 | w_{P,y}^0 \right\rangle_{L^2} + \left\langle l_y^1 | \mathrm{Re}(w_{P,y}^1) \right\rangle_{L^2} + i \left\langle l_y^1 | \Theta_K^{-2} \mathrm{Im}(w_{P,y}^1) \right\rangle_{L^2} \right) n_{0,1}(y) \mathrm{d}y \end{aligned} \tag{5.168}$$

where we used that l_y is real-valued. Note that $l_{-y}(-z) = l_y(z)$. As discussed in Remark 4, $n_{0,1}(y)$ is even, and using the arguments therein one can conclude that $\Theta_K^{-2}\mathrm{Im}(w_{P,y}^1)$ and $\mathrm{Im}(w_{P,y}^0)$ are odd functions on $\mathbb{R}^6$ since $(y,z) \mapsto \mathrm{Im}(w_{P,y})(z)$ is odd on this space, and hence

$$\int \left\langle l_y^0 | \mathrm{Im}(w_{P,y}^0) \right\rangle_{L^2} n_{0,1}(y) \mathrm{d}y = \int \left\langle l_y^1 | \Theta_K^{-2} \mathrm{Im}(w_{P,y}^1) \right\rangle_{L^2} n_{0,1}(y) \mathrm{d}y = 0. \tag{5.169}$$

Thus, with $\mathrm{Re}(w_{P,y}) = w_{0,y}$, and with

$$v(y) := \left\langle l_y | w_{0,y} \right\rangle_{L^2} \tag{5.170}$$

we finally have

$$\mathcal{E}_{21}^0 = \int \left\langle l_y^0 + l_y^1 | \, \mathrm{Re}(w_{P,y}^0) + \mathrm{Re}(w_{P,y}^1) \right\rangle_{L^2} n_{0,1}(y) \mathrm{d}y = \int v(y) n_{0,1}(y) \mathrm{d}y. \tag{5.171}$$

Note that $v \in L^1 \cap L^\infty$ since $y \mapsto \|l_y\|_{L^2}$ is, while $\|w_{0,y}\|_{L^2}$ is uniformly bounded in y. Because of $\varphi(z) = -\langle \psi | h.(z) \psi \rangle_{L^2}$ and $\nabla_z h(x-z) = -\nabla_x h(x-z)$ we have by integration by parts

$$\nabla \varphi = -2 \left\langle \nabla \psi | h.\psi \right\rangle_{L^2}. \tag{5.172}$$

Thus

$$l_y = -\frac{1}{2} y \nabla \varphi + \varphi(H(y) - 1) + \left\langle \psi | h.(T_y \psi - \psi - y \nabla \psi) \right\rangle_{L^2}. \tag{5.173}$$

Since ψ is a smooth function with uniformly bounded derivatives, there exists a $C > 0$ such that for all y

$$\|T_y \psi - \psi - y \nabla \psi\|_{L^\infty} \leq C y^2. \tag{5.174}$$

Moreover, for $k = 0, 1$ and every $z \in \mathbb{R}^3$,

$$x \mapsto (h.(z) \nabla^k \psi)(x) \in L^1(\mathbb{R}^3, \mathrm{d}x) \quad \text{and} \quad z \mapsto \|h.(z) \nabla^k \psi\|_{L^1} \in L^2(\mathbb{R}^3, \mathrm{d}z). \tag{5.175}$$

The first statement follows easily from Lemma 5.3.6; to show the second one, use

$$\int \mathrm{d}z \, \frac{1}{|u-z|^2 |v-z|^2} = \frac{1}{\pi^3 |u-v|} \tag{5.176}$$

and apply the Hardy–Littlewood–Sobolev inequality. This, together with (5.90), shows that there exists a function f in $L^2(\mathbb{R}^3, \mathrm{d}z)$ such that

$$|l_y(z) + \frac{1}{2} y \nabla\varphi(z)| \leq f(z) y^2. \tag{5.177}$$

Now let

$$b_y(z) := w_{0,y}(z) - y\nabla\varphi(z) = \int_0^1 \mathrm{d}s \int_0^s \mathrm{d}t\, (y\nabla)^2 \varphi(z - ty) \tag{5.178}$$

and note that $\|b_y\|_{L^2}^2 \leq \frac{1}{4} y^4 \|\Delta\varphi\|_{L^2}^2$ which is finite since $\Delta\varphi \in L^2$. This equation, together with (5.177), implies

$$\left| v(y) + \frac{1}{2} \|y\nabla\varphi\|_{L^2}^2 \right| \leq C(|y|^3 + |y|^4). \tag{5.179}$$

From this, and from $v \in L^1 \cap L^\infty$ it is also easy to deduce that $|\cdot|^{-2} v \in L^1 \cap L^\infty$. We can thus write

$$\int \mathrm{d}y\, v(y) n_{0,1}(y) = \int \mathrm{d}y\, v(y) e^{-\alpha^2 \lambda y^2} + \int \mathrm{d}y\, |y|^{-2} v(y) y^2 \Big(n_{0,1}(y) - e^{-\alpha^2 \lambda y^2} \Big) \tag{5.180}$$

and use Lemma 5.3.4 for $g = |\cdot|^{-2} |v|$ to bound

$$\left| \int \mathrm{d}y\, |y|^{-2} v(y) y^2 (n_{0,1}(y) - e^{-\alpha^2 \lambda y^2}) \right| \leq C\alpha^{-6}. \tag{5.181}$$

Using (5.179), the definition of $\lambda = \frac{1}{6} \|\nabla\varphi\|_{L^2}^2$ as well as $\int y^2 e^{-y^2} \mathrm{d}y = \frac{3}{2} \pi^{3/2}$, we further have that

$$\left| \int \mathrm{d}y\, v(y) e^{-\alpha^2 \lambda y^2} + \frac{3}{2\alpha^2} \left(\frac{\pi}{\lambda \alpha^2} \right)^{3/2} \right| \leq C\alpha^{-6} \tag{5.182}$$

which finally gives the estimate

$$\left| \mathcal{E}_{21}^0 + \left(\frac{3}{2\alpha^2} \right) \mathcal{N} \right| \leq C_\varepsilon \sqrt{K} \alpha^{-6+\varepsilon} \tag{5.183}$$

using Proposition 5.3.15.

In a similar fashion as for $\mathcal{E}_{21}^0$, we obtain

$$\mathcal{E}_{21}^P = \frac{1}{\alpha^2 M^{\mathrm{LP}}} \int \left\langle iP\nabla\varphi | w_{P,y}^0 \right\rangle_{L^2} H(y) n_{0,1}(y) \mathrm{d}y. \tag{5.184}$$

Explicit computation, using $\Pi_0 = \frac{3}{\|\nabla\varphi\|_{L^2}^2} \sum_{i=1}^3 |\partial_i \varphi\rangle\langle \partial_i \varphi|$ and $\langle \varphi | \nabla\varphi \rangle_{L^2} = 0$, gives

$$\frac{1}{3} w_{P,y}^0(z) = -\frac{(\varphi * \nabla\varphi)(y)}{\|\nabla\varphi\|_{L^2}^2} \nabla\varphi(z) + \frac{iP}{\alpha^2 M^{\mathrm{LP}}} \Big(\|\nabla\varphi\|_{L^2}^2 - (\nabla\varphi * \nabla\varphi)(y) \Big) \frac{\nabla\varphi(z)}{\|\nabla\varphi\|_{L^2}^2}. \tag{5.185}$$

Note that the real part of the above is odd as a function of y and hence

$$\int \left\langle \nabla\varphi | \mathrm{Re}(w_{P,y}^0) \right\rangle_{L^2} n_{0,1}(y) H(y) \mathrm{d}y = 0, \tag{5.186}$$

and, taking rotational invariance of φ into account, we arrive at

$$\mathcal{E}_{21}^{P} = \frac{P^2}{\alpha^4(M^{\mathrm{LP}})^2}\int \Big(\|\nabla\varphi\|_2^2 - (\nabla\varphi * \nabla\varphi)(y)\Big) n_{0,1}(y)H(y)\mathrm{d}y. \tag{5.187}$$

Further note that $|\|\nabla\varphi\|_{L^2}^2 - (\nabla\varphi * \nabla\varphi)(y)| \leq Cy^2$ and thus, by Lemma 5.3.6 and Corollary 5.3.5, one obtains

$$|\mathcal{E}_{21}^{P}| \leq C\frac{P^2}{\alpha^9} \leq \frac{C}{\alpha^7}. \tag{5.188}$$

This completes the analysis of $\mathcal{E}_{21}$.

In order to estimate the term $\mathcal{E}_{22}$, we proceed as before by splitting $\Upsilon_K = \Upsilon_K^{<} + \Upsilon_K^{>}$. Using (5.96) we can estimate

$$\begin{aligned}&\left|\alpha^{-1}\int \mathrm{d}y \left\langle \Upsilon_K^{>}|(\phi(l_y)+\pi(j_y))(e^{A_{P,y}}-1)W(\alpha w_{P,y})\Upsilon_K\right\rangle_{\mathcal{F}}\right|\\ &\quad\leq C\alpha^{-1}\int \mathrm{d}y\,(\|l_y\|_{L^2}+\|j_y\|_{L^2})\|(\mathbb{N}+1)^{1/2}\Upsilon_K^{>}\|_{\mathcal{F}} \leq C_\delta\,\alpha^{-11}\end{aligned} \tag{5.189}$$

where we used Corollary 5.3.12 and Lemmas 5.3.6 and 5.3.17. The term involving $\Upsilon_K^{<}$, we split again into two contributions,

$$\mathcal{E}_{22}^{0} = \alpha^{-1}\int \mathrm{d}y \left\langle \Upsilon_K^{<}|\phi(l_y)(e^{A_{P,y}}-1)W(\alpha w_{P,y})\Upsilon_K\right\rangle_{\mathcal{F}} \tag{5.190a}$$

$$\mathcal{E}_{22}^{P} = \alpha^{-1}\int \mathrm{d}y \left\langle \Upsilon_K^{<}|\pi(j_y)(e^{A_{P,y}}-1)W(\alpha w_{P,y})\Upsilon_K\right\rangle_{\mathcal{F}}. \tag{5.190b}$$

To bound the first one we proceed as in (5.159), i.e. use Lemma 5.3.13 and the fact that $\phi(l_y)$ changes the number of phonons at most by one. This leads to

$$\begin{aligned}|\mathcal{E}_{22}^{0}| &\leq \alpha^{-1}\int \mathrm{d}y\,\|e^{\kappa\mathbb{N}}\mathbb{U}_K(e^{-A_{P,y}}-1)\phi(l_y)\Upsilon_K^{<}\|_{\mathcal{F}}\,n_{\delta,\eta}(y)\\ &\leq \sqrt{2}\alpha^{-1}\int \mathrm{d}y\,\|(e^{-A_{P,y}}-1)\phi(l_y)\Upsilon_K^{<}\|_{\mathcal{F}}\,n_{\delta,\eta}(y).\end{aligned} \tag{5.191}$$

Furthermore, we have

$$\begin{aligned}\|(e^{-A_{P,y}}-1)\phi(l_y)\Upsilon_K^{<}\|_{\mathcal{F}} &\leq \|A_{P,y}\phi(l_y)\Upsilon_K^{<}\|_{\mathcal{F}} \leq \|\phi(l_y)A_{P,y}\Upsilon_K^{<}\|_{\mathcal{F}} + \|[A_{P,y},\phi(l_y)]\Upsilon_K^{<}\|_{\mathcal{F}}\\ &\leq C\alpha^{\delta/2}\left(\|l_y\|_{L^2}\|A_{P,y}\Upsilon_K\|_{\mathcal{F}} + \|y\nabla l_y\|_{L^2}\right)\end{aligned} \tag{5.192}$$

where we used $[iP_f y, \phi(f)] = \pi(y\nabla f)$ and $\Upsilon_K^{<} = 1(\mathbb{N}\leq\alpha^\delta)\Upsilon_K$. Note that in order to estimate the remaining expression, it is not sufficient to directly apply Corollary 5.3.5. To obtain a better bound, we first replace $n_{\delta,\eta}(y)$ by $e^{-\eta\lambda\alpha^{2(1-\delta)}y^2}$ and then, for the part containing the Gaussian, we use that $\|l_y\|_{L^2}$ and $\|\nabla l_y\|_{L^2}$ provide additional factors of $|y|$, as is shown below. More precisely, with Lemma 5.3.17 and the aid of Lemmas 5.3.4 and 5.3.14, we bound

$$\begin{aligned}\alpha^{\frac{\delta}{2}-1}\int \mathrm{d}y\,\|l_y\|_{L^2}\|A_{P,y}\Upsilon_K\|_{\mathcal{F}}\,n_{\delta,\eta}(y) &\leq C\alpha^{\frac{\delta}{2}-1}\int \mathrm{d}y\,\|l_y\|_{L^2}(\sqrt{K}|y|+\alpha|y|^3)n_{\delta,\eta}(y)\\ &\leq C\alpha^{\frac{\delta}{2}-1}\int \mathrm{d}y\,\|l_y\|_{L^2}(\sqrt{K}|y|+\alpha|y|^3)e^{-\eta\lambda\alpha^{2(1-\delta)}y^2} + C\sqrt{K}\alpha^{-6+\frac{9\delta}{2}}.\end{aligned} \tag{5.193}$$

Next we use that by Equation (5.177) there exists an L^2 function f such that

$$|l_y(z)| \leq \frac{1}{2}|y\nabla\varphi(z)| + f(z)y^2. \tag{5.194}$$

Hence, by integration

$$\alpha^{\delta/2-1}\int \mathrm{d}y\, \|l_y\|_{L^2}\left(\sqrt{K}|y|+\alpha|y|^3\right)e^{-\lambda\eta\alpha^{2(1-\delta)}y^2} \;\le\; C\sqrt{K}\alpha^{-6+11/2\delta}. \tag{5.195}$$

With regard to the second term in (5.192),

$$\alpha^{\delta/2-1}\int \mathrm{d}y\, |y|\|\nabla l_y\|_{L^2} n_{\delta,\eta}(y) \tag{5.196}$$

we proceed in a similar way, using that

$$\|\nabla l_y\|_{L^2} \;\le\; C(|y|+y^2). \tag{5.197}$$

In fact, since $\nabla\varphi(z) = -\langle\psi|h.(z)\nabla\psi\rangle_{L^2} - \langle\nabla\psi|h.(z)\psi\rangle_{L^2}$, we have the identity

$$\begin{aligned}\nabla l_y(z) \;&=\; H(y)\nabla\varphi(z) + \left\langle\nabla\psi|h.(z)T_y\psi\right\rangle_{L^2} + \left\langle\psi|h.(z)\nabla T_y\psi\right\rangle_{L^2} \\ &=\; (H(y)-1)\nabla\varphi(z) + \left\langle\nabla\psi|h.(z)(T_y-1)\psi\right\rangle_{L^2} + \left\langle\psi|h.(z)(T_y-1)\nabla\psi\right\rangle_{L^2}.\end{aligned} \tag{5.198}$$

Again using that ψ has bounded derivatives, we have

$$\|(T_y-1)\psi\|_{L^\infty} + \|(T_y-1)\nabla\psi\|_{L^\infty} \le C|y|, \tag{5.199}$$

and the desired inequality now follows from $|H(y)-1|\le Cy^2$ and (5.175). Given (5.166), we can use Lemma 5.3.4 to replace $n_{\delta,\eta}(y)$ in (5.196) with $e^{-\lambda\eta\alpha^{2(1-\delta)}y^2}$ at the energy penalty $C\alpha^{-6+9\delta/2}$, and then use (5.197) to bound the remaining integral involving the Gaussian factor, which yields an error of the same order. Altogether, this gives the estimate

$$|\mathcal{E}_{22}^0| \;\le\; C\sqrt{K}\alpha^{-6+\frac{11}{2}\delta}. \tag{5.200}$$

For the term $\mathcal{E}_{22}^P$ we proceed in exactly the same way as in (5.191):

$$\begin{aligned}|\mathcal{E}_{22}^P| \;&\le\; \sqrt{2}\alpha^{-1}\int \mathrm{d}y\, \|\left(e^{-A_{P,y}}-1\right)\pi(j_y)\Upsilon_K^{<}\|_{\mathcal{F}}\, n_{\delta,\eta}(y) \\ &\le\; C\alpha^{\delta/2-1}\int \mathrm{d}y\, \|j_y\|_{L^2}\|A_{P,y}\Upsilon_K\|_{\mathcal{F}}\, n_{\delta,\eta}(y) + C\alpha^{\delta/2-1}\int \mathrm{d}y\, \|y\nabla j_y\|_{L^2} n_{\delta,\eta}(y) \\ &\le\; C\alpha^{\delta/2-1}\frac{|P|}{\alpha^2}\int \mathrm{d}y\, H(y)\,(\sqrt{K}|y|+\alpha|y|^3)n_{\delta,\eta}(y) \\ &\quad + C\alpha^{\delta/2-1}\frac{|P|}{\alpha^2}\int \mathrm{d}y\, |y|H(y)\, n_{\delta,\eta}(y) \\ &\le\; C\alpha^{-6+\frac{9}{2}\delta}\sqrt{K}\end{aligned} \tag{5.201}$$

where the last estimate follows from Corollary 5.3.5 and the assumption $|P|\le c\alpha$.

Combining the relevant estimates, that is (5.155), (5.156), (5.158) and (5.162) for $\mathcal{E}_1$ as well as (5.183), (5.188), (5.189), (5.200) and (5.201) for $\mathcal{E}_2$, we arrive at the statement of Proposition 5.3.16, thus providing an appropriate bound for $\mathcal{E}$. □

Proof of Lemma 5.3.17. Since H has the desired properties, we need to show them for

$$l_y^{(1)} \;=\; \left\langle\psi|h.T_y\psi\right\rangle_{L^2}. \tag{5.202}$$

To this end we introduce

$$\mathcal{S} \;=\; \{f \in L^p(\mathbb{R}^3, (1+|y|^n)\mathrm{d}y) \quad \forall 1 \le p \le \infty, \quad \forall n \ge 0\} \tag{5.203}$$

and start with the following observation: Suppose f_1, f_2, f_3 and f_4 are functions in $\mathcal{S}$. Then

$$S(y) \;:=\; \iint \mathrm{d}u\mathrm{d}v \frac{f_1(u)f_2(v)f_3(u+y)f_4(v+y)}{|u-v|} \in \mathcal{S}. \tag{5.204}$$

In fact, $|S(y)| \le C\|f_4\|_{L^\infty}\|f_3\|_{L^\infty}\|f_1\|_{L^p}\|f_2\|_{L^q}$ for all $1 < p < 3/2, q = 3p/(5p-3)$ by the Hardy–Littlewood–Sobolev inequality. Since $\int \mathrm{d}y|y|^n f_3(u+y) \le 2^{n-1}\left(|u|^n\|f_3\|_{L^1} + \||\cdot|^n f_3\|_{L^1}\right)$, we have also

$$\int \mathrm{d}y|y|^n S(y) \;\le\; C\|f_4\|_{L^\infty}\left(\||\cdot|^n f_1\|_{L^p}\|f_2\|_{L^q}\|f_3\|_{L^1} + \|f_1\|_{L^p}\|f_2\|_{L^q}\||\cdot|^n f_3\|_{L^1}\right) \tag{5.205}$$

from which (5.204) follows. Moreover,

$$f \in \mathcal{S} \implies \sqrt{|f|} \in \mathcal{S}. \tag{5.206}$$

Indeed, we have for all $n \ge 0$,

$$\int |y|^n\sqrt{|f|}\mathrm{d}y \;\le\; \sqrt{\|f\|_{L^\infty}}\int_{|y|\le 1}|y|^n\mathrm{d}y + \frac{1}{2}\int |y|^{n+m}|f|\mathrm{d}y + \frac{1}{2}\int_{|y|>1}|y|^{n-m}\mathrm{d}y \;<\; \infty \tag{5.207}$$

since m can be chosen arbitrarily large by assumption. Thus, it suffices to prove the desired statement for the functions $\|\nabla^k l_y^{(1)}\|_{L^2}^2$. For $k=0$, we use (5.176) to compute

$$\|l_y^{(1)}\|_{L^2}^2 \;=\; \frac{1}{4\pi}\iint \mathrm{d}u\mathrm{d}v\frac{\psi(u)\psi(v)\psi(y+u)\psi(v+y)}{|u-v|}. \tag{5.208}$$

The statement now follows easily from (5.204) and Lemma 5.3.6. Arguing again via (5.206), for $k=1$ it suffices to show the statement for

$$\begin{aligned}\|\nabla l_y^{(1)}\|_{L^2}^2 \;&=\; \|\langle\nabla\psi|h.T_y\psi\rangle_{L^2} + \left\langle\psi|h.\nabla T_y\psi\right\rangle_{L^2}\|_{L^2}^2 \\ &\le\; 2\|\langle\nabla\psi|h.T_y\psi\rangle_{L^2}\|_{L^2}^2 + 2\|\langle\psi|h.\nabla T_y\psi\rangle_{L^2}\|_{L^2}^2\end{aligned} \tag{5.209}$$

(the first equality follows from $\nabla_z h_x(z) = -\nabla_x h_x(z)$ and integration by parts). Using (5.176), we find

$$\|\langle\nabla\psi|h.T_y\psi\rangle_{L^2}\|_{L^2}^2 \;\le\; C\iint \mathrm{d}u\mathrm{d}v\frac{|\nabla\psi(u)||\nabla\psi(v)|\psi(v+y)\psi(u+y)}{|u-v|}, \tag{5.210a}$$

$$\|\langle\psi|h.\nabla T_y\psi\rangle_{L^2}\|_{L^2}^2 \;\le\; C\iint \mathrm{d}u\mathrm{d}v\frac{|\nabla\psi(u+y)||\nabla\psi(v+y)|\psi(v)\psi(u)}{|u-v|}. \tag{5.210b}$$

We arrive at the desired conclusion by Lemma 5.3.6 and (5.204). □

5.3.7 Energy contribution $\mathcal{G}$

This energy contribution, defined in (5.60b), is evaluated by the following proposition.

Proposition 5.3.18. *Let* $\mathbb{H}_K$ *as in* (5.32), $\mathbb{N}_1 = \mathrm{d}\Gamma(\Pi_1)$ *and choose* $c > 0$. *For every* $\varepsilon > 0$ *there exists a constant* $C_\varepsilon > 0$ (*we omit the dependence on* c) *such that*

$$\left| \mathcal{G} - \mathcal{N}\frac{2}{\alpha^2}\Big\langle \Upsilon_K | (\mathbb{H}_K - \mathbb{N}_1)\Upsilon_K \Big\rangle_{\mathcal{F}} \right| \leq C_\varepsilon\, \alpha^\varepsilon \Big(\sqrt{K}\alpha^{-6} + K^{-1/2}\alpha^{-5}\Big) \tag{5.211}$$

for all $|P|/\alpha \leq c$ *and all* K, α *large enough.*

Proof. Using $h^{\mathrm{Pek}} G_K^0 = 0$ and $\mathbb{N} G_K^0 = \mathbb{N}_1 G_K^0$ we can decompose $\mathcal{G}$ into two terms

$$\begin{aligned} \mathcal{G} &= -\frac{2}{\alpha}\int \mathrm{d}y\ \mathrm{Re}\Big\langle G_K^0 | (\alpha^{-2}\mathbb{N}_1 + \alpha^{-1}\phi(h_\cdot + \varphi_P)) T_y e^{A_{P,y}} W(\alpha w_{P,y}) G_K^1 \Big\rangle_{\mathscr{H}} \\ &= \mathcal{G}_1 + \mathcal{G}_2, \end{aligned} \tag{5.212}$$

where the first term will contribute to the error while the second one provides an energy contribution of order α^{-2}. We proceed for each one separately.

Term $\mathcal{G}_1$. With the aid of (5.119), (5.132) and $(T_y e^{A_{P,y}})^\dagger = T_{-y} e^{-A_{P,y}}$, one finds

$$\mathcal{G}_1 = -\frac{2}{\alpha^3}\int \mathrm{d}y\ \mathrm{Re}\Big\langle R_{3,y}\psi \otimes \Big(\Upsilon_K^< + \Upsilon_K^>\Big) | W(\alpha w_{P,y}) G_K^0 \Big\rangle_{\mathscr{H}} = \mathcal{G}_1^< + \mathcal{G}_1^> \tag{5.213}$$

where we introduced the operator $R_{3,y} = R_{3,y}^1 + R_{3,y}^2$ with

$$R_{3,y}^1 = P_\psi \phi(h_{K,\cdot}^1) R u_\alpha T_{-y} P_\psi e^{-A_{P,y}} \mathbb{N}_1 \tag{5.214a}$$

$$R_{3,y}^2 = 2\alpha P_\psi \Big\langle h_{K,\cdot} | \mathrm{Re}(w_{P,y}^1) \Big\rangle_{L^2} R u_\alpha T_{-y} P_\psi e^{-A_{P,y}} \mathbb{N}_1. \tag{5.214b}$$

Proceeding similarly as for $R_{1,y}^1$ and $R_{2,y}^2$ in (5.134a)–(5.134b), one further verifies

$$\|R_{3,y}\Psi\|_{\mathscr{H}} \leq C\|u_\alpha T_{-y} P_\psi\|_{\mathrm{op}}\Big(1 + \alpha y^2\Big)\|(\mathbb{N}+1)^{3/2}\Psi\|_{\mathscr{H}}. \tag{5.215}$$

Recalling the definition $f_\alpha(y) = \|u_\alpha T_{-y} P_\psi\|_{\mathrm{op}}$ and (5.138), we can use Corollary 5.3.12 to find

$$|\mathcal{G}_1^>| \leq \frac{C}{\alpha^3}\|(\mathbb{N}+1)^{3/2}\Upsilon_K^>\|_{\mathcal{F}} \int \mathrm{d}y\, f_\alpha(y)(1+\alpha y^2) \leq C_\delta\, \alpha^{-7}. \tag{5.216}$$

In the first term we proceed with (5.126) and Lemma 5.3.13 to obtain

$$\begin{aligned} |\mathcal{G}_1^<| &\leq \frac{2}{\alpha^3}\int \mathrm{d}y\, \|e^{\kappa\mathbb{N}}\mathbb{U}_K(R_{3,y}\psi \otimes \Upsilon_K^<)\|_{\mathscr{H}}\, \|e^{-\kappa\mathbb{N}} W(\alpha\widetilde{w}_{P,y})\Omega\|_{\mathcal{F}} \\ &\leq \frac{2\sqrt{2}}{\alpha^3}\int \mathrm{d}y\, \|R_{3,y}\psi \otimes \Upsilon_K\|_{\mathscr{H}}\, n_{\delta,\eta}(y) \leq \frac{C}{\alpha^3}\int \mathrm{d}y\, f_\alpha(y)(1+\alpha y^2)\, n_{\delta,\eta}(y), \end{aligned} \tag{5.217}$$

which brings us again into a position to apply Corollary 5.3.5. Hence

$$|\mathcal{G}_1^<| \leq C\alpha^{-6+3\delta}. \tag{5.218}$$

Term $\mathcal{G}_2$. Here we have

$$\begin{aligned} \mathcal{G}_2 = &-\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\Big\langle G_K^0 | \phi(h_\cdot + \varphi_P) T_y W(\alpha w_{P,y}) G_K^1 \Big\rangle_{\mathscr{H}} \\ &- \frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\Big\langle G_K^0 | \phi(h_\cdot + \varphi_P) T_y (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) G_K^1 \Big\rangle_{\mathscr{H}} = \mathcal{G}_{21} + \mathcal{G}_{22}. \end{aligned} \tag{5.219}$$

To separate the leading order contribution in $\mathcal{G}_{21}$ we insert $1 = \mathbb{U}_K^\dagger \mathbb{U}_K$ next to G_K^0 and bring $\mathbb{U}_K^\dagger$ to the right side of the inner product. With $\mathbb{U}_K \Upsilon_K = \Omega$, (5.105c) and (5.115) this gives

$$\mathcal{G}_{21} = -\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle \psi\otimes\Omega | a(\underline{h_{\cdot}+\varphi_P}) T_y W(\alpha\widetilde{w}_{P,y}) u_\alpha R a^\dagger(\underline{h^1_{K,\cdot}})\psi\otimes\Omega\right\rangle_{\mathscr{H}}, \tag{5.220}$$

where $\underline{\cdot}$ is defined in (5.104a). Next we write $W(\alpha\widetilde{w}_{P,y}) = n_{0,1}(y) e^{a^\dagger(\alpha\widetilde{w}_{P,y})} e^{-a(\alpha\widetilde{w}_{P,y})}$ and move the first exponential to the left side and the second exponential to the right side until they act both on the Fock space vacuum. Using $e^{-a(f)}a^\dagger(g)e^{a(f)} = a^\dagger(g) - \langle f|g\rangle$ we find this way

$$\mathcal{G}_{21} = -\frac{2}{\alpha^2}\int \mathrm{d}y\, n_{0,1}(y)\ \mathrm{Re}\left\langle \psi\otimes\Omega | a(\underline{h_{\cdot}+\varphi_P}) T_y u_\alpha R a^\dagger(\underline{h^1_{K,\cdot}})\psi\otimes\Omega\right\rangle_{\mathscr{H}} \tag{5.221a}$$

$$+2\int \mathrm{d}y\, n_{0,1}(y)\ \mathrm{Re}\left\langle \psi\otimes\Omega | \langle \underline{h_{\cdot}+\varphi_P}|\widetilde{w}_{P,y}\rangle_{L^2} T_y u_\alpha R \langle \widetilde{w}_{P,y}|\underline{h^1_{K,\cdot}}\rangle_{L^2}\psi\otimes\Omega\right\rangle_{\mathscr{H}}. \tag{5.221b}$$

In the first line we write $h_{\cdot} + \varphi_P = h^0_{\cdot} + h^1_{\cdot} + \varphi + i\xi_P$, with $h^i_{\cdot} = (\Pi_i h)_{\cdot}$, and use that

$$\left\langle \psi\otimes\Omega | a(\underline{h^0_{\cdot}+i\xi_P}) T_y u_\alpha R a^\dagger(\underline{h^1_{K,\cdot}})\psi\otimes\Omega\right\rangle_{\mathscr{H}} = 0 \tag{5.222}$$

since $h^0_x + i\xi_P \in \mathrm{Ran}(\Pi_0)$ whereas $h^1_{K,x} \in \mathrm{Ran}(\Pi_1)$. Finally we can replace a and $a^\dagger$ by ϕ, and then transform back with $\mathbb{U}_K$, using (5.105c), in order to obtain

$$(5.221a) = -\frac{2}{\alpha^2}\int \mathrm{d}y\, n_{0,1}(y)\ \mathrm{Re}\left\langle \psi\otimes\Upsilon_K | \phi(h^1_{\cdot}+\varphi) T_y u_\alpha R \phi(h^1_{K,\cdot})\psi\otimes\Upsilon_K\right\rangle_{\mathscr{H}}. \tag{5.223}$$

To summarize, we have shown that

$$\mathcal{G}_{21} = -\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle G_K^0 | L_{2,y} G_K^0\right\rangle_{\mathscr{H}} n_{0,1}(y) + \int \mathrm{d}y\, \ell_2(y) n_{0,1}(y) = \mathcal{G}_{211} + \mathcal{G}_{212} \tag{5.224}$$

with

$$L_{2,y} = P_\psi \phi(h^1_{\cdot}+\varphi) T_y u_\alpha R \phi(h^1_{K,\cdot}) P_\psi \tag{5.225a}$$

$$\ell_2(y) = 2\,\mathrm{Re}\left\langle \psi | \langle \underline{h_{\cdot}+\varphi_P}|\widetilde{w}_{P,y}\rangle_{L^2} T_y u_\alpha R \langle \widetilde{w}^1_{P,y}|\underline{h^1_{K,\cdot}}\rangle_{L^2}\psi\right\rangle_{L^2}. \tag{5.225b}$$

In the first term we add and subtract the Gaussian,

$$\begin{aligned}\mathcal{G}_{211} &= -\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle G_K^0 | L_{2,y} G_K^0\right\rangle_{\mathscr{H}} e^{-\lambda\alpha^2 y^2}\\ &\quad -\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle G_K^0 | L_{2,y} G_K^0\right\rangle_{\mathscr{H}} \left(n_{0,1}(y) - e^{-\lambda\alpha^2 y^2}\right) = \mathcal{G}_{211}^{\mathrm{lo}} + \mathcal{G}_{211}^{\mathrm{err}},\end{aligned} \tag{5.226}$$

and proceed with $\mathcal{G}_{211}^{\mathrm{lo}}$ by inserting $h^1_{\cdot} = h^1_{K,\cdot} + (h^1_{\cdot} - h^1_{K,\cdot})$, $T_y = 1 + (T_y - 1)$ and $u_\alpha = 1 + (u_\alpha - 1)$,

$$\begin{aligned}\mathcal{G}_{211}^{\mathrm{lo}} &= -\frac{2}{\alpha^2}\mathrm{Re}\left\langle G_K^0 | \phi(h^1_{K,\cdot}+\varphi) R \phi(h^1_{K,\cdot}) G_K^0\right\rangle_{\mathscr{H}} \int \mathrm{d}y\, e^{-\lambda\alpha^2 y^2}\\ &\quad -\frac{2}{\alpha^2}\mathrm{Re}\left\langle G_K^0 | \phi(h^1_{K,\cdot}+\varphi)(u_\alpha - 1) R \phi(h^1_{K,\cdot}) G_K^0\right\rangle_{\mathscr{H}} \int \mathrm{d}y\, e^{-\lambda\alpha^2 y^2}\\ &\quad -\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle G_K^0 | \phi(h^1_{K,\cdot}+\varphi)(T_y - 1) u_\alpha R \phi(h^1_{K,\cdot}) G_K^0\right\rangle_{\mathscr{H}} e^{-\lambda\alpha^2 y^2}\\ &\quad -\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle G_K^0 | \phi(h^1_{\cdot} - h^1_{K,\cdot}) T_y u_\alpha R \phi(h^1_{K,\cdot}) G_K^0\right\rangle_{\mathscr{H}} e^{-\lambda\alpha^2 y^2}\\ &= \sum_{n=1}^{4} \mathcal{G}_{211}^{\mathrm{lo},n}.\end{aligned} \tag{5.227}$$

Since $P_\psi \phi(\varphi) R = 0$, we have $\mathcal{G}_{211}^{\mathrm{lo},1} = \frac{2}{\alpha^2}\left\langle \Upsilon_K | (\mathbb{H}_K - \mathbb{N}_1)\Upsilon_K \right\rangle_{\mathcal{F}} (\frac{\pi}{\lambda\alpha^2})^{3/2}$, cf. (5.32), and hence we can use Proposition 5.3.15 to conclude that

$$\left| \mathcal{G}_{211}^{\mathrm{lo},1} - \mathcal{N}\frac{2}{\alpha^2}\left\langle \Upsilon_K | (\mathbb{H}_K - \mathbb{N}_1)\Upsilon_K \right\rangle_{\mathcal{F}} \right| \le C_\varepsilon \sqrt{K} \alpha^{-6+\varepsilon}. \tag{5.228}$$

For the other terms, we shall show the combined error estimate

$$|\mathcal{G}_{211}^{\mathrm{lo},2}| + |\mathcal{G}_{211}^{\mathrm{lo},3}| + |\mathcal{G}_{211}^{\mathrm{lo},4}| \le C\Big(\sqrt{K}\alpha^{-6} + K^{-1/2}\alpha^{-5}\Big). \tag{5.229}$$

In the last term, we recall $h_\cdot(y) = h_{K=\infty,\cdot}(y)$, and apply Lemma 5.3.8 in combination with $\|R^{1/2} u_\alpha T_{-y} \nabla\|_{\mathrm{op}} \le C$. This gives

$$\begin{aligned} |\mathcal{G}_{211}^{\mathrm{lo},4}| &\le \frac{2}{\alpha^2}\int \mathrm{d}y\, e^{-\lambda\alpha^2 y^2}\, \|R^{1/2} u_\alpha T_{-y}\phi(h_\cdot^1 - h_{K,\cdot}^1) P_\psi G_K^0\|_{\mathscr{H}}\, \|R^{1/2}\phi(h_{K,\cdot}^1) P_\psi G_K^0\|_{\mathscr{H}} \\ &\le C\alpha^{-5} K^{-1/2}. \end{aligned} \tag{5.230}$$

Next we write $T_y - 1 = \int_0^1 \mathrm{d}s T_{sy}(y\nabla)$ in the third term to obtain an additional $|y|$,

$$\begin{aligned} |\mathcal{G}_{211}^{\mathrm{lo},3}| &\le \frac{2}{\alpha^2}\left(\int \mathrm{d}y\, |y| e^{-\lambda\alpha^2 y^2}\right) \|\nabla u_\alpha R^{1/2}\|_{\mathrm{op}}\, \|\phi(h_{K,\cdot}^1 + \varphi) G_K^0\|_{\mathscr{H}} \|R^{1/2}\phi(h_{K,\cdot}^1) G_K^0\|_{\mathscr{H}} \\ &\le C\alpha^{-6}\sqrt{K}, \end{aligned} \tag{5.231}$$

where the factor $\sqrt{K}$ comes from the L^2 norm of $h_{K,0}^1$ in the bound on the first field operator (since $\Delta R^{1/2}$ is unbounded, we can not apply the commutator method to this part). In the second term, we use $\psi(x) \le Ce^{-|x|/C}$ for some $C > 0$, and thus $\|(u_\alpha - 1)\psi\|_{L^2} \le Ce^{-\alpha/C}$, to estimate

$$|\mathcal{G}_{211}^{\mathrm{lo},2}| \le \frac{C}{\alpha^5}\|(u_\alpha - 1)\psi\|_{L^2}\, \|\phi(h_{K,\cdot}^1 + \varphi) R \phi(h_{K,\cdot}^1) G_K^0\|_{\mathscr{H}} \le C\sqrt{K} e^{-\alpha/C}. \tag{5.232}$$

This proves (5.229).

To bound the remaining contributions in $\mathcal{G}_{211}^{\mathrm{err}}$ and $\mathcal{G}_{212}$, we shall use

$$\left|\left\langle G_K^0 | L_{2,y} G_K^0 \right\rangle\right| \le C f_{2,\alpha}(y) \tag{5.233a}$$

$$|\ell_2(y)| \le C f_{2,\alpha}(y)(y^2 + \alpha^{-2})(|y| + |y|^3 + \alpha^{-2}) \tag{5.233b}$$

where

$$f_{2,\alpha}(y) = \|u_\alpha T_{-y} P_\psi\|_{\mathrm{op}} + \|\nabla u_\alpha T_{-y} P_\psi\|_{\mathrm{op}}. \tag{5.234}$$

Using the exponential decay of ψ and $|\nabla^k u_\alpha|(y) \le 1(|y| \le 2\alpha)$, for $k = 0, 1$, it is easy to show that

$$\|f_{2,\alpha}\|_{L^\infty} \le C \quad \text{and} \quad \||\cdot|^n f_{2,\alpha}\|_{L^1} \le C_n \alpha^{3+n} \quad \text{for all } n \in \mathbb{N}_0. \tag{5.235}$$

To verify (5.233a) and (5.233b), use $u_\alpha T_{-y}\phi(h_\cdot) = \phi(h_{\cdot - y}) u_\alpha T_{-y}$ and Cauchy–Schwarz to bound

$$\left|\left\langle G_K^0 | L_{2,y} G_K^0 \right\rangle_{\mathscr{H}}\right| \le \|R^{1/2}\phi(h_{\cdot - y}^1 + \varphi) u_\alpha T_{-y} P_\psi G_K^0\|_{\mathscr{H}}\, \|R^{1/2}\phi(h_{K,\cdot}^1) P_\psi G_K^0\|_{\mathscr{H}}. \tag{5.236}$$

Now we can use (5.96) and Lemma 5.3.8 to obtain (5.233a). To estimate $\ell_2(y)$, defined in (5.225b), we proceed with

$$|\ell_2(y)| \le 2\Big|\Big\langle \psi|T_y u_\alpha \langle \underline{h_{\cdot-y}}|\widetilde{w}_{P,y}\rangle_{L^2} R\langle \widetilde{w}^1_{P,y}|\underline{h^1_{K,\cdot}}\rangle_{L^2}\psi\Big\rangle_{L^2}\Big| \tag{5.237a}$$

$$+ 2\Big|\Big\langle \psi|T_y u_\alpha \langle \underline{\varphi_P}|\widetilde{w}_{P,y}\rangle_{L^2} R\langle \widetilde{w}^1_{P,y}|\underline{h^1_{K,\cdot}}\rangle_{L^2}\psi\Big\rangle_{L^2}\Big|, \tag{5.237b}$$

and considering the first line, we use Cauchy–Schwarz, write out the two inner products (in the phonon variable) and then use Cauchy–Schwarz again,

$$\begin{aligned} |(5.237\text{a})| &\le 2\int \mathrm{d}u\, |\widetilde{w}_{P,y}(u)|\, \|P_\psi T_y u_\alpha \underline{h_{\cdot-y}}(u) R^{1/2}\|_{\mathrm{op}} \int \mathrm{d}z\, |\widetilde{w}^1_{P,y}(z)|\, \|R^{1/2}\underline{h^1_{K,\cdot}}(z)\psi\| \\ &\le 2\|\widetilde{w}_{P,y}\|_{L^2}\|\widetilde{w}^1_{P,y}\|_{L^2}\left(\int \mathrm{d}u \|P_\psi T_y u_\alpha \underline{h_{\cdot-y}}(u) R^{1/2}\|^2_{\mathrm{op}} \int \mathrm{d}z \|R^{1/2}\underline{h^1_{K,\cdot}}(z)\psi\|^2_{L^2}\right)^{1/2} \\ &\le C f_{2,\alpha}(y)(|y| + y^3 + \alpha^{-2})(y^2+\alpha^{-2}), \end{aligned} \tag{5.238}$$

where the last step follows from Lemma 5.3.3 and Corollary 5.3.9 together with $\underline{h_{K,\cdot}} = h^0_{K,\cdot} + \Theta_K^{-1} h^1_{K,\cdot}$. Since the second line is estimated similarly, we arrive at (5.233b). With (5.233a) at hand we can apply Lemma 5.3.4 and (5.235) to get

$$|\mathcal{G}^{\mathrm{err}}_{211}| \le \frac{2}{\alpha^2}\int \mathrm{d}y \Big|\Big\langle G^0_K|L_{2,y}G^0_K\Big\rangle_{\mathscr{H}}\Big|\Big|n_{0,1}(y) - e^{-\lambda\alpha^2 y^2}\Big| \le C\alpha^{-6}, \tag{5.239}$$

and further, using (5.233b) and Corollary 5.3.5, we obtain

$$|\mathcal{G}_{212}| \le C\int \mathrm{d}y\, |\ell_2(y)|\, n_{0,1}(y) \le C\alpha^{-6}. \tag{5.240}$$

This completes the analysis of $\mathcal{G}_{21}$.

Next we introduce $R_{4,y} = R^1_{4,y} + R^2_{4,y}$ with

$$R^1_{4,y} = P_\psi \phi(h^1_{K,\cdot}) R^{\frac12}(e^{-A_{P,y}} - 1) R^{\frac12}\phi(h_{\cdot-y} + \varphi_P) u_\alpha T_{-y} P_\psi \tag{5.241a}$$

$$R^2_{4,y} = 2\alpha P_\psi \Big\langle h_{K,\cdot}|\operatorname{Re}(w^1_{P,y})\Big\rangle_{L^2} R^{\frac12}(e^{-A_{P,y}} - 1) R^{\frac12}\phi(h_{\cdot-y} + \varphi_P) u_\alpha T_{-y} P_\psi. \tag{5.241b}$$

Inserting (5.119) and (5.132) into (5.219) it follows that

$$\mathcal{G}_{22} = -\frac{2}{\alpha^2}\int \mathrm{d}y\, \operatorname{Re}\Big\langle R_{4,y}\psi \otimes \Big(\Upsilon^<_K + \Upsilon^>_K\Big)|W(\alpha w_{P,y})G^0_K\Big\rangle_{\mathscr{H}} = \mathcal{G}^<_{22} + \mathcal{G}^>_{22}. \tag{5.242}$$

With the aid of Lemma 5.3.8 we obtain

$$\|R^1_{4,y}\Psi\|_{\mathscr{H}} \le C\|(e^{-A_{P,y}} - 1)(\mathbb{N}+1)^{1/2} R^{1/2}\phi(h_{\cdot-y} + \varphi_P) u_\alpha T_{-y} P_\psi \Psi\|_{\mathscr{H}}, \tag{5.243}$$

and proceeding similarly as in (5.136), we find

$$\|R^2_{4,y}\Psi\|_{\mathscr{H}} \le C\alpha(y^2+\alpha^{-2})\|(e^{-A_{P,y}} - 1) R^{1/2}\phi(h_{\cdot-y} + \varphi_P) u_\alpha T_{-y} P_\psi \Psi\|_{\mathscr{H}}. \tag{5.244}$$

For $\Psi = \psi \otimes \Upsilon^>_K$, a second application of Lemma 5.3.8 (after using unitarity of $e^{-A_{P,y}}$) together with $\|\varphi_P\|^2_{L^2} \le C$ for $|P|/\alpha \le c$ and Corollary 5.3.12 is sufficient to find

$$\begin{aligned} \|R_{4,y}\psi \otimes \Upsilon^>_K\|_{\mathscr{H}} &\le C\Big(\|u_\alpha T_{-y}P_\psi\|_{\mathrm{op}} + \|\nabla u_\alpha T_{-y} P_\psi\|_{\mathrm{op}}\Big)(1+\alpha y^2)\|(\mathbb{N}+1)\Upsilon^>_K\|_{\mathcal{F}} \\ &\le C_\delta\, \alpha^{-10} f_{2,\alpha}(y)(1+\alpha y^2) \end{aligned} \tag{5.245}$$

with $f_{2,\alpha}$ defined in (5.234). Using this bound in $G_{22}^{>}$ and recalling Corollary 5.3.12 and (5.235) we thus obtain

$$|\mathcal{G}_{22}^{>}| \leq C_\delta\, \alpha^{-6}. \tag{5.246}$$

In $\mathcal{G}_{22}^{<}$ we proceed by inserting (5.122) and use (5.126) and Lemma 5.3.13. This gives

$$|\mathcal{G}_{22}^{<}| \;\leq\; \frac{2\sqrt{2}}{\alpha^2}\int \mathrm{d}y\, \|R_{4,y}\psi\otimes\Upsilon_K^{<}\|_{\mathscr{H}}\, n_{\delta,\eta}(y). \tag{5.247}$$

The derivation of a suitable bound for the norm in the integrand is more cumbersome, so we go through it step by step. To shorten the notation let $G_K^{0<}=\psi\otimes\Upsilon_K^{<}$. We start from (5.243) and (5.244) where we insert $h_\cdot = h_{K,\cdot}+(h_\cdot - h_{K,\cdot})$ and use the triangle inequality,

$$\begin{aligned}
\|R_{4,y}^1 G_K^{0<}\|_{\mathscr{H}} \;&\leq\; C\|(e^{-A_{P,y}}-1)(\mathbb{N}+1)^{1/2}R^{\frac12}\phi(h_{K,\cdot-y}+\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}} &(5.248a)\\
&\quad+\; C\|(e^{-A_{P,y}}-1)(\mathbb{N}+1)^{1/2}R^{\frac12}\phi(h_{\cdot-y}-h_{K,\cdot-y})u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}}, &(5.248b)\\
\|R_{4,y}^2 G_K^{0<}\|_{\mathscr{H}} \;&\leq\; C\alpha(y^2+\alpha^{-2})\|(e^{-A_{P,y}}-1)R^{\frac12}\phi(h_{K,\cdot-y}+\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}} &(5.248c)\\
&\quad+\; C\alpha(y^2+\alpha^{-2})\|(e^{-A_{P,y}}-1)R^{\frac12}u_\alpha\phi(h_{\cdot-y}-h_{K,\cdot-y})u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}}. &(5.248d)
\end{aligned}$$

For the second and fourth line, we apply Lemma 5.3.8 a second time (after bringing $(\mathbb{N}+1)^{1/2}$ to the right of a and $a^\dagger$) to find

$$\begin{aligned}
\text{(5.248b)}+\text{(5.248d)} \;&\leq\; CK^{-1/2}(1+\alpha y^2)(\|u_\alpha T_{-y}P_\psi\|_{\mathrm{op}}+\|\nabla u_\alpha T_{-y}P_\psi\|_{\mathrm{op}})\|(\mathbb{N}+1)\Upsilon_K^{<}\|_{\mathcal{F}}\\
&\leq\; CK^{-1/2}(1+\alpha y^2)f_{2,\alpha}(y). &(5.249)
\end{aligned}$$

In the first and third line, we use the functional calculus and write out $A_{P,y}=iP_f y+ig_P(y)$,

$$\begin{aligned}
\text{(5.248a)}+\text{(5.248c)} &\leq C\|(P_f y)(\mathbb{N}+1)^{1/2}R^{\frac12}\phi(h_{K,\cdot-y}+\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}} &(5.250a)\\
&\quad+C\alpha(y^2+\alpha^{-2})\|(P_f y)R^{\frac12}\phi(h_{K,\cdot-y}+\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}} &(5.250b)\\
&\quad+C|g_P(y)|\|(\mathbb{N}+1)^{1/2}R^{1/2}\phi(h_{K,\cdot-y}+\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}} &(5.250c)\\
&\quad+C\alpha(y^2+\alpha^{-2})|g_P(y)|\|R^{\frac12}\phi(h_{K,\cdot-y}+\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}}. &(5.250d)
\end{aligned}$$

Now we use $[iP_f y,\phi(f)]=\pi(y\nabla f)$ such that we can estimate the first line by

$$\begin{aligned}
\text{(5.250a)} \;\leq\; C\Big(&\|(\mathbb{N}+1)^{1/2}R^{1/2}\phi(h_{K,\cdot-y}+\varphi_P)(P_f y)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}}\\
&+\|(\mathbb{N}+1)^{1/2}R^{1/2}\pi(y\nabla h_{K,\cdot-y}+y\nabla\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}}\Big). &(5.251)
\end{aligned}$$

To bound the first line, we use again Lemma 5.3.8, while in the second line we use $(\nabla h_K)_\cdot = -\nabla(h_{K,\cdot})=-[\nabla,h_{K,\cdot}]$ and (5.96) together with $\|\nabla\varphi_P\|_{L^2}\leq C$ for $|P|/\alpha\leq c$. Together we obtain

$$\begin{aligned}
\text{(5.250a)} \;&\leq\; C|y|\Big(\|u_\alpha T_{-y}P_\psi\|_{\mathrm{op}}+\|\nabla u_\alpha T_{-y}P_\psi\|_{\mathrm{op}}\Big)\Big(\|(\mathbb{N}+1)P_f\Upsilon_K^{<}\|_{\mathcal{F}}+\sqrt{K}\|(\mathbb{N}+1)\Upsilon_K^{<}\|_{\mathcal{F}}\Big)\\
&\leq\; C\alpha^\delta|y|f_{2,\alpha}(y)\Big(\|P_f\Upsilon_K^{<}\|_{\mathcal{F}}+\sqrt{K}\Big)\\
&\leq\; C\alpha^\delta\sqrt{K}|y|f_{2,\alpha}(y), &(5.252)
\end{aligned}$$

where the factor $\sqrt{K}$ in the first step comes from the L^2-norm of $h_{K,0}$, and the last step follows from Lemma 5.3.14. In a similar fashion, one shows

$$\text{(5.250b)} \leq C\alpha^\delta \sqrt{K}|y|(1+\alpha y^2) f_{2,\alpha}(y), \tag{5.253}$$

and, with (5.129), one also verifies

$$\text{(5.250c)} + \text{(5.250d)} \leq C\alpha^\delta(\alpha^2|y|^5 + \alpha|y|^3) f_{2,\alpha}(y). \tag{5.254}$$

Collecting the estimates (5.249), (5.252), (5.253) and (5.254) we arrive at

$$\|R_{4,y}\psi \otimes \Upsilon_K^<\|_{\mathscr{H}} \leq C f_{2,\alpha}(y)\alpha^\delta\Big(K^{-\frac{1}{2}}(1+\alpha y^2) + \alpha^2|y|^5 + \sqrt{K}(|y| + \alpha|y|^3)\Big). \tag{5.255}$$

Now we can apply Corollary 5.3.5 together with (5.235) to bound the right side of (5.247). The result is

$$|\mathcal{G}_{22}^<| \leq C\alpha^{-2+\delta}\Big(K^{-1/2}\alpha^{-3} + \sqrt{K}\alpha^{-4+4\delta}\Big). \tag{5.256}$$

In view of the estimates (5.216), (5.218), (5.228), (5.229), (5.239), (5.240), (5.246) and (5.256), the proof of Proposition 5.3.18 is now complete. □

5.3.8 Energy contribution $\mathcal{K}$

Recall that $\mathcal{K}$ was defined in (5.60c).

Proposition 5.3.19. *Let* $\mathbb{H}_K$ *as in* (5.32), $\mathbb{N}_1 = \mathrm{d}\Gamma(\Pi_1)$ *and choose* $c > 0$. *For every* $\varepsilon > 0$ *there exists a constant* $C_\varepsilon > 0$ (*we omit the dependence on* c) *such that*

$$\left|\mathcal{K} + \mathcal{N}\frac{1}{\alpha^2}\Big\langle \Upsilon_K|(\mathbb{H}_K - \mathbb{N}_1)\Upsilon_K\Big\rangle_{\mathcal{F}}\right| \leq C_\varepsilon\, \alpha^\varepsilon\Big(\sqrt{K}\alpha^{-6} + K^{-1/2}\alpha^{-5}\Big) \tag{5.257}$$

for all $|P|/\alpha \leq c$ *and all* K, α *large enough.*

Proof. We split this contribution into three terms

$$\begin{aligned}\mathcal{K} &= \frac{1}{\alpha^2}\int \mathrm{d}y\,\Big\langle G_K^1|\Big(h^{\mathrm{Pek}} + \alpha^{-2}\mathbb{N} + \alpha^{-1}\phi(h_\cdot + \varphi_P)\Big)T_y e^{A_{P,y}}W(\alpha w_{P,y})G_K^1\Big\rangle_{\mathscr{H}} \\ &= \mathcal{K}_1 + \mathcal{K}_2 + \mathcal{K}_3,\end{aligned} \tag{5.258}$$

and note that $\mathcal{K}_1$ provides the energy contribution of order α^{-2}.

Term $\mathcal{K}_1$. We start again by writing

$$\begin{aligned}\mathcal{K}_1 &= \frac{1}{\alpha^2}\int \mathrm{d}y\,\Big\langle G_K^1|h^{\mathrm{Pek}}T_yW(\alpha w_{P,y})G_K^1\Big\rangle_{\mathscr{H}} \\ &\quad + \frac{1}{\alpha^2}\int \mathrm{d}y\,\Big\langle G_K^1|h^{\mathrm{Pek}}T_y(e^{A_{P,y}} - 1)W(\alpha w_{P,y})G_K^1\Big\rangle_{\mathscr{H}} = \mathcal{K}_{11} + \mathcal{K}_{12}.\end{aligned} \tag{5.259}$$

and proceed for the first term similarly as in the computation of $\mathcal{G}_2$, see (5.219). This leads to

$$\begin{aligned}\mathcal{K}_{11} &= \frac{1}{\alpha^2}\int \mathrm{d}y\,\Big\langle G_K^0|\phi(h_{K,\cdot}^1)Ru_\alpha h^{\mathrm{Pek}}T_yW(\alpha w_{P,y})u_\alpha R\phi(h_{K,\cdot}^1)G_K^0\Big\rangle_{\mathscr{H}} \\ &= \frac{1}{\alpha^2}\int \mathrm{d}y\,\Big\langle \psi\otimes\Omega|a(\underline{h_{K,\cdot}^1})Ru_\alpha h^{\mathrm{Pek}}T_yW(\alpha\widetilde{w}_{P,y})u_\alpha Ra^\dagger(\underline{h_{K,\cdot}^1})\psi\otimes\Omega\Big\rangle_{\mathscr{H}} \\ &= \frac{1}{\alpha^2}\int \mathrm{d}y\,\Big\langle G_K^0|L_{3,y}G_K^0\Big\rangle_{\mathscr{H}} n_{0,1}(y) - \int \mathrm{d}y\,\ell_3(y)n_{0,1}(y) = \mathcal{K}_{111} + \mathcal{K}_{112}\end{aligned} \tag{5.260}$$

where

$$L_{3,y} = P_\psi \phi(h^1_{K,\cdot}) R u_\alpha h^{\rm Pek} T_y u_\alpha R \phi(h^1_{K,\cdot}) P_\psi \quad (5.261a)$$

$$\ell_3(y) = \Big\langle \psi | \langle \underline{h^1_{K,\cdot}} | \widetilde{w}^1_{P,y}\rangle_{L^2} R u_\alpha h^{\rm Pek} T_y u_\alpha R \langle \widetilde{w}^1_{P,y} | \underline{h^1_{K,\cdot}}\rangle_{L^2} \psi \Big\rangle_{L^2}. \quad (5.261b)$$

We go on with

$$\mathcal{K}_{111} = \frac{1}{\alpha^2} \int \mathrm{d}y \, \Big\langle G^0_K | L_{3,y} G^0_K \Big\rangle_{\mathscr{H}} e^{-\lambda\alpha^2 y^2} + \frac{1}{\alpha^2} \int \mathrm{d}y \, \Big\langle G^0_K | L_{3,y} G^0_K \Big\rangle_{\mathscr{H}} \Big(n_{0,1}(y) - e^{-\lambda\alpha^2 y^2} \Big) = \mathcal{K}^{\rm lo}_{111} + \mathcal{K}^{\rm err}_{111}, \quad (5.262)$$

and in the leading-order term, we insert $T_y = 1 + (T_y - 1)$ and $u_\alpha = 1 + (u_\alpha - 1)$,

$$\begin{aligned} \mathcal{K}^{\rm lo}_{111} = & \frac{1}{\alpha^2} \Big\langle G^0_K | \phi(h^1_{K,\cdot}) R h^{\rm Pek} R \phi(h^1_{K,\cdot}) G^0_K \Big\rangle_{\mathscr{H}} \int \mathrm{d}y \, e^{-\lambda\alpha^2 y^2} \\ & + \frac{1}{\alpha^2} \Big\langle G^0_K | \phi(h^1_{K,\cdot}) R (u_\alpha - 1) h^{\rm Pek} R \phi(h^1_{K,\cdot}) G^0_K \Big\rangle_{\mathscr{H}} \int \mathrm{d}y \, e^{-\lambda\alpha^2 y^2} \\ & + \frac{1}{\alpha^2} \Big\langle G^0_K | \phi(h^1_{K,\cdot}) R u_\alpha h^{\rm Pek} (u_\alpha - 1) R \phi(h^1_{K,\cdot}) G^0_K \Big\rangle_{\mathscr{H}} \int \mathrm{d}y \, e^{-\lambda\alpha^2 y^2} \\ & + \frac{1}{\alpha^2} \int \mathrm{d}y \, \Big\langle G^0_K | \phi(h^1_{K,\cdot}) R u_\alpha h^{\rm Pek} (T_y - 1) u_\alpha R \phi(h^1_{K,\cdot}) G^0_K \Big\rangle_{\mathscr{H}} e^{-\lambda\alpha^2 y^2} \\ = & \sum_{n=1}^{4} \mathcal{K}^{\rm lo,n}_{111}. \end{aligned} \quad (5.263)$$

Since $Rh^{\rm Pek}R = R$, one finds $\mathcal{K}^{\rm lo,1}_{111} = -\frac{1}{\alpha^2}\Big\langle \Upsilon_K | (\mathbb{H}_K - \mathbb{N}_1) \Upsilon_K \Big\rangle_{\mathcal{F}} (\frac{\pi}{\lambda\alpha^2})^3$, cf. (5.32), and with the aid of Proposition 5.3.15, this gives the leading-order contribution

$$\left| \mathcal{K}^{\rm lo,1}_{111} + \mathcal{N} \frac{1}{\alpha^2} \Big\langle \Upsilon_K | (\mathbb{H}_K - \mathbb{N}_1) \Upsilon_K \Big\rangle_{\mathcal{F}} \right| \le C_\varepsilon \sqrt{K} \alpha^{-6+\varepsilon}. \quad (5.264)$$

For the other terms, we shall show that

$$|\mathcal{K}^{\rm lo,2}_{111}| + |\mathcal{K}^{\rm lo,3}_{111}| + |\mathcal{K}^{\rm lo,4}_{111}| \le C\sqrt{K}\alpha^{-6}. \quad (5.265)$$

In the second term we use $h^{\rm Pek} R = Q_\psi = 1 - P_\psi$ to write

$$K^{\rm lo,2}_{111} = \alpha^{-2} \Big\langle G^0_K | \phi(h^1_{K,\cdot}) R (u_\alpha - 1)(1 - P_\psi) \phi(h^1_{K,\cdot}) G^0_K \Big\rangle_{\mathscr{H}} \left(\frac{\pi}{\lambda\alpha^2} \right)^{3/2} \quad (5.266)$$

which is exponentially small in α, since $\|(u_\alpha - 1)\psi\|_{L^2} \le Ce^{-\alpha/C}$, and thus with Lemma 5.3.8 one obtains $|\mathcal{K}^{\rm lo,2}_{111}| \le C\sqrt{K} e^{-\alpha/C}$. In the next term we use $[h^{\rm Pek}, u_\alpha - 1] = -[\Delta, u_\alpha]$ and again $h^{\rm Pek} R = 1 - P_\psi$ to get

$$\begin{aligned} \mathcal{K}^{\rm lo,3}_{111} = & \alpha^{-2} \Big\langle G^0_K | \phi(h^1_{K,\cdot}) R u_\alpha (u_\alpha - 1)(1 - P_\psi) \phi(h^1_{K,\cdot}) G^0_K \Big\rangle_{\mathscr{H}} \left(\frac{\pi}{\lambda\alpha^2} \right)^{3/2} \\ & - \alpha^{-2} \Big\langle G^0_K | \phi(h^1_{K,\cdot}) R [\Delta, u_\alpha] R \phi(h^1_{K,\cdot}) G^0_K \Big\rangle_{\mathscr{H}} \left(\frac{\pi}{\lambda\alpha^2} \right)^{3/2}. \end{aligned} \quad (5.267)$$

Here the first line is bounded again exponentially in α, whereas in the second line we use $[\Delta, u_\alpha] = 2(\nabla u_\alpha)\nabla + (\Delta u_\alpha)$ and $\|\nabla u_\alpha\|_{L^\infty} + \|\Delta u_\alpha\|_{L^\infty} \le C\alpha^{-1}$, see (5.48). Together with Lemmas 5.3.7 and 5.3.8, this implies $|\mathcal{K}_{111}^{\mathrm{lo},3}| \leq C\alpha^{-6}$. In the last term we employ $T_y - 1 = \int_0^1 \mathrm{d}s T_{sy}(y\nabla)$, $[h^{\mathrm{Pek}}, u_\alpha] = -[\Delta, u_\alpha]$ and $h^{\mathrm{Pek}}R = Q_\psi$ to find

$$\begin{aligned}\mathcal{K}_{111}^{\mathrm{lo},4} &= \alpha^{-2}\int \mathrm{d}y \int_0^1 \mathrm{d}s \left\langle G_K^0 | \phi(h_{K,\cdot}^1) Q_\psi u_\alpha T_{sy}(y\nabla) u_\alpha R \phi(h_{K,\cdot}^1) G_K^0 \right\rangle_{\mathscr{H}} e^{-\lambda\alpha^2 y^2} \\ &\quad + \alpha^{-2}\int \mathrm{d}y \int_0^1 \mathrm{d}s \left\langle G_K^0 | \phi(h_{K,\cdot}^1) R [\Delta, u_\alpha] T_{sy}(y\nabla) u_\alpha R \phi(h_{K,\cdot}^1) G_K^0 \right\rangle_{\mathscr{H}} e^{-\lambda\alpha^2 y^2}.\end{aligned} \tag{5.268}$$

In both lines there is an additional factor y, and together with (5.48), we thus obtain

$$\begin{aligned}|\mathcal{K}_{111}^{\mathrm{lo},4}| &\leq C\alpha^{-6}\|\phi(h_{K,\cdot}^1)G_K^0\|_{\mathscr{H}}\,\|\nabla u_\alpha R^{1/2}\|_{\mathrm{op}}\|R^{1/2}\phi(h_{K,\cdot}^1)G_K^0\|_{\mathscr{H}} \\ &\quad + C\alpha^{-6}\|R^{1/2}\phi(h_{K,\cdot}^1)G_K^0\|_{\mathscr{H}}\|R^{1/2}[\Delta, u_\alpha]\|_{\mathrm{op}}\|\nabla u_\alpha R^{1/2}\|_{\mathrm{op}}\|R\phi(h_{K,\cdot}^1)G_K^0\|_{\mathscr{H}} \\ &\leq C(\alpha^{-6}\sqrt{K} + \alpha^{-7}).\end{aligned} \tag{5.269}$$

This proves (5.265).

To estimate $\mathcal{K}_{112}$ and $\mathcal{K}_{111}^{\mathrm{err}}$, we make use of

$$\left|\left\langle G_K^0 | L_{3,y} G_K^0 \right\rangle_{\mathscr{H}}\right| \leq C f_{3,\alpha}(y) \tag{5.270a}$$

$$|\ell_3(y)| \leq C f_{3,\alpha}(y)(y^4 + \alpha^{-4}) \tag{5.270b}$$

where

$$f_{3,\alpha}(y) = \|u_\alpha T_y u_\alpha\|_{\mathrm{op}} + \|(\nabla u_\alpha) T_y u_\alpha\|_{\mathrm{op}} + \|u_\alpha T_y (\nabla u_\alpha)\|_{\mathrm{op}} + \|(\nabla u_\alpha) T_y (\nabla u_\alpha)\|_{\mathrm{op}}. \tag{5.271}$$

Recalling that by definition $|\nabla^k u_\alpha(y)| \leq 1(|y| \leq 2\alpha)$ for $k = 0, 1$, it follows that $f_{3,\alpha}(y) \leq 41(|y| \leq 4\alpha)$ and thus

$$\|f_{3,\alpha}\|_{L^\infty} \leq 4 \quad \text{and} \quad \||\cdot|^n f_{3,\alpha}\|_{L^1} \leq C_n \alpha^{3+n} \quad \text{for all } n \in \mathbb{N}_0. \tag{5.272}$$

In order to verify (5.270a), use $h^{\mathrm{Pek}} = -\Delta + V^\varphi - \lambda^{\mathrm{Pek}}$ to write

$$\begin{aligned}R^{\frac12} u_\alpha T_y h^{\mathrm{Pek}} u_\alpha R^{\frac12} &= R^{\frac12} u_\alpha \Big((-i\nabla)T_y(-i\nabla) + T_y(V^\varphi - \lambda^{\mathrm{Pek}})\Big) u_\alpha R^{\frac12} \\ &= -R^{\frac12}(-i\nabla u_\alpha)T_y(-i\nabla u_\alpha)R^{\frac12} + R^{\frac12}(-i\nabla)u_\alpha T_y u_\alpha(-i\nabla)R^{\frac12} \\ &\quad + R^{\frac12}(-i\nabla)u_\alpha T_y(-i\nabla u_\alpha)R^{\frac12} - R^{\frac12}(-i\nabla u_\alpha)T_y u_\alpha(-i\nabla)R^{\frac12} \\ &\quad + R^{\frac12} u_\alpha T_y u_\alpha (V^\varphi - \lambda^{\mathrm{Pek}})R^{\frac12}.\end{aligned} \tag{5.273}$$

Since $\|V^\varphi R^{1/2}\|_{\mathrm{op}} \leq C(\|R\|_{\mathrm{op}} + \|\nabla R^{1/2}\|_{\mathrm{op}}) \leq C$, see Lemma 5.3.7, it thus follows that

$$\|R^{\frac12} u_\alpha T_y h^{\mathrm{Pek}} u_\alpha R^{\frac12}\|_{\mathrm{op}} \leq C f_{3,\alpha}(y). \tag{5.274}$$

With this at hand one applies Lemma 5.3.8 to conclude the bound stated in (5.270a). For $\ell_3(y)$ we proceed similarly as in (5.238), that is

$$\begin{aligned}|\ell_3(y)| &\leq \|R^{1/2} u_\alpha h^{\mathrm{Pek}} T_y u_\alpha R^{1/2}\|_{\mathrm{op}} \|R^{1/2}\langle \widetilde{w}_{P,y}^1 | \underline{h_{K,\cdot}^1}\rangle_{L^2}\psi\|_{L^2}^2 \\ &\leq f_{3,\alpha}(y)\,\|\widetilde{w}_{P,y}^1\|_{L^2}^2 \int \mathrm{d}z \|P_\psi \underline{h_{K,\cdot}^1}(z) R^{1/2}\|_{\mathrm{op}}^2 \leq C f_{3,\alpha}(y)(y^4 + \alpha^{-4}).\end{aligned} \tag{5.275}$$

Now we can apply Lemma 5.3.4 and (5.272) to estimate

$$|\mathcal{K}_{111}^{\mathrm{err}}| \leq \frac{C}{\alpha^2}\int \mathrm{d}y\, f_{3,\alpha}(y)\,|n_{0,1}(y) - e^{-\lambda\alpha^2 y^2}| \leq C\alpha^{-6}, \tag{5.276}$$

and further invoke Corollary 5.3.5 to obtain

$$|\mathcal{K}_{112}| \leq \int \mathrm{d}y\, f_{3,\alpha}(y)(|y|^4 + \alpha^{-4})n_{0,1}(y) \leq C\alpha^{-7}. \tag{5.277}$$

Next we come to $\mathcal{K}_{12}$ which we rewrite with the aid of (5.119) and (5.132) as

$$\mathcal{K}_{12} = \frac{1}{\alpha^2}\int \mathrm{d}y \left\langle R_{5,y}\psi \otimes \left(\Upsilon_K^< + \Upsilon_K^>\right)|W(\alpha w_{P,y})G_K^0\right\rangle_{\mathscr{H}} = \mathcal{K}_{12}^< + \mathcal{K}_{12}^> \tag{5.278}$$

with the operator $R_{5,y} = R_{5,y}^1 + R_{5,y}^2$ and

$$R_{5,y}^1 = P_\psi \phi(h_{K,\cdot}^1) R u_\alpha (e^{-A_{P,y}} - 1) T_{-y} h^{\mathrm{Pek}} u_\alpha R \phi(h_{K,\cdot}^1) P_\psi \tag{5.279a}$$

$$R_{5,y}^2 = 2\alpha P_\psi \left\langle h_{K,\cdot} | \operatorname{Re}(w_{P,y}^1)\right\rangle_{L^2} R u_\alpha (e^{-A_{P,y}} - 1) T_{-y} h^{\mathrm{Pek}} u_\alpha R \phi(h_{K,\cdot}^1) P_\psi. \tag{5.279b}$$

Utilizing Lemma 5.3.8 and (5.84a), we have

$$\|R_{5,y}^1 \Psi\|_{\mathscr{H}} \leq C\|(e^{-A_{P,y}} - 1)(\mathbb{N}+1)^{1/2} R^{\frac{1}{2}} u_\alpha T_{-y} h^{\mathrm{Pek}} u_\alpha R \phi(h_{K,\cdot}^1) P_\psi \Psi\|_{\mathscr{H}}, \tag{5.280}$$

and following the same steps as in (5.136),

$$\|R_{5,y}^2 \Psi\| \leq C\alpha(y^2 + \alpha^{-2})\|(e^{-A_{P,y}} - 1) R^{\frac{1}{2}} u_\alpha T_{-y} h^{\mathrm{Pek}} u_\alpha R \phi(h_{K,\cdot}^1) P_\psi \Psi\|_{\mathscr{H}}. \tag{5.281}$$

After using unitarity of $e^{-A_{P,y}}$ and (5.272), we can apply Lemma 5.3.8 another time to obtain

$$\|R_{5,y}\psi \otimes \Upsilon_K^>\|_{\mathscr{H}} \leq C f_{3,\alpha}(-y)(1 + \alpha y^2)\|(\mathbb{N}+1)\Upsilon_K^>\|_{\mathcal{F}}. \tag{5.282}$$

Thus we can estimate the tail with the aid of Corollary 5.3.12 and (5.272),

$$|\mathcal{K}_{12}^>| \leq \frac{C}{\alpha^2}\|(\mathbb{N}+1)\Upsilon_K^>\|_{\mathcal{F}} \int \mathrm{d}y\, f_{3,\alpha}(-y)(1 + \alpha y^2) \leq C_\delta\, \alpha^{-6}. \tag{5.283}$$

Then we use (5.115), (5.126) and apply Lemma 5.3.13 to get

$$\begin{aligned} |\mathcal{K}_{12}^<| &\leq \frac{1}{\alpha^2}\int \mathrm{d}y\, \|\mathbb{U}_K e^{\kappa\mathbb{N}} R_{5,y}\psi \otimes \Upsilon_K^<\|_{\mathscr{H}} \|e^{-\kappa\mathbb{N}} W(\alpha \widetilde{w}_{P,y})\Omega\|_{\mathcal{F}} \\ &\leq \frac{\sqrt{2}}{\alpha^2}\int \mathrm{d}y\, \|R_{5,y}\psi \otimes \Upsilon_K^<\|_{\mathscr{H}}\, n_{\delta,\eta}(y). \end{aligned} \tag{5.284}$$

To bound the norm in the integral, we proceed in close analogy to the steps following (5.247). We abbreviate again $G_K^{0<} = \psi \otimes \Upsilon_K^<$ and start from (5.280) and (5.281). With (5.272), the functional calculus and $A_{P,y} = iP_f y + i g_P(y)$, one finds

$$\begin{aligned} \|R_{5,y} G_K^{0<}\|_{\mathscr{H}} &\leq C\Big(f_{3,\alpha}(-y)\|(e^{-A_{P,y}} - 1)(\mathbb{N}+1)^{1/2} R^{\frac{1}{2}}\phi(h_{K,\cdot}^1) G_K^{0<}\|_{\mathscr{H}} \\ &\qquad + \alpha(y^2 + \alpha^{-2}) f_{3,\alpha}(-y)\|(e^{-A_{P,y}} - 1) R^{\frac{1}{2}}\phi(h_{K,\cdot}^1) G_K^{0<}\|_{\mathscr{H}}\Big) \\ &\leq C\Big(f_{3,\alpha}(-y)\Big(\|(yP_f)(\mathbb{N}+1)^{1/2} R^{\frac{1}{2}}\phi(h_{K,\cdot}^1) G_K^{0<}\|_{\mathscr{H}} && (5.285a) \\ &\qquad + f_{3,\alpha}(-y)|g_P(y)|(\mathbb{N}+1)^{1/2} R^{\frac{1}{2}}\phi(h_{K,\cdot}^1) G_K^{0<}\|_{\mathscr{H}} && (5.285b) \\ &\qquad + f_{3,\alpha}(-y)(\alpha y^2 + \alpha^{-1})\|(P_f y) R^{\frac{1}{2}}\phi(h_{K,\cdot}^1) G_K^{0<}\|_{\mathscr{H}} && (5.285c) \\ &\qquad + f_{3,\alpha}(-y)(\alpha y^2 + \alpha^{-1})|g_P(y)|\|R^{\frac{1}{2}}\phi(h_{K,\cdot}^1) G_K^{0<}\|_{\mathscr{H}}\Big). && (5.285d) \end{aligned}$$

In the second and fourth line, we use $|g_P(y)| \le C\alpha|y|^3$ and Lemma 5.3.8,

$$\begin{aligned}(5.285\text{b}) + (5.285\text{d}) \;&\le\; C(\alpha^2|y|^5 + \alpha|y|^3) f_{3,\alpha}(-y) \|(\mathbb{N}+1)\Upsilon_K^<\|_{\mathcal{F}} \\ &\le\; C(\alpha^2|y|^5 + \alpha|y|^3) f_{3,\alpha}(-y). \end{aligned} \tag{5.286}$$

In the first and third line, we employ the commutator $[iP_f y, \phi(f)] = \pi(y\nabla f)$ to get

$$\begin{aligned}(5.285\text{a}) + (5.285\text{c}) \;\le\; C\Big(& f_{3,\alpha}(-y)\|(\mathbb{N}+1)^{1/2} R^{\frac{1}{2}} \phi(h^1_{K,\cdot})(yP_f) G_K^{0<}\|_{\mathscr{H}} && (5.287\text{a})\\ &+ f_{3,\alpha}(-y)\|(\mathbb{N}+1)^{1/2} R^{\frac{1}{2}} \pi(y\nabla h^1_{K,\cdot}) G_K^{0<}\|_{\mathscr{H}} && (5.287\text{b})\\ &+ f_{3,\alpha}(-y)(\alpha y^2 + \alpha^{-1})\| R^{\frac{1}{2}} \phi(h^1_{K,\cdot})(yP_f) G_K^{0<}\|_{\mathscr{H}} && (5.287\text{c})\\ &+ f_{3,\alpha}(-y)(\alpha y^2 + \alpha^{-1})\| R^{\frac{1}{2}} \pi(y\nabla h^1_{K,\cdot}) G_K^{0<}\|_{\mathscr{H}}\Big). && (5.287\text{d})\end{aligned}$$

After another application of Lemma 5.3.8, we can use (5.119) and then Lemma 5.3.14 for the terms involving P_f,

$$\begin{aligned}(5.287\text{a}) + (5.287\text{c}) \;&\le\; C f_{3,\alpha}(-y)(\alpha y^2 + 1)\,|y|\,\|(\mathbb{N}+1) P_f \Upsilon_K^<\|_{\mathcal{F}} \\ &\le\; C f_{3,\alpha}(-y)(\alpha|y|^3 + |y|)\alpha^\delta \sqrt{K}, . \end{aligned} \tag{5.288}$$

while in the other two lines, we use $(\nabla h_K). = -[\nabla, h_{K,\cdot}]$, to obtain

$$\begin{aligned}(5.287\text{b}) + (5.287\text{d}) \;&\le\; C f_{3,\alpha}(-y)\,|y|\,(\alpha y^2 + 1)\|h_{K,0}\|_{L^2} \|(\mathbb{N}+1)\Upsilon_K^<\|_{\mathcal{F}} \\ &\le\; C f_{3,\alpha}(-y)(\alpha|y|^3 + |y|)\sqrt{K}. \end{aligned} \tag{5.289}$$

Collecting all estimates we have thus shown that

$$\|R_{5,y}\psi \otimes \Upsilon_K^<\|_{\mathscr{H}} \;\le\; C f_{3,\alpha}(-y)\alpha^\delta \Big(\alpha^2|y|^5 + \sqrt{K}(\alpha|y|^3 + |y|)\Big). \tag{5.290}$$

Using this bound in (5.284) we can invoke Corollary 5.3.5 together with (5.272) in order to obtain

$$|\mathcal{K}_{12}^<| \le C\sqrt{K}\alpha^{-6+5\delta}. \tag{5.291}$$

Term $\mathcal{K}_2$. Using (5.119) and (5.132), one finds

$$\mathcal{K}_2 \;=\; \frac{1}{\alpha^4}\int \mathrm{d}y \left\langle R_{6,y}\psi \otimes \left(\Upsilon_K^< + \Upsilon_K^>\right) | W(\alpha w_{P,y}) G_K^0 \right\rangle_{\mathscr{H}} \;=\; \mathcal{K}_2^< + \mathcal{K}_2^> \tag{5.292}$$

with the operator $R_{6,y} = R^1_{6,y} + R^2_{6,y}$ and

$$R^1_{6,y} \;=\; P_\psi \phi(h^1_{K,\cdot}) R u_\alpha \mathbb{N} T_{-y} e^{-A_{P,y}} u_\alpha R \phi(h^1_{K,\cdot}) P_\psi \tag{5.293a}$$

$$R^2_{6,y} \;=\; 2\alpha P_\psi \phi(h^1_{K,\cdot}) R u_\alpha \mathbb{N} T_{-y} e^{-A_{P,y}} u_\alpha R \langle \mathrm{Re}(w^1_{P,y}) | h_{K,\cdot}\rangle_{L^2} P_\psi. \tag{5.293b}$$

With Lemma 5.3.8 and (5.84a) it is not difficult to verify

$$\|R_{6,y}\Psi\|_{\mathscr{H}} \;\le\; C\|u_\alpha T_{-y} u_\alpha\|_{\mathrm{op}}(1 + \alpha y^2)\|(\mathbb{N}+1)^2\Psi\|_{\mathscr{H}}, \tag{5.294}$$

and since $\|u_\alpha T_{-y} u_\alpha\|_{\mathrm{op}} \le 1(|y| \le 4\alpha)$, we can use Corollary 5.3.12 to estimate the part with the tail by

$$|\mathcal{K}_2^>| \;\le\; \frac{C}{\alpha^4}\|(\mathbb{N}+1)^2\Upsilon_K^>\|_{\mathcal{F}} \int \mathrm{d}y\, 1(|y| \le 4\alpha)(1 + \alpha y^2) \;\le\; C_\delta\, \alpha^{-8}. \tag{5.295}$$

To treat $\mathcal{K}_2^<$ we proceed as in (5.284), that is

$$|\mathcal{K}_2^<| \leq \frac{\sqrt{2}}{\alpha^4} \int \mathrm{d}y \, \|R_{6,y}\psi \otimes \Upsilon_K^<\|_{\mathscr{H}} \, n_{\delta,\eta}(y) \leq \frac{C}{\alpha^4} \int \mathrm{d}y \, 1(|y| \leq \alpha)(1+\alpha y^2) \, n_{\delta,\eta}(y). \quad (5.296)$$

It now follows from Corollary 5.3.5 that

$$|\mathcal{K}_2^<| \leq C\alpha^{-7}. \quad (5.297)$$

Term $\mathcal{K}_3$. This term is similarly estimated as the previous one. With the aid of (5.119) and (5.132), we have

$$\mathcal{K}_3 \; = \; \frac{1}{\alpha^3} \int \mathrm{d}y \left\langle R_{7,y}\psi \otimes \left(\Upsilon_K^< + \Upsilon_K^>\right) | W(\alpha w_{P,y}) G_K^0 \right\rangle_{\mathscr{H}} \; = \; \mathcal{K}_3^< + \mathcal{K}_3^> \quad (5.298)$$

with the operator $R_{7,y} = R_{7,y}^1 + R_{7,y}^2$ and

$$R_{7,y}^1 \; = \; P_\psi \phi(h_{K,\cdot}^1) R u_\alpha e^{-A_{P,y}} T_{-y} \phi(h_\cdot + \varphi_P) u_\alpha R \phi(h_{K,\cdot}^1) P_\psi \quad (5.299a)$$

$$R_{7,y}^2 \; = \; 2\alpha P_\psi \langle \mathrm{Re}(w_{P,y}^1) | h_{K,\cdot} \rangle_{L^2} R u_\alpha e^{-A_{P,y}} T_{-y} \phi(h_\cdot + \varphi_P) u_\alpha R \phi(h_{K,\cdot}^1) P_\psi. \quad (5.299b)$$

Utilizing again Lemma 5.3.8 and (5.84a), one shows that

$$\|R_{7,y}\Psi\|_{\mathscr{H}} \; \leq \; C f_{3,\alpha}(-y)(1+\alpha y^2) \|(\mathbb{N}+1)^{3/2}\Psi\|_{\mathscr{H}} \quad (5.300)$$

with $f_{3,\alpha}$ defined in (5.271). Invoking Corollary 5.3.12 and (5.272) we thus find

$$|\mathcal{K}_3^>| \; \leq \; \frac{C}{\alpha^3} \|(\mathbb{N}+1)^{3/2}\Upsilon_K^>\|_{\mathcal{F}} \int \mathrm{d}y \, f_{3,\alpha}(-y)(1+\alpha y^2) \; \leq \; C_\delta \, \alpha^{-7}. \quad (5.301)$$

Similarly as in (5.284), we also obtain

$$|\mathcal{K}_3^<| \; \leq \; \frac{\sqrt{2}}{\alpha^3} \int \mathrm{d}y \, \|R_{7,y}\psi \otimes \Upsilon_K^<\|_{\mathscr{H}} \, n_{\delta,\eta}(y) \; \leq \; \frac{C}{\alpha^3} \int \mathrm{d}y \, f_{3,\alpha}(-y)(1+\alpha y^2) n_{\delta,\eta}(y). \quad (5.302)$$

By Corollary 5.3.5 and (5.271) it follows that

$$|\mathcal{K}_3^<| \leq C\alpha^{-6+3\delta}. \quad (5.303)$$

This completes the analysis of $\mathcal{K}$. The proof of Proposition 5.3.19 follows from combining (5.264), (5.265), (5.276), (5.277), (5.283), (5.291), (5.295), (5.297), (5.301) and (5.303). □

5.3.9 Concluding the proof of Proposition 5.2.4

Combining Propositions 5.3.16, 5.3.18 and 5.3.19, we arrive at

$$\left| \frac{\mathcal{E} + \mathcal{G} + \mathcal{K}}{\mathcal{N}} - \frac{\inf \sigma(\mathbb{H}_K)}{\alpha^2} + \frac{3}{2\alpha^2} \right| \leq C_\varepsilon \, \alpha^\varepsilon \left(\frac{K^{-1/2}\alpha^{-5} + \sqrt{K}\alpha^{-6}}{\mathcal{N}} \right). \quad (5.304)$$

Now for $K \leq \tilde{c}\alpha$ we know from Proposition 5.3.15 that $\mathcal{N} \geq C\alpha^3$ for some $C > 0$, such that the right side is bounded by $C_\varepsilon \, \alpha^\varepsilon r(K,\alpha)$. It remains to show that one can replace

$\alpha^{-2} \inf \sigma(\mathbb{H}_K)$ by $\alpha^{-2} \inf \sigma(\mathbb{H}_\infty)$ at the cost of an additional error. To this end, recall that $\inf \sigma(\mathbb{H}_K) = \langle \Upsilon_K | \mathbb{H}_K \Upsilon_K \rangle_\mathcal{F}$ and use the variational principle to find

$$\Big\langle \Upsilon_K | (\mathbb{H}_K - \mathbb{H}_\infty) \Upsilon_K \Big\rangle_\mathcal{F} \leq \inf \sigma(\mathbb{H}_K) - \inf \sigma(\mathbb{H}_\infty) \leq \Big\langle \Upsilon_\infty | (\mathbb{H}_K - \mathbb{H}_\infty) \Upsilon_\infty \Big\rangle_\mathcal{F}. \quad (5.305)$$

Writing

$$\mathbb{H}_K - \mathbb{H}_\infty = \Big\langle \psi | \phi(h^1_{K,\cdot} - h^1_\cdot) R \phi(h^1_{K,\cdot}) \psi \Big\rangle_{L^2} - \Big\langle \psi | \phi(h^1_\cdot) R \phi(h^1_\cdot - h^1_{K,\cdot}) \psi \Big\rangle_{L^2}, \quad (5.306)$$

and using Lemma 5.3.8, we can infer that for any $\Psi \in \mathcal{F}$

$$\Big| \Big\langle \Psi | (\mathbb{H}_K - \mathbb{H}_\infty) \Psi \Big\rangle_\mathcal{F} \Big| \leq C K^{-1/2} \Big\langle \Psi | (\mathbb{N}_1 + 1) \Psi \Big\rangle_\mathcal{F}. \quad (5.307)$$

By Corollary 5.3.12 we know that $\Big\langle \Upsilon_K | (\mathbb{N}_1 + 1) \Upsilon_K \Big\rangle_\mathcal{F} \leq C$ for all $K \in (K_0, \infty]$ with K_0 large enough, and thus $|\inf \sigma(\mathbb{H}_K) - \inf \sigma(\mathbb{H}_\infty)| \leq C K^{-1/2}$. In view of (5.304) and Lemma 5.3.1 this completes the proof of Proposition 5.2.4.

5.4 Remaining Proofs

Proof of Lemma 5.1.1. The form of the kernel is readily found using second order perturbation theory (we omit the details). (i) The lower bound $H^{\mathrm{Pek}} \geq 0$ follows from (5.19) whereas $H^{\mathrm{Pek}} \leq 1$ is a consequence of

$$\Big\langle v | (1 - H^{\mathrm{Pek}}) v \Big\rangle_{L^2} = 4 \Big\| \int \mathrm{d}y \, v(y) R^{1/2} h_\cdot(y) \psi \Big\|^2_{L^2}. \quad (5.308)$$

(ii) That Span$\{\partial_i \varphi : i = 1, 2, 3\} \subseteq$ KerH^{Pek} follows from translation invariance of the energy functional $\mathcal{F}$. To show equality we argue that there is a $\tau > 0$ such that $\langle v | H^{\mathrm{Pek}} v \rangle_{L^2} \geq \tau \|v\|^2_{L^2}$ for all $v \in L^2(\mathbb{R}^3)$ with $\langle v | \nabla \varphi \rangle_{L^2} = 0$ (note that this also implies (iii)). For that purpose we quote [61, Lemma 2.7] stating that there exists a constant $\tau > 0$ such that

$$\mathcal{F}(v) - \mathcal{F}(\varphi) \geq \tau \inf_{y \in \mathbb{R}^3} \|v - \varphi(\cdot - y)\|^2_{L^2} \quad (5.309)$$

for all $v \in L^2(\mathbb{R}^3)$. (a key ingredient in the proof of this quadratic lower bound are the results about the Hessian of the Pekar energy functional (5.12) that were obtained in [80]; see [61] for a detailed derivation). Combined with (5.19) this implies

$$\langle v | H^{\mathrm{Pek}} v \rangle_{L^2} \geq \tau \lim_{\varepsilon \to 0} \inf_{y \in \mathbb{R}^3} f_v(y, \varepsilon), \quad (5.310a)$$

$$f_v(y, \varepsilon) = \|v\|^2_{L^2} + \varepsilon^{-2} \|\varphi - \varphi(\cdot - y)\|^2_{L^2} + 2\varepsilon^{-1} \operatorname{Re} \langle v | \varphi - \varphi(\cdot - y) \rangle_{L^2}. \quad (5.310b)$$

Given any v satisfying $\langle v | \nabla \varphi \rangle_{L^2} = 0$, we choose $y^*(\varepsilon)$ such that $f_v(y^*(\varepsilon), \varepsilon)$ is minimal. Furthermore, note that for every zero sequence $(\varepsilon_n)_{n \in \mathbb{N}}$ such that

$$\lim_{n \to \infty} \|\varphi(\cdot - y^*(\varepsilon_n)) - \varphi\|_{L^2} > 0, \quad (5.311)$$

it follows that $\lim_{n \to \infty} f_v(y^*(\varepsilon_n), \varepsilon_n) = \infty$, and hence we can conclude that $|y^*(\varepsilon)| \to 0$ as $\varepsilon \to 0$. To proceed, let $\eta(\varepsilon) := \varphi - \varphi(\cdot - y^*(\varepsilon))$ and assume $|y^*(\varepsilon)| > 0$ (for if $y^*(\varepsilon) = 0$ it follows directly that $f_v(y^*(\varepsilon), \varepsilon) = \|v\|^2_{L^2}$). With this we can estimate

$$\begin{aligned} f_v(y^*(\varepsilon), \varepsilon) &\geq \|v\|^2_{L^2} + \varepsilon^{-2} \|\eta(\varepsilon)\|^2_{L^2} - 2\varepsilon^{-1} |\langle v | \eta(\varepsilon) \rangle_{L^2}| \\ &\geq \|v\|^2_{L^2} - |\langle v | \frac{\eta(\varepsilon)}{\|\eta(\varepsilon)\|_{L^2}} \rangle_{L^2}|^2. \end{aligned} \quad (5.312)$$

To bound the right side, write

$$\eta(\varepsilon)(z) = \int_0^1 \mathrm{d}s \, (y^*(\varepsilon)\nabla)\varphi(z - sy^*(\varepsilon)) \tag{5.313}$$

and use, by dominated convergence, that

$$\frac{\| \int_0^1 \mathrm{d}s \, (y\nabla)\varphi(\cdot - sy) - (y\nabla)\varphi\|_{L^2}}{\| \int_0^1 \mathrm{d}s \, (y\nabla)\varphi(\cdot - sy)\|_{L^2}} \to 0 \quad \text{as} \quad |y| \to 0. \tag{5.314}$$

Combining the last statement with $|y^*(\varepsilon)| \to 0$ as $\varepsilon \to 0$ and $\langle v|\nabla\varphi\rangle_{L^2} = 0$ we conclude that

$$\lim_{\varepsilon\to 0} f_v(y^*(\varepsilon), \varepsilon) \geq \|v\|_{L^2}^2. \tag{5.315}$$

This completes the proof of items (ii) and (iii). Property (iv) follows from $H^{\mathrm{Pek}} \leq (H^{\mathrm{Pek}})^{1/2}$ and $\mathsf{Tr}_{L^2}(1 - H^{\mathrm{Pek}}) < \infty$, see Lemma 5.2.2 for $K = \infty$. □

Proof of Lemma 5.2.2. (i) The bound $H_K^{\mathrm{Pek}} \restriction \mathsf{Ran}(\Pi_1) \leq 1$ follows analogously to (5.308) and $H_K^{\mathrm{Pek}} \restriction \mathsf{Ran}(\Pi_0) = 0$ holds by definition. The lower bound on $\mathsf{Ran}(\Pi_1)$ is a consequence of $(H^{\mathrm{Pek}} - \tau) \restriction \mathsf{Ran}(\Pi_1) \geq 0$ for some $\tau > 0$, see Lemma 5.1.1, in combination with

$$\pm(H^{\mathrm{Pek}} - H_K^{\mathrm{Pek}}) \ \leq \ CK^{-1/2}. \tag{5.316}$$

To verify the latter, let $v \in \mathsf{Ran}(\Pi_1)$, $\Pi_v = |v\rangle\langle v|$ and write

$$\begin{aligned}\Big\langle v|(H_K^{\mathrm{Pek}} - H^{\mathrm{Pek}})v\Big\rangle_{L^2} \ =\ & 4\int \mathrm{d}y \ \mathrm{Re}\Big\langle \psi|\Big(h_{K,\cdot}(y) - h_{\cdot})(y)\Big)R(\Pi_v h_{K,\cdot})(y)\psi\Big\rangle_{L^2} \\ & + 4\int \mathrm{d}y \ \mathrm{Re}\Big\langle \psi|(\Pi_v h_{\cdot})(y)R\Big(h_{K,\cdot}(y) - h_{\cdot}(y)\Big)\psi\Big\rangle_{L^2}.\end{aligned} \tag{5.317}$$

With Cauchy–Schwarz it follows that

$$\begin{aligned}\Big|\Big\langle v|(H_K^{\mathrm{Pek}} - H^{\mathrm{Pek}})v\Big\rangle_{L^2}\Big| \leq\ & 4K^{1/2}\int \mathrm{d}y \, \|R^{1/2}(h_{K,\cdot}(y) - h_{\cdot}(y))P_\psi\|_{\mathrm{op}}^2 \\ & + 4K^{-1/2}\int \mathrm{d}y \, \Big(\|R^{1/2}(\Pi_v h_{K,\cdot})(y)P_\psi\|_{\mathrm{op}}^2 + \|R^{1/2}(\Pi_v h_{\cdot})(y)P_\psi\|_{\mathrm{op}}^2\Big),\end{aligned} \tag{5.318}$$

and from Corollary 5.3.9, we obtain

$$\Big|\Big\langle v|(H_K^{\mathrm{Pek}} - H^{\mathrm{Pek}})v\Big\rangle_{L^2}\Big| \leq CK^{-1/2}. \tag{5.319}$$

(ii) On $\mathsf{Ran}(\Pi_0)$ the inequality holds trivially, whereas on $\mathsf{Ran}(\Pi_1)$, it follows from $\Theta_K \leq 1$, $B_K^2 \leq \frac{1}{4}(\Theta_K^{-2} - 1)$, $\Theta_K^{-2} = (1 - (1 - H_K^{\mathrm{Pek}}))^{-1/2}$ and the elementary inequality $(1 - x)^{-1/2} \leq 1 + \beta^{-3/2}x$ for all $x \in (0, 1 - \beta)$.

(iii) Here we use $\mathsf{Tr}_{\mathsf{Ran}(\Pi_0)}(1 - H_K^{\mathrm{Pek}}) = 3$, write

$$\mathsf{Tr}_{\mathsf{Ran}(\Pi_1)}(1 - H_K^{\mathrm{Pek}}) = \int \mathrm{d}y \, \Big\langle \psi|h_{K,\cdot}^1(y)Rh_{K,\cdot}^1(y)\psi\Big\rangle_{L^2} = \int \mathrm{d}y \, \|R^{1/2}h_{K,\cdot}^1(y)P_\psi\|_{\mathrm{op}}^2 \tag{5.320}$$

and apply Corollary 5.3.9.

(iv) Since $1 - H_K^{\mathrm{Pek}} = \Pi_0 + \Pi_1(1 - H_K^{\mathrm{Pek}})\Pi_1 = \Pi_0 + 4T_K$, cf. (5.35a) and (5.35b), we can write

$$\mathsf{Tr}_{L^2}((-i\nabla)(1 - H_K^{\mathrm{Pek}})(-i\nabla)) = \mathsf{Tr}_{L^2}\Big(\nabla\Pi_0\nabla\Big) + 4\mathsf{Tr}_{L^2}\Big(\nabla T_K\nabla\Big). \tag{5.321}$$

Using the explicit form of Π_0, one shows that the first term is given by

$$\mathrm{Tr}_{L^2}\Big(\nabla\Pi_0\nabla\Big) = \frac{3}{\|\nabla\varphi\|_{L^2}^2}\sum_{j=1}^{3}\mathrm{Tr}_{L^2}\Big(\nabla|\nabla_j\varphi\rangle\langle\nabla_j\varphi|\nabla\Big) \le 3\frac{\|\Delta\varphi\|_{L^2}^2}{\|\nabla\varphi\|_{L^2}^2}, \tag{5.322}$$

which is finite since $\Delta\varphi \in L^2$. For the second term it follows from a short computation that

$$\mathrm{Tr}_{L^2}\Big(\nabla T_K\nabla\Big) \;=\; \int \mathrm{d}y\, \Big\langle\psi|[\nabla, h^1_{K,\cdot}(y)]R[\nabla, h^1_{K,\cdot}(y)]|\psi\Big\rangle_{L^2}. \tag{5.323}$$

Using the Cauchy–Schwarz inequality and $\|\nabla\psi\|_{L^2}+\|R^{1/2}\|_{\mathrm{op}}+\|R^{1/2}\nabla\|_{\mathrm{op}}<\infty$, see Lemmas 5.3.6 and 5.3.7, we can estimate the last expression by

$$\begin{aligned}\int \mathrm{d}y\,\|R^{1/2}[\nabla, h^1_{K,\cdot}(y)]\psi\|_{L^2}^2 \;&\le\; C\int \mathrm{d}y\,\Big(\|h^1_{K,\cdot}(y)\psi\|_{L^2}^2 + \|h^1_{K,\cdot}(y)\nabla\psi\|_{L^2}^2\Big)\\ &\le\; C\int \mathrm{d}y\,|h^1_{K,0}(y)|^2 \;\le\; C\|h_{K,0}\|_{L^2}^2 \;=\; CK.\end{aligned} \tag{5.324}$$

This completes the proof of the lemma. □

Proof of Lemma 5.2.3. We recall that $H_K^{\mathrm{Pek}} \restriction \mathrm{Ran}(\Pi_0) = 0$ and $T_K = \frac{1}{4}(H_K^{\mathrm{Pek}} - \Pi_1)$, and set $S_K = \frac{1}{2}(\Pi_1 + H_K^{\mathrm{Pek}})$. For $(u_n)_{n\in\mathbb{N}}$ an orthonormal basis of $\mathrm{Ran}(\Pi_1)$, we further set $a_n = a(u_n)$ and use this to write the Bogoliubov Hamiltonian as

$$\mathbb{H}_K \;=\; \sum_{n,m=1}^{\infty}\bigg(\Big\langle u_n|S_K u_m\Big\rangle_{L^2} a_n^\dagger a_m + \Big(\Big\langle u_n|T_K\overline{u_m}\Big\rangle_{L^2} a_n^\dagger a_m^\dagger + \mathrm{h.c.}\Big)\bigg) + \mathrm{Tr}_{L^2}(T_K). \tag{5.325}$$

Applying the transformation (5.39), a straightforward computation leads to

$$\begin{aligned}\mathbb{U}_K\mathbb{H}_K\mathbb{U}_K^\dagger \;=\; \sum_{n,m=1}^{\infty}&\bigg(\Big\langle u_n|(A_KS_KA_K + B_KS_KB_K + 4A_KT_KB_K)u_m\Big\rangle_{L^2} a_n^\dagger a_m\\ &+\Big(\Big\langle u_n|(A_KS_KB_K + A_KT_KA_K + B_KT_KB_K)\overline{u_m}\Big\rangle_{L^2} a_n^\dagger a_m^\dagger + \mathrm{h.c.}\Big)\bigg)\\ &+ \mathrm{Tr}_{\mathrm{Ran}(\Pi_1)}\Big(T_K + B_KS_KB_K + 2A_KT_KB_K\Big).\end{aligned} \tag{5.326}$$

The statement of the lemma now follows from

$$\Pi_1(A_KS_KA_K + B_KS_KB_K + 4A_KT_KB_K)\Pi_1 \;=\; \sqrt{H_K^{\mathrm{Pek}}} \tag{5.327a}$$

$$\Pi_1(A_KS_KB_K + A_KT_KA_K + B_KT_KB_K)\Pi_1 \;=\; 0 \tag{5.327b}$$

$$\Pi_1(T_K + B_KS_KB_K + 2A_KT_KB_K)\Pi_1 \;=\; \frac{1}{2}\Big(\sqrt{H_K^{\mathrm{Pek}}} - \Pi_1\Big). \tag{5.327c}$$

□

Proof of Lemma 5.3.3. To bound $\|w^1_{P,y}\|_{L^2}^2$ we expand

$$\begin{aligned}w^1_{P,y} \;=\; \Pi_1(1-e^{-y\nabla})(\varphi + i\xi_P) \;=\; &\int_0^1 \mathrm{d}s_1\int_0^{s_1}\mathrm{d}s_2\,\Pi_1 e^{-s_2y\nabla}(y\nabla)^2\varphi\\ &+\frac{i}{\alpha^2M^{\mathrm{LP}}}\int_0^1 \mathrm{d}s\,\Pi_1 e^{-sy\nabla}(y\nabla)(P\nabla)\varphi,\end{aligned} \tag{5.328}$$

where we used $\Pi_1(y\nabla)\varphi = 0$. Thus, since $\Delta\varphi \in L^2$, we easily arrive at

$$\|w^1_{P,y}\|^2_{L^2} \le C\Big(y^4 + \alpha^{-4}y^2P^2\Big) \tag{5.329}$$

for some constant $C > 0$, and with $|P| \le \alpha c$ we obtain the stated estimated. The bound for $\|\widetilde{w}^1_{P,y}\|^2_{L^2}$ follows from

$$\|\widetilde{w}^1_{P,y}\|^2_{L^2} = \|\Theta_K \operatorname{Re}(w^1_{P,y})\|^2_{L^2} + \|\Theta_K^{-1} \operatorname{Im}(w^1_{P,y})\|^2_{L^2} \le C\|w^1_{P,y}\|^2_{L^2}, \tag{5.330}$$

where we used that Θ_K is real-valued and satisfies

$$0 < \beta \le \Theta_K^2 \le 1 \tag{5.331}$$

when restricted to Ran(Π_1); see Lemma 5.2.2. To bound $\|w^0_{P,y}\|^2_{L^2}$ we use

$$\|w^0_{P,y}\|^2_{L^2} = \|w^0_{0,y}\|^2_{L^2} + \|\Pi_0(1 - e^{-y\nabla})\xi_P\|^2_{L^2}, \tag{5.332}$$

since φ, ξ_P and Π_0 are all real-valued. Expanding $1 - e^{-y\nabla}$ as in (5.328), it is easy to conclude that $\|\Pi_0(1 - e^{-y\nabla})\xi_P\|^2_{L^2} \le CP^2y^2\alpha^{-4}$. Using the explicit form of Π_0 and $\langle\nabla\varphi|\varphi\rangle_{L^2} = 0$, we can write

$$\|w^0_{0,y}\|^2_{L^2} = \frac{3}{\|\nabla\varphi\|^2_{L^2}} \sum_{i=1}^3 \Big|\Big\langle \nabla_i\varphi | e^{-y\nabla}\varphi\Big\rangle_{L^2}\Big|^2. \tag{5.333}$$

Using the Fourier representation and rotation invariance, we have

$$\Big|\Big\langle \nabla_i\varphi | e^{-y\nabla}\varphi\Big\rangle_{L^2}\Big| = \left|\int p_i |\hat{\varphi}(p)|^2 \sin(py)\, \mathsf{d}y\right|. \tag{5.334}$$

By the elementary inequality $|\sin z - z| \le Cz^3$, the formula $\|(y\nabla)\varphi\|^2_{L^2} = 2\lambda y^2$ and the finiteness of $\|\Delta\varphi\|_{L^2}$, we conclude that

$$\Big|\|w^0_{P,y}\|^2_{L^2} - 2\lambda y^2\Big| \le C\Big(y^4 + y^6 + \alpha^{-4}y^2P^2\Big). \tag{5.335}$$

To prove the last bound, we use

$$\|\widetilde{w}_{P,y}\|^2_{L^2} = \|w^0_{P,y}\|^2_{L^2} + \|\Theta_K \operatorname{Re}(w^1_{P,y})\|^2_{L^2} + \|\Theta_K^{-1} \operatorname{Im}(w^1_{P,y})\|^2_{L^2}, \tag{5.336}$$

and hence with (5.331),

$$\beta\|w^1_{P,y}\|^2_{L^2} \le \|\widetilde{w}_{P,y}\|^2_{L^2} - \|w^0_{P,y}\|^2_{L^2} \le \beta^{-1}\|w^1_{P,y}\|^2_{L^2}. \tag{5.337}$$

The desired bound now follows from (5.329) and (5.335). □

Proof of Lemma 5.3.4. From Lemma 5.3.3, we have

$$\Big|\|\widetilde{w}_{P,y}\|^2_{L^2} - 2\lambda y^2\Big| \le C(\alpha^{-2}y^2 + y^4 + y^6) \le C\frac{y^2}{\alpha} \quad \text{for all} \quad \frac{|P|}{\alpha} \le c,\ y^2 \le \alpha^{-1}. \tag{5.338}$$

Hence there is a constant $\mu > 0$ such that for all $y^2 \le \alpha^{-1}$ the weight function (5.85) satisfies

$$n_{\delta,\eta}(y) \le \exp(-(\lambda\eta\alpha^{2(1-\delta)} - \mu\alpha^{-2\delta+1})y^2) \tag{5.339a}$$

$$n_{\delta,\eta}(y) \ge \exp(-(\lambda\eta\alpha^{2(1-\delta)} + \mu\alpha^{-2\delta+1})y^2). \tag{5.339b}$$

In the remainder let us abbreviate $f_n(y) = |y|^n g(y)$ and $Z(y) = |n_{\delta,\eta}(y) - e^{-\lambda\eta\alpha^{2(1-\delta)}y^2}|$. We then decompose the integral into

$$\int \mathrm{d}y\, f_n(y)Z(y) \;=\; \int_{B_\alpha} \mathrm{d}y\, f_n(y)Z(y) + \int_{B_\alpha^c} \mathrm{d}y\, f_n(y)Z(y) \tag{5.340}$$

with $B_\alpha = \{y \in \mathbb{R}^3 : y^2 \le \alpha^{-1}\}$. The bounds (5.339a) and (5.339b) imply that

$$|Z(y)| \le e^{-\lambda\eta\alpha^{2(1-\delta)}} \left(e^{\mu\alpha^{-2\delta+1}y^2} - 1\right) \quad \forall y \in B_\alpha \tag{5.341}$$

and thus by $|e^z - 1| \le ze^z$ for $z > 0$, we obtain

$$\int_{B_\alpha} \mathrm{d}y\, f_n(y)Z(y) \;\le\; \mu\alpha^{-2\delta+1} \int \mathrm{d}y\, f_n(y)y^2 e^{-(\eta\lambda-\mu\alpha^{-1})\alpha^{2(1-\delta)}y^2}. \tag{5.342}$$

The last expression is further bounded by

$$\begin{aligned}\int \mathrm{d}y\, f_n(y)y^2 e^{-(\eta\lambda-\mu\alpha^{-1})\alpha^{2(1-\delta)}y^2} \;&\le\; \|g\|_{L^\infty} \int \mathrm{d}y\, |y|^{n+2} e^{-(\eta\lambda-\mu\alpha^{-1})\alpha^{2(1-\delta)}y^2} \\ &=\; \frac{C_n\|g\|_{L^\infty}}{\alpha^{(5+n)(1-\delta)}} \left(\eta\lambda - \mu\alpha^{-1}\right)^{-(n+5)/2}\end{aligned} \tag{5.343}$$

and since the resulting expression is uniformly bounded in $\eta \ge \eta_0$ and α large, we get

$$\int_{B_\alpha} \mathrm{d}y\, f_n(y)Z(y) \;\le\; C_n \frac{\|g\|_{L^\infty}}{\alpha^{(4+n)(1-\delta)+\delta}}. \tag{5.344}$$

To bound the second term in (5.340), we estimate

$$\int_{B_\alpha^c} \mathrm{d}y\, f_n(y)Z(y) \;\le\; \int_{B_\alpha^c} \mathrm{d}y\, f_n(y)n_{\delta,\eta}(y) + e^{-\lambda\eta\alpha^{-2\delta+1}} \int \mathrm{d}y\, f_n(y). \tag{5.345}$$

To see that the first summand is exponentially small as well, we use (5.336), (5.331) and $\mathrm{Re}(w_{P,y}^i) = \Pi_i \,\mathrm{Re}(w_{P,y}) = \Pi_i \,\mathrm{Re}(w_{0,y})$ for $i = 0, 1$,

$$\|\widetilde{w}_{P,y}\|_{L^2}^2 \ge \|\mathrm{Re}(w_{P,y}^0)\|_{L^2}^2 + \beta\|\mathrm{Re}(w_{P,y}^1)\|_{L^2}^2 \ge \beta\|\mathrm{Re}(w_{0,y})\|_{L^2}^2 = \beta\|(1 - e^{-y\nabla})\varphi\|_{L^2}^2, \tag{5.346}$$

and hence

$$n_{\delta,\eta}(y) \;\le\; \exp\Big(- \eta\beta\alpha^{2(1-\delta)}q(y)\Big) \quad \text{with} \quad q(y) \;=\; \frac{1}{2}\|(1 - e^{-y\nabla})\varphi\|_{L^2}^2. \tag{5.347}$$

Since φ is real-valued, we have $\langle\varphi|e^{-y\nabla}|\varphi\rangle_{L^2} = \langle\varphi|e^{y\nabla}|\varphi\rangle_{L^2} = (\varphi * \varphi)(y)$ and thus

$$q(y) = \|\varphi\|_{L^2}^2 - (\varphi * \varphi)(y). \tag{5.348}$$

Recall that, as shown in [83], the electronic Pekar minimizer ψ is radial and non-increasing and hence φ, cf. (5.14), is radial and non-increasing as well, as convolutions of radial non-increasing functions are themselves radial non-increasing functions. Consequently, $q(y)$ is radial and monotone non-decreasing, and thus $q(y) \ge q(y')$ for all $y \in B_\alpha^c$, $y' \in B_\alpha$. On the other hand, by a simple computation, using the regularity of φ, one finds that $q(y) \ge C_0 y^2$ for some $C_0 > 0$ and all $|y|$ small enough, and thus $q(y) \ge C_0\alpha^{-1}$ for all $y \in B_\alpha^c$ and α large. Therefore

$$\begin{aligned}\int_{B_\alpha^c} \mathrm{d}y\, f_n(y)n_{\delta,\eta}(y) \;&\le\; \int_{B_\alpha^c} \mathrm{d}y\, f_n(y)e^{-\eta\beta\alpha^{2(1-\delta)}q(y)} \\ &\le\; e^{-C_0\eta\beta\alpha^{2(1-\delta)-1}} \int \mathrm{d}y\, f_n(y) \;\le\; e^{-d\alpha^{-2\delta+1}} \int \mathrm{d}y\, f_n(y)\end{aligned} \tag{5.349}$$

for some $d > 0$, which completes the proof of the lemma. □

Proof of Lemma 5.3.14. Let $p = -i\nabla$. By a straightforward computation using the transformation property (5.39), we arrive at

$$\mathbb{U}_K P_f \mathbb{U}_K^\dagger \Omega = \sum_n a^\dagger(A_K u_n) a^\dagger(B_K p \overline{u_n})\Omega + \mathrm{Tr}_{L^2}(B_K p B_K)\Omega \tag{5.350}$$

for some orthonormal basis $(u_n)_{n\in\mathbb{N}}$ of $L^2(\mathbb{R}^3)$. That $B_K p B_K$ is trace-class can be seen via

$$\mathrm{Tr}_{L^2}|B_K p B_K| \,\leq\, \|B_K\|_{\mathrm{HS}}\, \|p B_K\|_{\mathrm{HS}} \,\leq\, CK, \tag{5.351}$$

where the second step follows from Lemma 5.2.2, implying $\|B_K\|_{\mathrm{HS}} \leq C$, and

$$\|p B_K\|_{\mathrm{HS}}^2 \,=\, \mathrm{Tr}_{L^2}(p B_K B_K p) \,\leq\, \mathrm{Tr}_{L^2}(p(1 - H_K^{\mathrm{Pek}})p) \,\leq\, CK. \tag{5.352}$$

By rotation invariance $\mathrm{Tr}_{L^2}(B_K p B_K) = 0$. The first term in (5.350), on the other hand, is seen to be a two-particle wave function Φ_K given by

$$\Phi_K(x,y) = \frac{1}{\sqrt{2}} \left(A_K p B_K + B_K p A_K\right)(x,y). \tag{5.353}$$

Thus

$$\left\langle \Upsilon_K | (P_f)^2 \Upsilon_K \right\rangle_{\mathcal{F}} \,=\, \frac{1}{2}\|A_K p B_K + B_K p A_K\|_{\mathrm{HS}}^2 \,\leq\, 2\|A_K\|_{\mathrm{op}}^2 \|p B_K\|_{\mathrm{HS}}^2 \,\leq\, CK, \tag{5.354}$$

where we invoked again (5.352). □

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