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

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June 13, 2019

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.

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

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

acting on $L^2(\Omega) \otimes \mathcal{F}$, where $\mathcal{F}$ is the bosonic Fock space over $L^2(\Omega)$. Here $\Omega \subset \mathbb{R}^3$ is the region occupied by the crystal, $x \in \Omega$ 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 $y \in \Omega$, and $\alpha > 0$ is the coupling constant. In the generic case, one is concerned with $\Omega = \mathbb{R}^3$ and passes to the Fourier space, in which the so-called Fröhlich Hamiltonian arises

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

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 (2), $E(\alpha)$, in the case of the strong coupling limit, i.e. $\alpha \gg 1$. Despite the fact that (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 and then proven by Donsker and Varadhan that $\lim_{\alpha\to\infty} E(\alpha)/\alpha^2 = e_p$, where $e_p \approx -0.109$ is the *Pekar constant*. Then, in 1997 Lieb and Thomas 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 for the case of the confined model, that is, for the case 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.

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 $\Omega = \mathbb{R}^3$.

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 effectively into the creation and annihilation operators. These operators, for $f, g \in L^2$, commute to

$$[a_f, a_g^\dagger] = \frac{(f,g)}{\alpha^2}, \tag{3}$$

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

$$\mathbb{H} = p^2 + \mathbb{N} - (2\pi)^{-3/2}\int_{\mathbb{R}^3} dk \frac{1}{|k|} e^{ikx} a_k + h.c; \tag{4}$$

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 $h(k)$ being an L^2-function of the phonon variables, we denote $h_x = h(k)e^{ikx}$ 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 $v := |k|^{-1}$ and $w_x := v_x\chi_{|k|\geq K}$ 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, and some ideas used in this work were first developed there. Finally, we use the now standard 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.

2 Auxiliary considerations, main result and proof strategy

For $K > 0$, write the Hamiltonian as

$$\mathbb{H} = p^2 + \mathbb{N}_- + \mathbb{N}_+ - V_+ - V_- \tag{5}$$

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 $\mathbb{H}_K := p^2 + N_- - V_-$. Since we are interested in the lower bound, we can drop the $\mathbb{N}_+$ due to its positivity. The paper of Lieb and Thomas (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 2.1. *For any $E > 0, P > 0$ and $K > 0$ and $\delta > 0$ sufficiently small, we have*

$$\inf \mathrm{spec}\mathbb{H}_K - e_p \geqslant c_1\delta - E + c_2\frac{P^2K}{\delta E} + c_3\frac{K^3}{\alpha^2P^3} \tag{6}$$

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 $|e^{ikx} - e^{ik_B x}| \leqslant |(k - k_B)x| \lesssim PE^{-1/2}$ and the obvious positivity of $(\sqrt{\delta} a_k^\dagger - \delta^{-1/2}|k|^{-1}(e^{ikx} - e^{ik_B x}))(hc)$ for any δ, one replaces $\mathbb{H}_K$ with $H'_K = p^2 + \sum_i \int_{B_i} dk (1-\delta) a_k^\dagger a_k + \frac{a_k e^{ik_B x}}{|k|} + hc.)$ at the energy penalty $\sim \frac{P^2 K}{\delta E}$.

3. One introduces $A_{B_i} = \int_{B_i} dk a_k |k|^{-1} / \sqrt{\int_{B_i} dk |k|^{-1}}$ with $A_{B_i}^\dagger A_{B_i} \leqslant \int_{B_i} a_k^\dagger a_k dk$. 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_p, as desired. The $-\frac{K^3}{\alpha^2 P^3}$ term stems from the application of the coherent state ansatz, which replaces $A_B^\dagger A_B$ 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 2.2. *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*

$$\inf \mathrm{spec} \mathbb{H} - e_p \gtrsim -\alpha^\epsilon \tag{7}$$

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,

$$\inf \operatorname{spec} \mathbb{H} - e_p \geqslant c_1 \delta - E + c_2 \frac{P^2 K}{\delta E} + c_3 \frac{K^3}{\alpha^2 P^3} - cK^{-\beta}. \tag{8}$$

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 $\alpha \gg 1$. $\square$

Remark 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 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 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

$$\inf \operatorname{spec} \mathbb{H} - e_p \geqslant c_1 \delta + c_2 |\Omega|^{2/3} \frac{P^2 K}{\delta} + c_3 \frac{K^3}{\alpha^2 P^3} - cK^{-\beta}. \tag{9}$$

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

$$\inf \mathrm{spec}\mathbb{H} \geq \inf \mathrm{spec}\mathbb{H}_K - \mathrm{const.}(K^{-5/2} + \alpha^{-1}K^{-3/2} + \alpha^{-2}K^{-1}). \tag{10}$$

Taking now $K \sim \alpha^\kappa$ with $0 < \kappa < 1$, which is consistent with the statement and proof of Theorem 2.2, we see that the leading term is $K^{-5/2}$. Therefore, given the above considerations, it directly leads to the main result:

Corollary 2.4. *For the Fröhlich Hamiltonian in free space, we have the following lower bound for the ground state energy asymptotics*

$$\inf \mathrm{spec}\mathbb{H} \geqslant e_p - const.\alpha^{-20/73} \tag{11}$$

for $\alpha \gg 1$.

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

$$-V_+ = \sum_j \left[p_j, a\left(\frac{k_j}{|k|^2} w_x\right) - h.c. \right]. \tag{12}$$

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

$$-V_+ \gtrsim -\frac{\tilde{c}_1}{K} p^2 - \mathbb{N}_+ - \frac{3}{2\alpha^2} \tag{13}$$

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

$$-V_+ \gtrsim -\left(p^2 + \mathbb{N} + 1\right)^2 K^{-5/2}; \tag{14}$$

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 (14) with

$$V_+ \gtrsim -(\mathbb{H}^2 + C^2)K^{-5/2} \tag{15}$$

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 $\inf \mathrm{spec}\mathbb{H}$, then $(\Psi, \mathbb{H}^2\Psi)$ can be chosen to be of order e_p^2, independently of α. This observation immediately leads to

$$\inf \mathrm{spec}\mathbb{H} \geqslant \inf \mathrm{spec}\mathbb{H}_K - \mathrm{const.}K^{-5/2}, \tag{16}$$

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 (14). Secondly, we apply the Gross transformation to the original Hamiltonian, estimate the additional terms which arise, and finally prove (15). 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.

3 The ultraviolet cutoff

3.1 The triple Lieb - Yamazaki bound

As announced, this section gives rise to the following

Proposition 3.1. *For any $K > 0$ and α large enough, we have*

$$-V_+ \gtrsim -\left(p^2 + \mathbb{N} + 1\right)^2 \left(K^{-5/2} + \alpha^{-1}K^{-3/2}\right). \tag{17}$$

Proof. Clearly, with $p = -\mathrm{i}\nabla_x$,

$$V_+ = \sum_{rst} \left[p_r, \left[p_s, \left[p_t, a^\dagger\left(\frac{k_s k_r k_t}{|k|^6} w_x\right) - a\left(\frac{k_s k_r k_t}{|k|^6} w_x\right)\right]\right]\right]. \tag{18}$$

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

$$AC + C^\dagger A^\dagger \leqslant \epsilon A A^\dagger + \frac{1}{\epsilon} C^\dagger C \tag{19}$$

for any A, C and arbitrary $\epsilon > 0$. We get

$$V_+ = \sum_{rst} (p_r p_s [p_t, B_{rst}] + [p_t, B_{rst}] p_r p_s) - 2 \left(p_r p_s B_{rst} p_t + p_t B_{rst}^\dagger p_r p_s \right). \tag{20}$$

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

$$-\left(p_r p_s B_{rst} p_t + p_t B_{rst}^\dagger p_r p_s \right) \leqslant \epsilon p_r^2 p_s^2 + \frac{1}{\epsilon} p_t B_{rst}^\dagger B_{rst} p_t \tag{21}$$

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

$$B_{rst}^\dagger B_{rst} \lesssim K^{-5}(4\mathbb{N} + \frac{2}{\alpha^2}). \tag{22}$$

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

$$C_{rs}^2 \leqslant 4a^\dagger \left(\frac{k_r k_s}{|k|^4} w_x \right) a \left(\frac{k_r k_s}{|k|^4} w_x \right) + \frac{2}{\alpha^2} || \frac{k_r k_s}{|k|^4} w_x ||^2. \tag{23}$$

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 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 $\Psi \in L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)$,

$$||a(f)\Psi||^2 = \int dp | \int dk f(k) \Phi(p-k, k)|^2; \tag{24}$$

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

$$||a(f)\Psi||^2 \leqslant \int dp \left(\int dk \frac{|f(k)|^2}{|k-p|^2} \right) \left(\int dk |k-p|^2 |\Phi(p-k, k)|^2 \right) \leqslant \left(\sup_q \int dk \frac{|f(k)|^2}{|k-q|^2} \right) (\Psi, p^2 \mathbb{N} \Psi). \tag{25}$$

The prefactor is now estimated directly:

$$\int dk|f(k)|^2|k-q|^{-2} = \int_{B(q,R)} dk|f(k)|^2|k-p|^{-2} + \int_{B^c(q,R)} dk|f(k)|^2|p-k|^{-2} \leq ||f^2||_\infty 4\pi R + \frac{||f||_2^2}{R}; \tag{26}$$

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

$$V_+ \lesssim K^{-5/2}(|p|^4 + 3p^2(\mathbb{N} + 2\alpha^{-2})) + (K^{-5/2} + \alpha^{-1}K^{-3/2})(|p|^4 + p^2\mathbb{N} + 1/2). \tag{27}$$

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. □

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 (16) will be true. We will achieve this result by (15). To get there, we need

Proposition 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*

$$(1+\epsilon)||(p^2+\mathbb{N})\Psi|| + C||\Psi|| \geqslant ||U^\dagger_{K',\alpha}\mathbb{H}U_{K',\alpha}\Psi|| \geqslant (1-\epsilon)||(p^2+\mathbb{N})\Psi|| - C||\Psi||, \tag{28}$$

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

$$U = e^{\alpha^2(a(f_x) - a^\dagger(f_x))}. \tag{29}$$

Using the easy to prove formulae, valid for any h s.t. $(h, f_x) < \infty$,

$$Ua_hU^\dagger = a_h + (h, f_x) \quad Ua_h^\dagger U^\dagger = a_h^\dagger + (f_x, h), \tag{30}$$

as well as

$$[p,U]=(-i\nabla_x U),\quad (-i\nabla_x a)(f_x)=-a(pf_x),\quad (-i\nabla_x a^\dagger)(f_x)=a^\dagger(pf_x) \tag{31}$$

and the formula

$$\frac{de^{A(x)}}{dx}=\int_0^1 e^{tA(x)}A'(x)e^{(1-t)A(x)}dt \tag{32}$$

one finds

$$U\mathbb{H}U^\dagger=p^2+\mathbb{N}+\alpha^4(a^\dagger(pf_x)+a(pf_x))^2+2\alpha^2 pa(pf_x)+2\alpha^2a^\dagger(pf_x)p+$$
$$+a(\alpha^2p^2f_x+f_x-v_x)+a^\dagger(\alpha^2p^2f_x+f_x-v_x)+||f_x||_2^2-2\mathrm{Re}(v_x,f_x)\equiv p^2+\mathbb{N}+\tilde{V},$$

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

$$\alpha^2p^2f_x+f_x-v_x=-\frac{\chi_{k\leqslant K'}e^{ikx}}{|k|}\equiv g_x.$$

Writing down the relevant integrals, we readily have the following estimates:

$$||g_x||_2^2\lesssim K',\quad ||f_x||_2^2\lesssim\alpha^{-4}K'^{-3} \tag{33}$$

and

$$(v_x,f_x)\lesssim\alpha^{-2}K'^{-1},\quad ||pf_x||_2^2\lesssim\alpha^{-4}K'^{-1}. \tag{34}$$

We are now able to estimate every term in $\tilde{V}$. We have, by similar computations as in Proposition 3.1

$$||(a(g_x)+a^\dagger(g_x))\Psi||\leqslant||g_x||_2\left|\left|\sqrt{(\mathbb{N}+\alpha^{-2})}\Psi\right|\right|\lesssim\delta||(\mathbb{N}+\alpha^{-2})\Psi||+\delta^{-1}K'||\Psi|| \tag{35}$$

for any $\delta>0$. Similarly,

$$\alpha^4||(a^\dagger(pf_x)+a(pf_x))^2\Psi||\lesssim K'^{-1}||(\mathbb{N}+\alpha^{-2})\Psi||. \tag{36}$$

The cross-terms give, by $pa_fa_f^\dagger p\lesssim p^2(\mathbb{N}+\alpha^{-2})||f||_2^2\lesssim(p^2+\mathbb{N}+\alpha^{-2})^2||f||_2^2$,

$$\alpha^2||a^\dagger(pf_x)p\Psi||\lesssim K'^{-1/2}||(p^2+\mathbb{N}+\alpha^{-2})\Psi||. \tag{37}$$

The term $\alpha^2pa(pf_x)$ requires a bit more work. "Commuting the p through", we get that it can be bounded using the former estimate, and an estimate on $\alpha^2a(p^2f_x)$. $p^2f_x\notin L^2$, however, so we split it as

$$\alpha^2p^2f_x=g_x-f_x+e^{ikx}\left(\frac{1}{|k|}-\frac{1}{\sqrt{K'^2+|k|^2}}\right)+\frac{e^{ikx}}{\sqrt{K'^2+|k|^2}}. \tag{38}$$

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

$$||a((K'^2 + |k|^2)^{-1/2} e^{ikx})\Psi|| \leqslant \sqrt{\left(\sup_p \int dk \frac{1}{(K'^2 + |k|^2)|k-p|^2}\right)(\Psi, \mathbb{N}p^2\Psi)}. \tag{39}$$

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,

$$||a((K'^2 + |k|^2)^{-1/2} e^{ikx})\Psi|| \lesssim K'^{-1/2}||(p^2 + \mathbb{N})\Psi||. \tag{40}$$

The remaining estimates are

$$||a(g_x)\Psi|| \lesssim K'^{1/2}||\mathbb{N}^{1/2}\Psi|| \leqslant \delta||\mathbb{N}\Psi|| + \delta^{-1}K'||\Psi||, \tag{41}$$

$$||a(f_x)\Psi|| \lesssim \alpha^{-2}K'^{-3/2}||\sqrt{\mathbb{N}}\Psi|| \leqslant \delta||\mathbb{N}\Psi|| + \delta^{-1}\alpha^{-4}K'^{-3}||\Psi|| \tag{42}$$

and

$$||a(j_x)\Psi|| \lesssim \delta||\mathbb{N}\Psi|| + \delta^{-1}K'||\Psi|| \tag{43}$$

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

$$-UV_+U^\dagger \gtrsim -U(p^2 + \mathbb{N})^2 U^\dagger \left(K^{-5/2} + \alpha^{-1}K^{-3/2}\right). \tag{44}$$

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 $U(p^2+\mathbb{N})^2 U^\dagger \leqslant \frac{2}{(1-\epsilon)^2}(\mathbb{H}^2 + C^2)$ and hence

$$-V_+ \gtrsim -(\mathbb{H}^2 + C^2)\left(K^{-5/2} + \alpha^{-1}K^{-3/2}\right) - \alpha^{-2}K^{-1}. \tag{45}$$

We can now always choose Ψ' such that both $(\Psi', \mathbb{H}, \Psi')$ is arbitrarily close to $\inf \mathrm{spec}\mathbb{H}$ and $(\Psi', \mathbb{H}^2\Psi')$ can be bounded by a constant independent of Ψ' and α. Choosing such Ψ', we have finally

$$\inf \mathrm{spec}\mathbb{H} \geqslant \inf \mathrm{spec}\mathbb{H}_K - const.(K^{-5/2} + \alpha^{-1}K^{-3/2} + \alpha^{-2}K^{-1}) \tag{46}$$

This is precisely the result that has been claimed.

4 Acknowledgements

The author thanks Dario Feliciangeli for friendly and fruitful discussions.