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The Bipolaron in the Strong Coupling Limit

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Abstract. The bipolaron are two electrons coupled to the elastic deformations of an ionic crystal. We study this system in the Fröhlich approximation. If the Coulomb repulsion dominates, the lowest energy states are two well separated polarons. Otherwise the electrons form a bound pair. We prove the validity of the Pekar–Tomasevich energy functional in the strong coupling limit, yielding estimates on the coupling parameters for which the binding energy is strictly positive. Under the condition of a strictly positive binding energy we prove the existence of a ground state at fixed total momentum P, provided P is not too large.

1. Introduction

The polaron is an electron coupled to the elastic deformations of an ionic crystal. We rely here on the approximation proposed by H. Fröhlich [6], where the phonons are represented as a Bose field over $\mathbb{R}^3$, the dispersion relation is constant, $\omega(k) = \omega_0$, and the coupling function is proportional to $1/|k|$ in wave number space. The Hilbert space of the polaron is then $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathfrak{F}(L^2(\mathbb{R}^3))$ with $\mathfrak{F}(L^2(\mathbb{R}^3))$ the bosonic Fock space and the hamiltonian is given by

$$H_{\mathrm{p}} = -\frac{1}{2}\Delta_x \otimes 1\!\!1 + \sqrt{\alpha}\lambda_0 \int_{\mathbb{R}^3} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|} \Big[\mathrm{e}^{\mathrm{i}k\cdot x} \otimes a(k) + \mathrm{e}^{-\mathrm{i}k\cdot x} \otimes a(k)^*\Big] + 1\!\!1 \otimes N_{\mathrm{f}}$$

with $\lambda_0 = (2\sqrt{2}\pi)^{1/2}$. Here Δ_x is the Laplacian, N_{f} is the number operator, and $a(k), a(k)^*$ are the bosonic annihilation and creation operators with commutation relations

$$\big[a(k), a(k')^*\big] = \delta(k-k')\,, \quad \big[a(k), a(k')\big] = 0 = \big[a(k)^*, a(k')^*\big]\,.$$

(The complete definition of H_{p} will be recalled in the subsequent section.) We use units in which $\hbar = 1, \omega_0 = 1$, and the bare mass of the electron $m_{\mathrm{e}} = 1$.

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Since the coupling function is pure power, the only parameter in the model is the dimensionless coupling constant $\sqrt{\alpha}$.

The bipolaron, the subject of our paper, consists of *two* electrons coupled to the elastic deformations of an ionic crystal. The Hilbert space is then $\mathcal{H} = L^2(\mathbb{R}^6) \otimes \mathfrak{F}(L^2(\mathbb{R}^3))$ and, in the Fröhlich approximation, the hamiltonian reads

$$H_{\rm bp} = \sum_{j=1,2} \left\{ -\frac{1}{2}\Delta_{x_j} \otimes 1\!\!1 + \sqrt{\alpha}\lambda_0 \int_{\mathbb{R}^3} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|} \left[\mathrm{e}^{\mathrm{i}k\cdot x_j} \otimes a(k) + \mathrm{e}^{-\mathrm{i}k\cdot x_j} \otimes a(k)^* \right] \right\} + \frac{\alpha U}{|x_1 - x_2|} \otimes 1\!\!1 + 1\!\!1 \otimes N_{\rm f}\,.$$

$x_j \in \mathbb{R}^3$, $j = 1, 2$, are the coordinates of the two electrons. The electrons are spinless and no statistics is imposed. In addition to the interaction with the phonons, the electrons repel each other through a static Coulomb interaction, which is proportional to e^2. Since $\sqrt{\alpha}$ is proportional to e, the strength of the Coulomb repulsion is written as αU with U a second dimensionless coupling parameter $U \geq 0$. As explained in [4], e.g., $U \geq \sqrt{2}$ in the Fröhlich approximation. For the purpose of our study, we regard α, U as independent parameters, $\alpha \geq 0, U \geq 0$.

The phonons induce an effective attraction between the electrons which competes with the Coulomb repulsion. If the latter dominates we expect the low energy states of $H_{\rm p}$ to consist of two far apart polarons, while if the coupling to the phonon field dominates the electrons should form a bound pair. More precisely, let $E_{\rm p}(\alpha)$ and $E_{\rm bp}(\alpha, U)$ be the lowest energy of $H_{\rm p}$ and $H_{\rm bp}$, respectively. We define the bipolaron binding energy as

$$E_{\rm bin}(\alpha, U) = 2E_{\rm p}(\alpha) - E_{\rm bp}(\alpha, U)\,.$$

One basic problem is then to characterize in the quadrant of couplings (α, U) a domain with $E_{\rm bin} = 0$ (two widely separated polarons) and a domain with $E_{\rm bin} > 0$ (bound pair).

If α is small, one could use iterative techniques in the spirit of [1], see also [10, 11], to approach the issue of a strictly positive binding energy. In this paper we investigate the strong coupling regime, $\alpha \to \infty$.

We first establish that $H_{\rm p}$ is a properly defined self-adjoint operator and that, for $E_{\rm p}(\alpha) = \inf \mathrm{spec}(H_{\rm p})$, one has $\lim_{\alpha\to\infty} E_{\rm p}(\alpha)/\alpha^2 = c_{\rm p}$ with $c_{\rm p}$ a constant defined as the minimum of the Pekar functional. (Numerically, one finds $c_{\rm p} = -0.1085\ldots$ [19].) The strong coupling limit has been studied before by Donsker and Varadhan [5], using functional integration, and by Lieb and Thomas [15, 16] based on operator techniques. In fact, we slightly improve their results. In [5, 15, 16] the authors consider a suitable cutoff version of $H_{\rm p}$ with ground state energy $E^{(\kappa)}(\alpha)$, κ denoting the ultraviolet cutoff. They define $E(\alpha) = \lim_{\kappa\to\infty} E^{(\kappa)}(\alpha)$ and prove that $\lim_{\alpha\to\infty} E(\alpha)/\alpha^2 = c_{\rm p}$. Secondly we consider the bipolaron and establish that in the strong coupling limit its ground state energy is given through minimizing the Pekar–Tomasevich functional [22], see [27] for a review. An analysis of the Pekar–Tomasevich variational problem yields an information on the binding energy for large α.

From our investigaton of the strong coupling limit it is a small step to study the existence of a ground state for the bipolaron at constant total momentum P following the strategy developed in [17]. We will prove that, if $E_{\mathrm{bin}} > 0$, then H_{bp} at total momentum P has a ground state, provided P is not too large (specified quantitatively).

The bipolaron is a very well studied system, both experimentally and theoretically. We refer to [27] for a survey and to [12] for a listing of theoretical investigations. Spectral properties of the Fröhlich polaron are investigated in [20, 29].

The paper is organized as follows: Section 3 deals with the strong coupling limit $\alpha \to \infty$ and Section 4 with the existence of a ground state. In the Appendices A and B removal of the ultraviolet cutoff and self-adjointness are discussed. In Appendix C it is established that the bipolaron hamiltonian is bounded from below and in Appendix D a localization estimate is proved.

2. Main results

In general we denote the inner product and the norm of a Hilbert space $\mathfrak{h}$ by $\langle\cdot,\cdot\rangle_{\mathfrak{h}}$ and $\|\cdot\|_{\mathfrak{h}}$ respectively. If there is no danger of confusion, then we omit the subscript $\mathfrak{h}$ in $\langle\cdot,\cdot\rangle_{\mathfrak{h}}$ and $\|\cdot\|_{\mathfrak{h}}$. For a linear operator T on a Hilbert space, we denote its domain by $\mathrm{dom}(T)$. For a self-adjoint operator A on a Hilbert space, we denote its spectrum (resp. essential spectrum) by $\mathrm{spec}(A)$ (resp. $\mathrm{ess.\,spec}(A)$).

Let $\mathfrak{h}$ be a Hilbert space. The Fock space over $\mathfrak{h}$ is defined by

$$\mathfrak{F}(\mathfrak{h}) = \oplus_{n=0}^{\infty} \otimes_{\mathrm{s}}^{n} \mathfrak{h}\,,$$

where $\otimes_{\mathrm{s}}^{n}\mathfrak{h}$ means the n-fold symmetric tensor product of $\mathfrak{h}$ with the convention $\otimes_{\mathrm{s}}^{0}\mathfrak{h} = \mathbb{C}$. The vector $\Omega = 1 \oplus 0 \oplus \cdots \in \mathfrak{F}(\mathfrak{h})$ is called the Fock vacuum.

We denote by $a(f)$ the annihilation operator on $\mathfrak{F}(\mathfrak{h})$ with test vector $f \in \mathfrak{h}$ [24, Sect. X.7]. By definition, $a(f)$ is densely defined, closed, and antilinear in f. The adjoint $a(f)^*$ is the adjoint of $a(f)$ and called the creation operator. We frequently write $a(f)^{\#}$ to denote either $a(f)$ or $a(f)^*$. Creation and annihilation operators satisfy the canonical commutation relations

$$\big[a(f), a(g)^*\big] = \langle f, g\rangle_{\mathfrak{h}} \mathbb{1}\,, \quad \big[a(f), a(g)\big] = 0 = \big[a(f)^*, a(g)^*\big]$$

on the finite particle subspace

$$\mathfrak{F}_0(\mathfrak{h}) = \bigcup_{m=1}^{\infty} \big\{\varphi = \varphi_0 \oplus \varphi_1 \oplus \cdots \in \mathfrak{F}(\mathfrak{h}) \,|\, \varphi_n = 0, \ \text{for}\, n \geq m\big\}\,,$$

where $\mathbb{1}$ denotes the identity operator. In the case of $\mathfrak{h} = L^2(\mathbb{R}^3)$, we often use the symbolic notation for the annihilation and creation operator by the kernel:

$$a(f) = \int_{\mathbb{R}^3} \mathrm{d}k\, f(k)^* a(k)\,, \quad a(f)^* = \int_{\mathbb{R}^3} \mathrm{d}k\, f(k) a(k)^*\,.$$

We introduce a further important subspace of $\mathfrak{F}(\mathfrak{h})$. Let $\mathfrak{s}$ be a subspace of $\mathfrak{h}$. We define

$$\mathfrak{F}_{\mathrm{fin}}(\mathfrak{s}) = \mathrm{Lin}\big\{a(f_1)^* \dots a(f_n)^*\Omega,\ \Omega \,|\, f_1, \dots, f_n \in \mathfrak{s},\ n \in \mathbb{N}\big\}\,,$$

where $\mathrm{Lin}\{\cdots\}$ means the linear span of the set $\{\cdots\}$. If $\mathfrak{s}$ is dense in $\mathfrak{h}$, so is $\mathfrak{F}_{\mathrm{fin}}(\mathfrak{s})$ in $\mathfrak{F}(\mathfrak{h})$.

Let b be a contraction operator from $\mathfrak{h}_1$ to $\mathfrak{h}_2$, i.e., $\|b\| \le 1$. The linear operator $\Gamma(b) : \mathfrak{F}(\mathfrak{h}_1) \to \mathfrak{F}(\mathfrak{h}_2)$ is defined by

$$\Gamma(b) \restriction \otimes_{\mathrm{s}}^n \mathfrak{h}_1 = \otimes^n b$$

with the convention $\otimes^0 b = \mathbb{1}$.

For a densely defined closable operator c on $\mathfrak{h}$, $\mathrm{d}\Gamma(c) : \mathfrak{F}(\mathfrak{h}) \to \mathfrak{F}(\mathfrak{h})$ is defined by

$$\mathrm{d}\Gamma(c) \restriction \hat{\otimes}_{\mathrm{s}}^n \mathrm{dom}(c) = \sum_{j=1}^{n} \mathbb{1} \otimes \cdots \otimes \underset{j\,\mathrm{th}}{c} \otimes \cdots \otimes \mathbb{1}$$

and

$$\mathrm{d}\Gamma(c)\Omega = 0$$

where $\hat{\otimes}$ means the algebraic tensor product. Here in the j-th summand c is at the j-th entry. Clearly $\mathrm{d}\Gamma(c)$ is closable and we denote its closure by the same symbol. As a typical example, the number operator N_{f} is given by $N_{\mathrm{f}} = \mathrm{d}\Gamma(\mathbb{1})$.

The bipolaron Hamiltonian with an ultraviolet cutoff $\kappa > 0$ is defined as

$$\begin{aligned} H_{\mathrm{bp},\kappa} = \sum_{j=1,2} \Bigg\{ -\frac{1}{2}\Delta_{x_j} \otimes \mathbb{1} + \sqrt{\alpha}\lambda_0 \int_{|k|\le\kappa} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|} \Big[\mathrm{e}^{\mathrm{i}k\cdot x_j} \otimes a(k) + \mathrm{e}^{-\mathrm{i}k\cdot x_j} \otimes a(k)^* \Big] \Bigg\} \\ + \frac{\alpha U}{|x_1 - x_2|} \otimes \mathbb{1} + \mathbb{1} \otimes N_{\mathrm{f}} \end{aligned}$$

with $\alpha, U \ge 0$. This linear operator acts in the Hilbert space $L^2(\mathbb{R}^6, \mathrm{d}x_1 \otimes \mathrm{d}x_2) \otimes \mathfrak{F}(L^2(\mathbb{R}^3))$. By the bound

$$\|a(f)^{\#}(N_{\mathrm{f}} + \mathbb{1})^{-1/2}\| \le \|f\| \tag{1}$$

and the Kato–Rellich theorem, it is easy to see that, for all $0 < \kappa < \infty$ and $0 < \alpha < \infty$, $H_{\mathrm{bp},\kappa}$ is self-adjoint on the domain of the self-adjoint operator $L_{\mathrm{bp}} = -\sum_{j=1,2} \Delta_{x_j} \otimes \mathbb{1} + \mathbb{1} \otimes N_{\mathrm{f}}$, bounded from below, and essentially self-adjoint on any core for L_{bp}. We note that $H_{\mathrm{bp},\kappa}$ strongly commutes with the total momentum operator

$$P_{\mathrm{tot}} = -\mathrm{i}\nabla_{x_1} \otimes \mathbb{1} - \mathrm{i}\nabla_{x_2} \otimes \mathbb{1} + \mathbb{1} \otimes P_{\mathrm{f}}\,, \tag{2}$$

where $P_{\mathrm{f}} = (\mathrm{d}\Gamma(k_1), \mathrm{d}\Gamma(k_2), \mathrm{d}\Gamma(k_3))$, that is to say, $\mathrm{e}^{\mathrm{i}a\cdot P_{\mathrm{tot}}} H_{\mathrm{bp},\kappa} \subseteq H_{\mathrm{bp},\kappa} \mathrm{e}^{\mathrm{i}a\cdot P_{\mathrm{tot}}}$ for all $a \in \mathbb{R}^3$.

Let $(x_{\mathrm{r}}, x_{\mathrm{c}})$ be the center of mass coordinates defined by

$$x_{\mathrm{r}} = x_1 - x_2\,, \quad x_{\mathrm{c}} = \frac{x_1 + x_2}{2}$$

and let U_C be the unitary operator from $L^2(\mathbb{R}^6, \mathrm{d}x_1 \otimes \mathrm{d}x_2)$ to $L^2(\mathbb{R}^6, \mathrm{d}x_\mathrm{r} \otimes \mathrm{d}x_\mathrm{c})$ given by

$$(U_C f)(x_\mathrm{r}, x_\mathrm{c}) = f\left(x_\mathrm{c} + \frac{x_\mathrm{r}}{2}, x_\mathrm{c} - \frac{x_\mathrm{r}}{2}\right)$$

for $f(x_1, x_2) \in L^2(\mathbb{R}^6, \mathrm{d}x_1 \otimes \mathrm{d}x_2)$. We introduce a unitary operator $\mathcal{U}$ by

$$\mathcal{U} = (\mathcal{F}_{x_\mathrm{c}} \otimes \mathbb{1})\, \mathrm{e}^{\mathrm{i}x_\mathrm{c}\cdot P_\mathrm{f}} (U_C \otimes \mathbb{1})\,,$$

where $\mathcal{F}_{x_\mathrm{c}}$ is the Fourier transformation with respect to x_c, i.e.,

$$(\mathcal{F}_{x_\mathrm{c}} f)(P, x_\mathrm{r}) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} \mathrm{d}x_\mathrm{c}\, \mathrm{e}^{-\mathrm{i}x_\mathrm{c}\cdot P} f(x_\mathrm{r}, x_\mathrm{c})$$

for $f(x_\mathrm{r}, x_\mathrm{c}) \in L^2(\mathbb{R}^6, \mathrm{d}x_\mathrm{r} \otimes \mathrm{d}x_\mathrm{c})$. The unitary operator $\mathcal{U}$ induces the identification $L^2(\mathbb{R}^6, \mathrm{d}x_1 \otimes \mathrm{d}x_2) \otimes \mathfrak{F}(L^2(\mathbb{R}^3))$ with $\int_{\mathbb{R}^3}^{\oplus} L^2(\mathbb{R}^3, \mathrm{d}x_\mathrm{r}) \otimes \mathfrak{F}(L^2(\mathbb{R}^3))\, \mathrm{d}P$, that is concretely written as

$$\begin{aligned}
&(\mathcal{U}\varphi)^{(n)}(P, x_\mathrm{r}, k_1, \ldots, k_n) \\
&\quad = (2\pi)^{-3/2} \int_{\mathbb{R}^3} \mathrm{d}x_\mathrm{c}\, \mathrm{e}^{-\mathrm{i}x_\mathrm{c}\cdot (P - \sum_{j=1}^n k_j)} \varphi^{(n)}\left(x_\mathrm{c} + \frac{x_\mathrm{r}}{2}, x_\mathrm{c} - \frac{x_\mathrm{r}}{2}, k_1, \ldots, k_n\right)
\end{aligned}$$

for $\varphi = \oplus_{n=0}^{\infty} \varphi^{(n)} \in L^2(\mathbb{R}^6, \mathrm{d}x_1 \otimes \mathrm{d}x_2) \otimes \mathfrak{F}(L^2(\mathbb{R}^3))$. It is easily shown that

$$\mathcal{U} P_\mathrm{tot} \mathcal{U}^* = \int_{\mathbb{R}^3}^{\oplus} P\, \mathrm{d}P\,.$$

Hence the unitary operator $\mathcal{U}$ provides the direct integral decomposition of $L^2(\mathbb{R}^6, \mathrm{d}x_1 \otimes \mathrm{d}x_2) \otimes \mathfrak{F}(L^2(\mathbb{R}^3))$ with respect to the value of the total momentum.

Since $H_{\mathrm{bp},\kappa}$ strongly commutes with P_tot, $\mathcal{U} H_{\mathrm{bp},\kappa} \mathcal{U}^*$ is decomposable and can be represented by the fiber direct integral

$$\mathcal{U} H_{\mathrm{bp},\kappa} \mathcal{U}^* = \int_{\mathbb{R}^3}^{\oplus} H_\kappa(P)\, \mathrm{d}P\,,$$

where

$$\begin{aligned}
H_\kappa(P) &= \frac{1}{4}(P - \mathbb{1} \otimes P_\mathrm{f})^2 - \Delta_{x_\mathrm{r}} \otimes \mathbb{1} + \frac{\alpha U}{|x_\mathrm{r}|} \otimes \mathbb{1} + \mathbb{1} \otimes N_\mathrm{f} \\
&\quad + 2\sqrt{\alpha}\lambda_0 \int_{|k|\le\kappa} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|} \cos\frac{k\cdot x_\mathrm{r}}{2} \otimes \left[a(k) + a(k)^*\right]\,. \qquad (3)
\end{aligned}$$

By the Kato–Rellich's theorem, $H_\kappa(P)$ is self-adjoint on $\mathrm{dom}(-\Delta_{x_\mathrm{r}} \otimes \mathbb{1}) \cap \mathrm{dom}(\mathbb{1} \otimes P_\mathrm{f}^2) \cap \mathrm{dom}(\mathbb{1} \otimes N_\mathrm{f})$ for all $\kappa < \infty$ and $\alpha < \infty$, and bounded from below. Further, $H_\kappa(P)$ is essentially self-adjoint on any core for the self-adjoint operator

$$L = -\Delta_{x_\mathrm{r}} \otimes \mathbb{1} + \mathbb{1} \otimes P_\mathrm{f}^2 + \mathbb{1} \otimes N_\mathrm{f}\,. \qquad (4)$$

We state our main results. Our first result concerns the existence of the limiting Hamiltonians. Namely, we remove the ultraviolet cutoff from $H_{\mathrm{bp},\kappa}$ and $H_\kappa(P)$. No energy renormalization is required.

Theorem 2.1.

(i) *For all $\alpha < \infty$ and $U < \infty$, there exists a self-adjoint operator $H_{\rm bp}$ that is bounded from below such that $H_{{\rm bp},\kappa}$ converges to $H_{\rm bp}$ in the strong resolvent sense as $\kappa \to \infty$.*

(ii) *For all $\alpha < \infty$, $U < \infty$ and $P \in \mathbb{R}^3$, there exists a self-adjoint operator $H(P)$ that is bounded from below such that $H_\kappa(P)$ converges to $H(P)$ in the strong resolvent sense as $\kappa \to \infty$.*

(iii) *$\mathcal{U} H_{\rm bp} \mathcal{U}^*$ is decomposable and*

$$\mathcal{U} H_{\rm bp} \mathcal{U}^* = \int_{\mathbb{R}^3}^{\oplus} H(P)\,\mathrm{d}P\,. \tag{5}$$

Let $H_{{\rm p},\kappa}$ be the Hamiltonian for a single polaron with the ultraviolet cutoff κ,

$$H_{{\rm p},\kappa} = -\frac{1}{2}\Delta_x \otimes 1\!\!1 + \sqrt{\alpha}\lambda_0 \int_{|k|\le\kappa} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|}\left[\mathrm{e}^{\mathrm{i}k\cdot x}\otimes a(k) + \mathrm{e}^{-\mathrm{i}k\cdot x}\otimes a(k)^*\right] + 1\!\!1 \otimes N_{\rm f}\,.$$

The linear operator $H_{{\rm p},\kappa}$ acts in the Hilbert space $L^2(\mathbb{R}^3)\otimes\mathfrak{F}(L^2(\mathbb{R}^3))$. Moreover, for all $0<\kappa<\infty$ and $0<\alpha<\infty$, $H_{{\rm p},\kappa}$ is self-adjoint on the domain of the self-adjoint operator $L_{\rm p} = -\Delta_x \otimes 1\!\!1 + 1\!\!1 \otimes N_{\rm f}$, bounded from below, and essentially self-adjoint on any core for $L_{\rm p}$. In a way similar to the proof of Theorem 2.1 (i), we can show the following.

Proposition 2.2. *For any coupling α, there exists a self-adjoint operator $H_{\rm p}$, bounded from below, such that $H_{{\rm p},\kappa}$ converges to $H_{\rm p}$ in the strong resolvent sense as $\kappa \to \infty$.*

Let

$$E_{\rm bp} = \inf \mathrm{spec}(H_{\rm bp})\,, \quad E_{\rm p} = \inf \mathrm{spec}(H_{\rm p})\,.$$

The *binding energy* $E_{\rm bin}$ is defined by

$$E_{\rm bin} = 2E_{\rm p} - E_{\rm bp}\,.$$

In order to display the dependence on α and U, we also denote the binding energy by $E_{\rm bin}(\alpha, U)$.

We introduce the *Pekar energy functional* by

$$\mathcal{E}_{\rm p}(\varphi) = \frac{1}{2}\int \mathrm{d}x\,|\nabla_x\varphi(x)|^2 - \frac{1}{\sqrt{2}}\int \mathrm{d}x\mathrm{d}y\,\frac{|\varphi(x)|^2|\varphi(y)|^2}{|x-y|} \tag{6}$$

for $\varphi\in W^1(\mathbb{R}^3)$, where $W^1(\mathbb{R}^d)$ is the space of functions on $\mathbb{R}^d$ such that $\|\nabla\varphi\|_{L^2(\mathbb{R}^d)}$ and $\|\varphi\|_{L^2(\mathbb{R}^d)}$ are finite. For $U \ge 0$, the *Pekar–Tomasevich energy functional* is defined by

$$\begin{aligned}\mathcal{E}^U_{\mathrm{bp}}(\varphi) = \frac{1}{2}\int \mathrm{d}x_1\mathrm{d}x_2\,|\nabla_{x_1}\varphi(x_1,x_2)|^2 + \frac{1}{2}\int \mathrm{d}x_1\mathrm{d}x_2\,|\nabla_{x_2}\varphi(x_1,x_2)|^2 \\ + U\int \mathrm{d}x_1\mathrm{d}x_1\,\frac{|\varphi(x_1,x_2)|^2}{|x_1-x_2|} \\ - \frac{1}{\sqrt{2}}\sum_{i,j=1,2}\int \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}y_1\mathrm{d}y_2\,\frac{|\varphi(x_1,x_2)|^2|\varphi(y_1,y_2)|^2}{|x_i-y_j|}\end{aligned} \tag{7}$$

for $\varphi \in W^1(\mathbb{R}^6)$.

Theorem 2.3. *Let*

$$c_{\mathrm{p}} = \inf\left\{\mathcal{E}_{\mathrm{p}}(\varphi)\,|\,\varphi\in W^1(\mathbb{R}^3), \|\varphi\|_{L^2(\mathbb{R}^3)}=1\right\}, \tag{8}$$

$$c_{\mathrm{bp}}(U) = \inf\left\{\mathcal{E}^U_{\mathrm{bp}}(\varphi)\,|\,\varphi\in W^1(\mathbb{R}^6),\ \|\varphi\|_{L^2(\mathbb{R}^6)}=1\right\}. \tag{9}$$

For any Coulomb strength $U \geq 0$,

$$\lim_{\alpha\to\infty}\frac{E_{\mathrm{bin}}(\alpha,U)}{\alpha^2} = 2c_{\mathrm{p}} - c_{\mathrm{bp}}(U)\,.$$

The Pekar energy functional is studied in [13]. In a separate work [18] we investigate the Pekar–Tomasevich energy functional and quote only

Theorem 2.4 ([18]).

(i) *For all $U \geq 0$, $2c_{\mathrm{p}} - c_{\mathrm{bp}}(U) \geq 0$. Moreover, $2c_{\mathrm{p}} - c_{\mathrm{bp}}(U)$ is monotone decreasing, convex and continuous in U.*

(ii) *Let $U_{\mathrm{c}} = \sup\{U\in[0,\infty)\,|\,2c_{\mathrm{p}} - c_{\mathrm{bp}}(U) > 0\}$. Then $\sqrt{2} < U_{\mathrm{c}}$.*

Remark 2.5. If $\varphi(x_1,x_2) = \phi_0(x_1)\phi_0(x_2)$ with ϕ_0 the minimizer of $\mathcal{E}_{\mathrm{p}}(\cdot)$, up to translation, then $\mathcal{E}^{\sqrt{2}}_{\mathrm{bp}}(\varphi) = 2c_{\mathrm{p}}$. Theorem 2.4 asserts that the energy is lowered through correlations. Numerically one uses trial functions [28] or variational actions [4]. On this basis the value for U_{c} is approximately $(1.1)\sqrt{2}$.

Returning to finite α we characterize the existence of the ground state for $H(P)$ in terms of the binding energy in the following way.

Theorem 2.6. *For all P, coupling strength α and Coulomb strength U, one has*

$$\inf \mathrm{ess.\,spec}\big(H(P)\big) - \inf \mathrm{spec}\big(H(P)\big) \geq \min\left\{1, E_{\mathrm{bin}}\right\} - \frac{P^2}{4}\,.$$

Thus, if $E_{\mathrm{bin}} > 0$, then $H(P)$ has a ground state provided

$$|P| < 2\min\left\{1, \sqrt{E_{\mathrm{bin}}}\right\}.$$

Combining both theorems yields a domain of coupling parameters and P for which $H(P)$ has a ground state.

Corollary 2.7. *Suppose that the strength U of the Coulomb interaction satisfies $U < U_{\mathrm{c}}$. Then, there exists an α_{c} such that, for any $\alpha > \alpha_{\mathrm{c}}$, $H(P)$ has a ground state for $|P| < 2$.*

3. Strong coupling limit

3.1. The Pekar variational problem

In this subsection we summarize properties of the Pekar–Tomasevich energy functional. They are proven in [18].

Lemma 3.1.

(i) *There exists a constant* $A_{\mathrm{p}} > -\infty$ *such that for all* $\varphi \in W^1(\mathbb{R}^3)$ *with* $\|\varphi\|_{L^2(\mathbb{R}^3)} = 1$ *the bound* $\mathcal{E}_{\mathrm{p}}(\varphi) \ge A_{\mathrm{p}}$ *holds. Hence,* $c_{\mathrm{p}} > -\infty$.

(ii) *There exists a constant* $A_{\mathrm{bp}} > -\infty$ *such that for all* $\varphi \in W^1(\mathbb{R}^6)$ *with* $\|\varphi\|_{L^2(\mathbb{R}^6)} = 1$ *the bound* $\mathcal{E}^U_{\mathrm{bp}}(\varphi) \ge A_{\mathrm{bp}}$ *holds. Hence,* $c_{\mathrm{bp}}(U) > -\infty$.

Lemma 3.2.

(i) $c_{\mathrm{p}} = \inf\big\{\mathcal{E}_{\mathrm{p}}(\varphi)\,|\,\varphi \in C_0^\infty(\mathbb{R}^3),\ \|\varphi\|_{L^2(\mathbb{R}^3)} = 1\big\}$.

(ii) $c_{\mathrm{bp}}(U) = \inf\big\{\mathcal{E}^U_{\mathrm{bp}}(\varphi)\,|\,\varphi \in C_0^\infty(\mathbb{R}^6),\ \|\varphi\|_{L^2(\mathbb{R}^6)} = 1\big\}$ *for all* $U \ge 0$.

Lemma 3.3. $c_{\mathrm{bp}}(U)$ *is continuous in* $U \ge 0$.

3.2. Infinimum of spectrum for $\alpha \to \infty$

Lemma 3.4. *For all* $\alpha > 0$ *and Coulomb strength* U*, we have the following.*

(i) $E_{\mathrm{p}} \le c_{\mathrm{p}}\alpha^2$.

(ii) $E_{\mathrm{bp}} \le c_{\mathrm{bp}}(U)\alpha^2$.

Proof. (i) We will apply the variational principle. Let $\varphi \in C_0^\infty(\mathbb{R}^3)$ with $\|\varphi\|_{L^1(\mathbb{R}^3)} = 1$. Set

$$\rho(k) = \frac{1}{(2\pi)^{3/2}}\int \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}k\cdot x}|\varphi(x)|^2 .$$

We choose $\xi = \varphi \otimes \Psi$ as a trial function, where

$$\Psi = \exp\left\{\mathrm{i}\lambda\int_{|k|\le\kappa}\frac{\mathrm{d}k}{|k|}\Big[-\mathrm{i}\bar{\rho}(k)a(k) + \mathrm{i}\rho(k)a(k)^*\Big]\right\}\Omega$$

with $\lambda = \sqrt{\alpha}\lambda_0$. By the standard calculation, we have

$$\langle\xi, H_{\mathrm{p},\kappa}\xi\rangle = \frac{1}{2}\int \mathrm{d}x\,|\nabla_x\varphi(x)|^2 - \lambda^2\int_{|k|\le\kappa}\mathrm{d}k\,\frac{|\rho(k)|^2}{|k|^2} .$$

Thus

$$E_{\mathrm{p},\kappa} \le \frac{1}{2}\int \mathrm{d}x\,|\nabla_x\varphi(x)|^2 - \lambda^2\int_{|k|\le\kappa}\mathrm{d}k\,\frac{|\rho(k)|^2}{|k|^2} .$$

Here $E_{\mathrm{p},\kappa}$ is the ground state energy for $H_{\mathrm{p},\kappa}$. Taking the limit $\kappa \to \infty$, we have

$$\begin{aligned} E_{\mathrm{p}} &\le \frac{1}{2}\int \mathrm{d}x\,|\nabla_x\varphi(x)|^2 - \lambda^2\int \mathrm{d}k\,\frac{|\rho(k)|^2}{|k|^2} \\ &= \frac{1}{2}\int \mathrm{d}x\,|\nabla_x\varphi(x)|^2 - \frac{\alpha}{\sqrt{2}}\int \mathrm{d}x\mathrm{d}y\frac{|\varphi(x)|^2|\varphi(y)|^2}{|x-y|} \end{aligned}$$

by Proposition B.1 (ii). Here we use the following fact [14]:

$$\int_{\mathbb{R}^3} \mathrm{d}k \frac{\bar{\hat{f}}(k)\hat{g}(k)}{k^2} = \frac{1}{4\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \mathrm{d}x\mathrm{d}y\, \frac{\bar{f}(x)g(y)}{|x-y|}\,, \tag{10}$$

for $f, g \in L^{6/5}(\mathbb{R}^3)$, where $\hat{f}(k) = (2\pi)^{-3/2}\int_{\mathbb{R}^3} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}k\cdot x} f(x)$. Finally we remark that, by the scaling argument and Lemma 3.2 (i), we get

$$\inf\left\{\frac{1}{2}\int \mathrm{d}x\, |\nabla_x \varphi(x)|^2 - \frac{\alpha}{\sqrt{2}}\int \mathrm{d}x\mathrm{d}y\, \frac{|\varphi(x)|^2|\varphi(y)|^2}{|x-y|}\,\Big|\, \varphi\in C_0^\infty(\mathbb{R}^3),\ \|\varphi\|_{L^2}=1\right\} = c_{\mathrm{p}}\alpha^2\,.$$

(ii) The proof of (ii) is almost same as (i). Our choice of the trial function is

$$\xi = \varphi\otimes\Psi\,,\quad \varphi\in C_0^\infty(\mathbb{R}^6)\ \text{ with }\ \|\varphi\|_{L^2(\mathbb{R}^6)} = 1\,,$$

$$\Psi = \exp\left\{\mathrm{i}\lambda\int_{|k|\le\kappa}\frac{\mathrm{d}k}{|k|}\Big[-\mathrm{i}\bar{\rho}(k)a(k) + \mathrm{i}\rho(k)a(k)^*\Big]\right\}\Omega \quad \text{with}\quad \lambda = \sqrt{\alpha}\lambda_0\,,$$

$$\rho(k) = \rho_1(k) + \rho_2(k)\,,$$

$$\rho_1(k) = \frac{1}{(2\pi)^{3/2}}\int \mathrm{d}x_1\mathrm{d}x_2\, \mathrm{e}^{-\mathrm{i}k\cdot x_2}|\varphi(x_1,x_2)|^2\,,$$

$$\rho_2(k) = \frac{1}{(2\pi)^{3/2}}\int \mathrm{d}x_1\mathrm{d}x_2\, \mathrm{e}^{-\mathrm{i}k\cdot x_1}|\varphi(x_1,x_2)|^2\,.$$

Then, we get

$$\langle\xi, H_{\mathrm{bp},\kappa}\xi\rangle = T_{\mathrm{bp}}(\varphi) + \alpha U\int \mathrm{d}x_1\mathrm{d}x_2\, \frac{|\varphi(x_1,x_2)|^2}{|x_1-x_2|} - \lambda^2\int_{|k|\le\kappa}\mathrm{d}k\, \frac{|\rho(k)|^2}{k^2}$$

with $T_{\mathrm{bp}}(\varphi) = \frac{1}{2}\int \mathrm{d}x_1\mathrm{d}x_2\, |\nabla_{x_1}\varphi(x_1,x_2)|^2 + \frac{1}{2}\int \mathrm{d}x_1\mathrm{d}x_2\, |\nabla_{x_2}\varphi(x_1,x_2)|^2$. Accordingly, by Proposition B.1 (i), we obtain that

$$E_{\mathrm{bp}} \le T_{\mathrm{bp}}(\varphi) + \alpha U\int \mathrm{d}x_1\mathrm{d}x_2\, \frac{|\varphi(x_1,x_2)|^2}{|x_1-x_2|} - \lambda^2\int \mathrm{d}k\, \frac{|\rho(k)|^2}{k^2}\,.$$

Let $\rho_1(k;x_1) := (2\pi)^{-3/2}\int \mathrm{d}x_2 \mathrm{e}^{-\mathrm{i}k\cdot x_2}|\varphi(x_1,x_2)|^2$. Then, by Fubini's theorem and (10),

$$\begin{aligned}\lambda^2\int \mathrm{d}k\, \frac{|\rho_1(k)|^2}{k^2} &= \lambda^2\int \mathrm{d}x_1\mathrm{d}y_1\int \mathrm{d}k\, \frac{\bar{\rho}_1(k;x_1)\rho_1(k;y_1)}{k^2}\\ &= \lambda^2\int \mathrm{d}x_1\mathrm{d}y_1\left(\frac{1}{4\pi}\int \mathrm{d}x_2\mathrm{d}y_2 \frac{|\varphi(x_1,x_2)|^2|\varphi(y_1,y_2)|^2}{|x_2-y_2|}\right)\\ &= -\frac{\alpha}{\sqrt{2}}\int \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}y_1\mathrm{d}y_2 \frac{|\varphi(x_1,x_2)|^2|\varphi(y_1,y_2)|^2}{|x_2-y_2|}\end{aligned}$$

Calculating the other terms contained in $\lambda^2\int \mathrm{d}k\, |\rho(k)|^2/k^2$ by the similar way, we obtain

$$-\lambda^2\int \mathrm{d}k \frac{|\rho(k)|^2}{k^2} = -\sum_{i,j=1,2}\frac{\alpha}{\sqrt{2}}\int \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}y_1\mathrm{d}y_2 \frac{|\varphi(x_1,x_2)|^2|\varphi(y_1,y_2)|^2}{|x_i-y_j|}$$

Now the assertion follows from Lemma 3.2 (ii) and the scaling argument. □

Lemma 3.5.
(i) $E_{\mathrm{p}} \ge c_{\mathrm{p}}\alpha^2 + \mathcal{O}(\alpha^{9/5})$.
(ii) $E_{\mathrm{bp}} \ge c_{\mathrm{bp}}((1-c_1\alpha^{-1/5})(1-c_2\alpha^{-1/5})U)\alpha^2 + \mathcal{O}(\alpha^{9/5})$, *where* c_1 *and* c_2 *are positive constants.*

Proof. The assertion (i) has been proven in [15,16], essentially. Although the authors consider a finite volume model, their arguments are still valid in our case. More precisely, first we apply the methods in [15,16] to $H_{\mathrm{p},\kappa}$, and obtain the bound

$$E_{\mathrm{p},\kappa} \ge c_{\mathrm{p}}\alpha^2 + \mathcal{O}\left(\alpha^{9/5}\right)$$

for sufficiently large κ. The important point is that the error term $\mathcal{O}(\alpha^{9/5})$ is independent of κ. Now taking the limit $\kappa \to \infty$, we have the desired result by Proposition B.1 (ii). The details of the argument are provided in Appendix C. As for (ii), one can extend the proof of (i) to the bipolaron Hamiltonian $H_{\mathrm{bp},\kappa}$ with some slight modifications. For the convenience of the reader, we give a sketch of the proof in Appendix C. □

Proof of Theorem 2.3. By Lemma 3.4 and 3.5, we have

$$\begin{aligned}2c_{\mathrm{p}}\alpha^2 - c_{\mathrm{bp}}\Big(\big(1-c_1\alpha^{-1/5}\big)\big(1-c_2\alpha^{-1/5}\big)U\Big)\alpha^2 + \mathcal{O}\big(\alpha^{9/5}\big) \;&\ge\; 2E_{\mathrm{p}} - E_{\mathrm{bp}}\\ &\ge\; 2c_{\mathrm{p}}\alpha^2 - c_{\mathrm{bp}}\big(U\big)\alpha^2 + \mathcal{O}\big(\alpha^{9/5}\big)\,.\end{aligned}$$

Taking Lemma 3.3 into consideration, we get

$$\lim_{\alpha\to\infty}\frac{E_{\mathrm{bin}}(\alpha,U)}{\alpha^2} = 2c_{\mathrm{p}} - c_{\mathrm{bp}}(U)\,.$$ □

4. Existence of a ground state

4.1. Properties of the ground state energy

Let $E_{\mathrm{bp},\kappa}$ and $E_{\mathrm{p},\kappa}$ be the ground state energy for $H_{\mathrm{bp},\kappa}$ and $H_{\mathrm{p},\kappa}$ respectively. Further we denote $\inf\operatorname{spec}(H_\kappa(P))$, resp. $\inf\operatorname{spec}(H(P))$, by $E_\kappa(P)$, resp. $E(P)$.

Proposition 4.1. *For all* $\alpha, U > 0$ *and* $\kappa \le \infty$, *the following holds.*
(i) $E_\kappa(P) \le E_\kappa(0) + P^2/4$ *for all* P.
(ii) $E_\kappa(0) \le E_\kappa(P)$ *for all* P.
(iii) $E_\kappa(0) = E_{\mathrm{bp},\kappa}$.

Proof. These are well-known relations. However, for the reader's convenience, we give a proof.

(i) Let T be the time reversal operator which is defined by complex conjugation the wave function, reversing all phonon momenta. T is antiunitary and $TH_\kappa(P)T = H_\kappa(-P)$. Thus we conclude that

$$E_\kappa(-P) = E_\kappa(P)\,. \tag{11}$$

Let $F(P) := E_\kappa(P) - P^2/4$. Since $\langle\varphi, [H_\kappa(P) - P^2/4]\varphi\rangle$ is linear in P, F is concave. Moreover, by (11), $F(-P) = F(P)$. Thus,

$$F(0) = F\left(\frac{P}{2} - \frac{P}{2}\right) \geq \frac{1}{2}F(P) + \frac{1}{2}F(-P) = F(P)\,.$$

(ii) Let

$$K(P) = \frac{1}{4}(P - \mathbb{1}\otimes P_{\mathrm{f}})^2$$

and

$$H = -\Delta_{x_{\mathrm{r}}} \otimes \mathbb{1} + \frac{\alpha U}{|x_{\mathrm{r}}|} \otimes \mathbb{1} + \mathbb{1} \otimes N_{\mathrm{f}} + 2\sqrt{\alpha}\lambda_0 \int_{|k|\leq\kappa} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|} \cos\frac{k\cdot x_{\mathrm{r}}}{2} \otimes \left[a(k) + a(k)^*\right].$$

Then, $H_\kappa(P) = K(P)\dot{+}H$, where $\dot{+}$ means the form sum. We consider the Schrödinger representation $L^2(Q, \mathrm{d}\mu)$ of the Fock space $\mathfrak{F}(L^2(\mathbb{R}^3))$, where $\mathrm{d}\mu$ is the Gaussian measure with mean 0 and covariance $1/2$. Let ϑ be the unitary operator which gives the natural identification from $L^2(\mathbb{R}^3) \otimes \mathfrak{F}(L^2(\mathbb{R}^3))$ onto $L^2(\mathbb{R}^3 \times Q, \mathrm{d}x_{\mathrm{r}} \otimes \mathrm{d}\mu)$. We note that $\vartheta \mathrm{e}^{-tH}\vartheta^*$ is positivity preserving, see, e.g., [2]. Moreover, since

$$\mathrm{e}^{-t(P_j - \mathbb{1}\otimes P_{\mathrm{f},j})^2/4} = \int \mathrm{d}\mu_G(\lambda)\, \mathrm{e}^{\mathrm{i}\lambda(P_j - \mathbb{1}\otimes P_{\mathrm{f},j})}\,, \quad j = 1, 2, 3\,,$$

where μ_G is the Gaussian measure with mean zero and variance $t/2$, and $\vartheta\mathrm{e}^{-\mathrm{i}\lambda P_{\mathrm{f},j}}\vartheta^*$ is positivity preserving (see, e.g., [26]), we get

$$\begin{aligned}\left|\vartheta \mathrm{e}^{-t(P_j - \mathbb{1}\otimes P_{\mathrm{f},j})^2/4}\vartheta^*\varphi\right| &\leq \int \mathrm{d}\mu_G(\lambda)\, |\vartheta \mathrm{e}^{-\mathrm{i}\lambda \mathbb{1}\otimes P_{\mathrm{f},j}}\vartheta^*\varphi| \\ &\leq \int \mathrm{d}\mu_G(\lambda)\, \vartheta \mathrm{e}^{-\mathrm{i}\lambda \mathbb{1}\otimes P_{\mathrm{f},j}}\vartheta^*|\varphi| \\ &\leq \vartheta \mathrm{e}^{-t\mathbb{1}\otimes P_{\mathrm{f},j}^2/4}\vartheta^*|\varphi|\,.\end{aligned}$$

(Here we use the following fact: if A is positivity preserving, then $|A\varphi| \leq A|\varphi|$.) Therefore we conclude that

$$|\vartheta \mathrm{e}^{-tK(P)}\vartheta^*\varphi| \leq \vartheta \mathrm{e}^{-tK(0)}\vartheta^*|\varphi|\,. \tag{12}$$

Let $T_n = (\mathrm{e}^{-tK(P)/n}\mathrm{e}^{-tH/n})^n$. By the Trotter product formula, $\lim_{n\to\infty} T_n(P) = \mathrm{e}^{-tH_\kappa(P)}$. On the other hand, by the positivity preserving property for $\vartheta\mathrm{e}^{-tH}\vartheta^*$ and (12), we get $|\vartheta T_n(P)\vartheta^*\varphi| \leq \vartheta T_n(0)\vartheta^*|\varphi|$. Taking the limit $n \to \infty$, we arrive at $|\vartheta \mathrm{e}^{-tH_\kappa(P)}\vartheta^*\varphi| \leq \mathrm{e}^{-tH_\kappa(0)}|\varphi|$ which implies that

$$\left\langle \varphi, \vartheta \mathrm{e}^{-tH_\kappa(P)}\vartheta^*\varphi\right\rangle \leq \left\langle |\varphi|, \vartheta \mathrm{e}^{-tH_\kappa(0)}\vartheta^*|\varphi|\right\rangle\,. \tag{13}$$

Now we can derive (iii) from the above inequality.

(iii) To show $E_\kappa(0) \geq E_{\mathrm{bp},\kappa}$ is easy. To prove the converse, we just note that, by (ii),

$$\begin{aligned}\left\langle \varphi, H_{\mathrm{bp},\kappa}\varphi \right\rangle &= \int \mathrm{d}P \left\langle (\mathcal{U}\varphi)(P), H_\kappa(P)(\mathcal{U}\varphi)(P) \right\rangle_{L^2(\mathbb{R}^3)\otimes\mathfrak{F}(L^2(\mathbb{R}^3))} \\ &\geq \int \mathrm{d}P E_\kappa(P) \left\| (\mathcal{U}\varphi)(P) \right\|^2_{L^2(\mathbb{R}^3)\otimes\mathfrak{F}(L^2(\mathbb{R}^3))} \\ &\geq E_\kappa(0)\|\varphi\|^2 .\end{aligned}$$

□

4.2. Properties of the ionization energy

We introduce the ionization energy $\Sigma_\kappa(P)$ by

$$\Sigma_\kappa(P) = \lim_{R\to\infty} \inf_{\varphi\in\mathcal{D}_R,\, \|\varphi\|=1} \left\langle \varphi, H_\kappa(P)\varphi \right\rangle ,$$

where $\mathcal{D}_R = \big\{\varphi \in \mathrm{dom}\big(H_\kappa(P)\big) \mid \varphi(x) = 0 \text{ if } |x_{\mathrm{r}}| < R\big\}$.

Proposition 4.2. *For all $\alpha, U > 0$ and $\kappa < \infty$, the following holds.*

(i) $\Sigma_\kappa(P) \geq \Sigma_\kappa(0)$ *for all* P.

(ii) $\Sigma_\kappa(0) \geq 2E_{\mathrm{p},\kappa}$.

Remark 4.3. We can apply similar arguments in [8] to our model and see that $\Sigma_\kappa(0) = 2E_{\mathrm{p},\kappa}$. However the above inequality in (ii) is enough for our purpose.

Proof. (i) We consider the Schrödinger representation introduced in the previous subsection. By (13), we have

$$\frac{1}{t}\left\langle \varphi, \left(\mathbb{1} - \vartheta \mathrm{e}^{-t(H_\kappa(P)-E_\kappa(0))}\vartheta^*\right)\varphi \right\rangle \geq \frac{1}{t}\left\langle |\varphi|, \left(\mathbb{1} - \vartheta \mathrm{e}^{-t(H_\kappa(0)-E_\kappa(0))}\vartheta^*\right)|\varphi| \right\rangle \geq 0$$

for all $t>0$. By taking the limit $t \searrow 0$, we can conclude that if $\varphi\in\mathrm{dom}(\vartheta|H_\kappa(P)|^{1/2}\vartheta^*)$, then $|\varphi| \in \mathrm{dom}(\vartheta|H_\kappa(0)|^{1/2}\vartheta^*)$ and

$$\left\langle \varphi, \vartheta H_\kappa(P)\vartheta^*\varphi \right\rangle \geq \left\langle |\varphi|, \vartheta H_\kappa(0)\vartheta^*|\varphi| \right\rangle \tag{14}$$

as an inequality of forms. Let

$$\begin{aligned}\tilde{\Sigma}_{R,\kappa}(P) = \inf\Big\{ \left\langle \varphi, H_\kappa(P)\varphi \right\rangle \,\big|\, \varphi \in \mathrm{dom}\big(|H_\kappa(P)|^{1/2}\big)\,, \\ \|\varphi\| = 1 \ \text{ and } \ \varphi(x_{\mathrm{r}}) = 0 \ \text{ if } \ |x_{\mathrm{r}}| < R \Big\} .\end{aligned} \tag{15}$$

Then, by (14), we get

$$\tilde{\Sigma}_{R,\kappa}(P) \geq \tilde{\Sigma}_{R,\kappa}(0) . \tag{16}$$

Since, by Lemma 4.4 below, $\lim_{R\to\infty}\tilde{\Sigma}_{R,\kappa}(P) = \Sigma_\kappa(P)$, we conclude the desired assertion.

(ii) Let

$$\begin{aligned}\Sigma\left(H_{\mathrm{bp},\kappa}\right) = \lim_{R\to\infty} \inf\Big\{ \left\langle \varphi, H_{\mathrm{bp},\kappa}\varphi \right\rangle \,\big|\, \varphi \in \mathrm{dom}(H_{\mathrm{bp},\kappa}), \|\varphi\| = 1 \\ \text{and } \ \varphi(x_1, x_2) = 0 \ \text{ if } \ |x_1 - x_2| < R \Big\} .\end{aligned}$$

The inequality $\Sigma_\kappa(P) \geq \Sigma(H_{\mathrm{bp},\kappa})$ has been essentially proven in [7]. Namely assume that there exists P_0 such that $\Sigma_\kappa(P_0) < \Sigma(H_{\mathrm{bp},\kappa})$. Then there exists an $R > 0$ such that $\Sigma_{\kappa,R}(P_0) < \Sigma_R(H_{\mathrm{bp},\kappa})$, where

$$\Sigma_{\kappa,R}(P) = \inf\Big\{\big\langle\varphi, H_\kappa(P)\varphi\big\rangle \,|\, \varphi \in \mathcal{D}_R,\ \|\varphi\| = 1\Big\},$$

$$\Sigma_R(H_{\mathrm{bp},\kappa}) = \inf\Big\{\big\langle\varphi, H_{\mathrm{bp},\kappa}\varphi\big\rangle \,|\, \varphi \in \mathrm{dom}(H_{\mathrm{bp},\kappa}), \|\varphi\| = 1 \ \text{ and } \ \varphi(x_1,x_2) = 0 \ \text{ if } \ |x_1 - x_2| < R\Big\}.$$

Set $\gamma_R = \Sigma_R(H_{\mathrm{bp},\kappa}) - \Sigma_{\kappa,R}(P_0) > 0$. There exists a $\varphi \in \mathcal{D}_R$ so that $\|\varphi\| = 1$ and $\langle\varphi, H_\kappa(P_0)\varphi\rangle \leq \Sigma_R(H_{\mathrm{bp},\kappa}) - \gamma_R/2$. Since $\langle\varphi, H_\kappa(P)\varphi\rangle$ is continuous in P, there is a $\delta > 0$ such that, for all P with $|P - P_0| \leq \delta$, $\langle\varphi, H_\kappa(P)\varphi\rangle \leq \Sigma_R(H_{\mathrm{bp},\kappa}) - \gamma_R/4$. Choose $f \in C_0^\infty(\mathbb{R}^3)$ as $\mathrm{supp} f \subseteq \{P \in \mathbb{R}^3 \,|\, |P - P_0| \leq \delta\}$ with $\|f\| = 1$ and define $\varphi_f = f \times \varphi$ for $\varphi \in \mathcal{D}_R$ with $\|\varphi\| = 1$. Then we have $\langle\varphi_f, \mathcal{U}H_{\mathrm{bp},\kappa}\mathcal{U}^*\varphi_f\rangle \leq \Sigma_R(H_{\mathrm{bp},\kappa}) - \gamma_R/4$. Notice that $(\mathcal{U}^*\varphi_f)(x_1,x_2) = 0$ if $|x_1 - x_2| < R$. Hence one arrives at $\Sigma_R(H_{\mathrm{bp},\kappa}) \leq \Sigma_R(H_{\mathrm{bp},\kappa}) - \gamma_R/4$ which means a contradiction.

On the other hand, for $\varphi \in \mathrm{dom}(H_{\mathrm{bp},\kappa})$ such that $\|\varphi\| = 1$ and $\varphi(x_1,x_2) = 0$ if $|x_1 - x_2| < R$, we have that, by (16),

$$\begin{aligned}\langle\varphi, H_{\mathrm{bp},\kappa}\varphi\rangle &= \int \mathrm{d}P \big\langle(\mathcal{U}\varphi)(P), H_\kappa(P)(\mathcal{U}\varphi)(P)\big\rangle_{L^2(\mathbb{R}^3)\otimes\mathfrak{F}(L^2(\mathbb{R}^3))} \\ &\geq \int \mathrm{d}P\, \tilde{\Sigma}_{R,\kappa}(P)\big\|(\mathcal{U}\varphi)(P)\big\|^2_{L^2(\mathbb{R}^3)\otimes\mathfrak{F}(L^2(\mathbb{R}^3))} \\ &\geq \tilde{\Sigma}_{R,\kappa}(0),\end{aligned}$$

which implies $\Sigma(H_{\mathrm{bp},\kappa}) \geq \Sigma_\kappa(0)$ by Lemma 4.4 below. Hence we obtain that $\Sigma_\kappa(0) = \Sigma(H_{\mathrm{bp},\kappa})$.

Let $\bar{\phi}$ be the smooth nonnegative function on $\mathbb{R}^3$, identically one outside the ball of radius 2 and vanishing inside the unit ball. Set $\bar{\phi}_R(x_1,x_2) = \bar{\phi}(|x_1 - x_2|/R)$. By Lemma D.1, we have that

$$\big\langle\bar{\phi}_R\varphi, H_{\mathrm{bp},\kappa}\bar{\phi}_R\varphi\big\rangle \geq 2E_{\mathrm{p},\kappa}\|\bar{\phi}_R\varphi\|^2 + O(1),$$

where $O(1)$ is the error term satisfying $|O(1)| \leq G(R)(\langle\varphi, H_{\mathrm{bp},\kappa}\varphi\rangle + b\|\varphi\|^2)$ with $G(R)$ vanishing as $R \to \infty$, and some positive constant $b > E_{\mathrm{bp},\kappa}$. Choose $\varphi \in \mathrm{dom}(H_{\mathrm{bp},\kappa})$ with $\|\varphi\| = 1$ and $\varphi(x) = 0$ if $|x_1 - x_2| < 2R$. (Note that $\bar{\phi}_R\varphi = \varphi$.) Then, by the above inequality, we have that $(1 + G(R))\Sigma_{2R}(H_{\mathrm{bp},\kappa}) \geq 2E_{\mathrm{p},\kappa} - bG(R)$. Taking $R \to \infty$, we conclude that $\Sigma(H_{\mathrm{bp},\kappa}) \geq 2E_{\mathrm{p},\kappa}$. □

Lemma 4.4. *Let* $\tilde{\Sigma}_{R,\kappa}(P)$ *be given by* (15)*. Then,*

$$\lim_{R\to\infty} \tilde{\Sigma}_{R,\kappa}(P) = \Sigma_\kappa(P).$$

Proof. It is clear that $\tilde{\Sigma}_{R,\kappa}(P) \leq \Sigma_{R,\kappa}(P)$ which implies $\lim_{R\to\infty}\tilde{\Sigma}_{R,\kappa}(P) \leq \Sigma_\kappa(P)$. We will prove the converse. Fix R for a while. For arbitrary $\varepsilon > 0$, there exists $\varphi \in \mathrm{dom}(|H_\kappa(P)|^{1/2})$ such that $\|\varphi\| = 1$, $\varphi(x_\mathrm{r}) = 0$ if $x_\mathrm{r} < R$ and

$$\langle \varphi, H_\kappa(P)\varphi \rangle \le \tilde{\Sigma}_{R,\kappa}(P) + \frac{\varepsilon}{2}\,.$$

For this φ, there exists a sequence $\{\varphi_n\} \subset \mathrm{dom}(H_\kappa(P))$ such that $\|\varphi_n\| = 1$, $\lim_{n\to\infty} \|\varphi - \varphi_n\| = 0$ and

$$\langle \varphi_n, H_\kappa(P)\varphi_n \rangle \le \langle \varphi, H_\kappa(P)\varphi \rangle + \frac{\varepsilon}{2}$$

for all sufficiently large n. Let χ and $\bar{\chi}$ be the two localization functions with $\chi^2 + \bar{\chi}^2 = 1$, χ is identically one on the unit ball and vanishing outside the ball of radius 2. We introduce $\chi_R(x_\mathrm{r}) = \chi(2x_\mathrm{r}/R)$ and $\bar{\chi}_R(x_\mathrm{r}) = \bar{\chi}(2x_\mathrm{r}/R)$. Then, since $\bar{\chi}_R\varphi_n \in \mathrm{dom}(H_\kappa(P))$ and $(\bar{\chi}_R\varphi_n)(x_\mathrm{r}) = 0$ if $|x_\mathrm{r}| < R/2$, we get, by the IMS localization formula, that

$$\begin{aligned}\langle \varphi_n, H_\kappa(P)\varphi_n \rangle &= \langle \varphi_n, \chi_R H_\kappa(P)\chi_R\varphi_n \rangle + \langle \varphi_n, \bar{\chi}_R H_\kappa(P)\bar{\chi}_R\varphi_n \rangle \\ &\quad - \langle \varphi_n, (\nabla_{x_\mathrm{r}}\chi_R)^2\varphi_n \rangle - \langle \varphi_n, (\nabla_{x_\mathrm{r}}\bar{\chi_R})^2\varphi_n \rangle \\ &\ge E_\kappa(P)\|\chi_R\varphi_n\|^2 + \Sigma_{R/2,\kappa}(P)\|\bar{\chi}_R\varphi\|^2 - \frac{C}{R^2}\,,\end{aligned}$$

where C is a positive constant independent of n and ε. Combining these results, we arrive at

$$E_\kappa(P)\|\chi_R\varphi_n\|^2 + \Sigma_{R/2,\kappa}(P)\|\bar{\chi}_R\varphi_n\|^2 - \frac{C}{R^2} \le \tilde{\Sigma}_{R,\kappa}(P) + \varepsilon\,.$$

First, we take $n \to \infty$. Notice that $\text{s-lim}_{n\to\infty} \chi_R\varphi_n = 0$ and $\text{s-lim}_{n\to\infty} \bar{\chi}_R\varphi_n = \varphi$. Hence,

$$\Sigma_{R/2,\kappa}(P) - \frac{C}{R^2} \le \tilde{\Sigma}_{R,\kappa}(P) + \varepsilon\,.$$

Since ε is arbitrary, we have that $\Sigma_{R/2,\kappa}(P) - C/R^2 \le \tilde{\Sigma}_{R,\kappa}(P)$. Next, we take $R \to \infty$, then we get the desired result. □

4.3. Existence of a ground state under the ultraviolet cutoff

We define the binding energy with the ultraviolet cutoff κ by

$$E_{\mathrm{bin},\kappa} = 2E_{\mathrm{p},\kappa} - E_{\mathrm{bp},\kappa}\,.$$

We remark that, by Proposition B.1, $\lim_{\kappa\to\infty} E_{\mathrm{bin},\kappa} = E_\mathrm{bin}$. In this subsection, we will prove the following proposition.

Proposition 4.5.

$$\inf \mathrm{ess.\,spec}\big(H_\kappa(P)\big) - E_\kappa(P) \ge \min\{1, E_{\mathrm{bin},\kappa}\} - \frac{P^2}{4}\,. \tag{17}$$

Remark 4.6. Since the phonon dispersion relation is constant, we can not apply the method developed in [3, 9, 17] directly. The main purpose of this subsection is to show how to overcome this difficulty.

Before we enter the proof, we note the following.

Proof of Theorem 2.6. The assertion directly follows from Proposition 4.5, B.1 and B.2. $\square$

Let j_1 and j_2 be two smooth localization functions so that $j_1^2 + j_2^2 = 1$ and j_1 is supported in a ball of radius L. We introduce a linear operator j from $L^2(\mathbb{R}^3)$ to $L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$ by

$$jf = j_1(-\mathrm{i}\nabla_k)f \oplus j_2(-\mathrm{i}\nabla_k)f$$

for $f \in L^2(\mathbb{R}^3)$. Note that $j^*j = \mathbb{1}$. Let U be the unitary operator from $\mathfrak{F}(L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3))$ to $\mathfrak{F}(L^2(\mathbb{R}^3)) \otimes \mathfrak{F}(L^2(\mathbb{R}^3))$ defined by

$$\begin{aligned}\mathsf{U}a(f_1 \oplus g_1)^* \cdots a(f_n \oplus g_n)^*\Omega = \big[a(f_1)^* \otimes \mathbb{1} + \mathbb{1} \otimes a(g_1)^*\big] \cdots \\ \big[a(f_n)^* \otimes \mathbb{1} + \mathbb{1} \otimes a(g_n)^*\big]\Omega \otimes \Omega\,, \mathsf{U}\Omega = \Omega \otimes \Omega\,.\end{aligned}$$

We set

$$\check{\Gamma}(j) = \mathsf{U}\Gamma(j) \,:\, \mathfrak{F}\big(L^2(\mathbb{R}^3)\big) \to \mathfrak{F}\big(L^2(\mathbb{R}^3)\big) \otimes \mathfrak{F}\big(L^2(\mathbb{R}^3)\big)\,.$$

Then $\check{\Gamma}(j)$ is also isometry and we have the following localization formula in a similar way to [17], see also [9, Lemma A.1]. (We also remark that essential idea here was first established in [3].)

Lemma 4.7. *Let $H_\kappa^\otimes(P)$ be the self-adjoint operator on $L^2(\mathbb{R}^3) \otimes \mathfrak{F}(L^2(\mathbb{R}^3)) \otimes \mathfrak{F}(L^2(\mathbb{R}^3))$ defined by*

$$\begin{aligned}&\frac{1}{4}\big(P - \mathbb{1} \otimes P_\mathrm{f} \otimes \mathbb{1} - \mathbb{1} \otimes \mathbb{1} \otimes P_\mathrm{f}\big)^2 + \left(-\Delta_{x_\mathrm{r}} + \frac{\alpha U}{|x_\mathrm{r}|}\right) \otimes \mathbb{1} \otimes \mathbb{1} \\ &\quad + \mathbb{1} \otimes N_\mathrm{f} \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{1} \otimes N_\mathrm{f} \\ &\quad + 2\sqrt{\alpha}\lambda_0 \int_{|k|\le\kappa} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|} \cos\frac{k\cdot x_\mathrm{r}}{2} \otimes \big[a(k) + a(k)^*\big] \otimes \mathbb{1}\,.\end{aligned}$$

(i) *Let χ be a smooth nonnegative function on $\mathbb{R}^3$ that is compactly supported. Then, for $\varphi \in C_0^\infty(\mathbb{R}^3)\hat{\otimes}\mathfrak{F}_\mathrm{fin}(C_0^\infty(\mathbb{R}^3))$,*

$$\big\langle \chi\varphi, H_\kappa(P)\chi\varphi\big\rangle = \big\langle \check{\Gamma}(j)\chi\varphi, H_\kappa^\otimes(P)\check{\Gamma}(j)\chi\varphi\big\rangle + o_L(\varphi)\,,$$

where $o_L(\varphi)$ is the error term which satisfies

$$\big|o_L(\varphi)\big| \le \tilde{o}(L^0)\big(\|H_\kappa(P)\varphi\|^2 + \|\varphi\|^2\big)\,.$$

Here $\tilde{o}_L(L^0)$ is a function of L does not depend on φ and vanishes as $L \to \infty$.

(ii) *Let $\Delta_\kappa(P) = E_\kappa(0) - E_\kappa(P) + 1$. For $\varphi \in \mathrm{dom}(H_\kappa^\otimes(P))$,*

$$\big\langle \varphi, H_\kappa^\otimes(P)\varphi\big\rangle \ge \Big\langle \varphi, \big[E_\kappa(P) + (\mathbb{1} - P_\Omega)\Delta_\kappa(P)\big]\varphi\Big\rangle\,,$$

where P_Ω is the orthogonal projection onto $L^2(\mathbb{R}^3) \otimes \mathfrak{F}(L^2(\mathbb{R}^3)) \otimes \Omega$.

Let ϕ and $\bar{\phi}$ be smooth nonnegative functions with $\phi^2 + \bar{\phi}^2 = 1$, ϕ identically one on the unit ball, and vanishing outside the ball of radius 2. Define $\phi_R(x_{\rm r}) = \phi(x_{\rm r}/R)$ and $\bar{\phi}_R(x_{\rm r}) = \bar{\phi}(x_{\rm r}/R)$. It is not hard to see that, for $\Psi \in C_0^\infty(\mathbb{R}^3)\hat{\otimes}\mathfrak{F}_{\rm fin}(C_0^\infty(\mathbb{R}))$,

$$\begin{aligned}\big\langle \Psi, H_\kappa(P)\Psi\big\rangle &= \big\langle \phi_R\Psi, H_\kappa(P)\phi_R\Psi\big\rangle + \big\langle \bar{\phi}_R\Psi, H_\kappa(P)\bar{\phi}_R\Psi\big\rangle \\ &\quad - \big\langle \Psi, (\nabla_{x_{\rm r}}\phi_R)^2\Psi\big\rangle - \big\langle \Psi, (\nabla_{x_{\rm r}}\bar{\phi}_R)^2\Psi\big\rangle\,. \end{aligned} \tag{18}$$

By Proposition 4.2, we get

$$\begin{aligned}\big\langle \bar{\phi}_R\Psi, H_\kappa(P)\bar{\phi}_R\Psi\big\rangle &\geq \Sigma_{\kappa,R}(P)\|\bar{\phi}_R\Psi\|^2 \\ &\geq \Sigma_\kappa(P)\|\bar{\phi}_R\Psi\|^2 + \tilde{o}(R^0)\|\Psi\|^2 \\ &\geq \Sigma_\kappa(0)\|\bar{\phi}_R\Psi\|^2 + \tilde{o}(R^0)\|\Psi\|^2 \\ &\geq 2E_{{\rm p},\kappa}\|\bar{\phi}_R\Psi\|^2 + \tilde{o}(R^0)\|\Psi\|^2\,, \end{aligned} \tag{19}$$

where $\Sigma_{\kappa,R}(P) = \inf_{\varphi\in\mathcal{D}_R,\|\varphi\|=1}\langle\varphi, H_\kappa(P)\varphi\rangle$. On the other hand, by Lemma 4.7 and the fact $\|P_\Omega\phi_R\otimes\check{\Gamma}(j)\Psi\| = \|\phi_R\otimes\Gamma(j_1(-{\rm i}\nabla_k))\Psi\|$, we obtain

$$\begin{aligned}\big\langle \phi_R\Psi, H_\kappa(P)\phi_R\Psi\big\rangle &\geq \big(E_\kappa(P) + \Delta_\kappa(P)\big)\|\phi_R\Psi\|^2 \\ &\quad - \Delta_\kappa(P)\|\phi_R\otimes\Gamma\big(j_1(-{\rm i}\nabla_k)\big)\Psi\|^2 + \tilde{o}(L^0)\|\Psi\|^2_{H_\kappa(P)}\,, \end{aligned} \tag{20}$$

where $\|\varphi\|_A^2 = \|A\varphi\|^2 + \|\varphi\|^2$ for a self-adjoint operator A. To summarize, by combining (18), (19), (20) and the facts $\Delta_\kappa(P) \geq 1 - P^2/4$ and $2E_{{\rm p},\kappa} - E_\kappa(P) \geq E_{{\rm bin},\kappa} - P^2/4$ which follow from Proposition 4.1 (i), we have the following.

Lemma 4.8. *For $\Psi \in {\rm dom}(H_\kappa(P))$,*

$$\begin{aligned}\big\langle \Psi, H_\kappa(P)\Psi\big\rangle &\geq \left(E_\kappa(P) + \min\{1, E_{{\rm bin},\kappa}\} - \frac{P^2}{4}\right)\|\Psi\|^2 \\ &\quad - \Delta_\kappa(P)\|\phi_R\otimes\Gamma\big(j_1(-{\rm i}\nabla_k)\big)\Psi\|^2 + o(1)\|\Psi\|^2_{H_\kappa(P)}\,, \end{aligned} \tag{21}$$

where $o(1)$ is the error term vanishing uniformly in Ψ as both $L, R \to \infty$.

We set

$$\mathbb{R}^3_{\leq\kappa} = \big\{k\in\mathbb{R}^3 \,|\, |k|\leq\kappa\big\}\,, \quad \mathbb{R}^3_{>\kappa} = \big\{k\in\mathbb{R}^3 \,|\, |k|>\kappa\big\}$$

for each $\kappa > 0$. It is well-known that there exists a unitary operator V_κ such that

$$V_\kappa\mathfrak{F}\big(L^2(\mathbb{R}^3)\big) = \mathfrak{F}\big(L^2(\mathbb{R}^3_{\leq\kappa})\big)\otimes\mathfrak{F}\big(L^2(\mathbb{R}^3_{>\kappa})\big)\,, \tag{22}$$

$$V_\kappa a(f)V_\kappa^* = a(f_{\leq\kappa})\otimes 1\!\!1 + 1\!\!1\otimes a(f_{>\kappa}) \tag{23}$$

with $f_{\leq\kappa} = \chi_\kappa f$ and $f_{>\kappa} = (1-\chi_\kappa)f$. (Here $\chi_\kappa(k) = 1$ for $|k|\leq\kappa$, $\chi_\kappa(k) = 0$ otherwise.) We also note that, for a multiplication operator h by the function $h(k)$,

$$V_\kappa {\rm d}\Gamma(h)V_\kappa^* = {\rm d}\Gamma(h_{\leq\kappa})\otimes 1\!\!1 + 1\!\!1\otimes{\rm d}\Gamma(h_{>\kappa})\,.$$

In particular,

$$V_\kappa N_{\rm f}V_\kappa^* = N_{\leq\kappa}\otimes 1\!\!1 + 1\!\!1\otimes N_{>\kappa} \tag{24}$$

where $N_{\le\kappa}$ and $N_{>\kappa}$ are the number operators on $\mathfrak{F}(L^2(\mathbb{R}^3_{\le\kappa}))$ and $\mathfrak{F}(L^2(\mathbb{R}^3_{>\kappa}))$, respectively. For notational simplicity, we denote the unitary operator $\mathbb{1}\otimes V_\kappa$ acting in $L^2(\mathbb{R}^3)\otimes\mathfrak{F}(L^2(\mathbb{R}^3))$ by the symbol V_κ. Let $\mathcal{H}_\kappa = L^2(\mathbb{R}^3)\otimes\mathfrak{F}(L^2(\mathbb{R}^3_{\le\kappa}))$. Then, we can easily see that

$$\begin{aligned} V_\kappa L^2(\mathbb{R}^3)\otimes\mathfrak{F}\big(L^2(\mathbb{R}^3)\big) &= \mathcal{H}_\kappa\otimes\mathfrak{F}\big(L^2(\mathbb{R}^3_{>\kappa})\big) \\ &= \mathcal{H}_\kappa\oplus\bigoplus_{n=1}^{\infty}\Big[\mathcal{H}_\kappa\otimes\big(\otimes_{\mathrm{s}}^n L^2(\mathbb{R}^3_{>\kappa})\big)\Big] \\ &= \mathcal{H}_\kappa\oplus\bigoplus_{n=1}^{\infty} L^2_{\mathrm{sym}}\Big(\underbrace{\mathbb{R}^3_{>\kappa}\times\cdots\times\mathbb{R}^3_{>\kappa}}_{n};\mathcal{H}_\kappa\Big)\,, \end{aligned} \tag{25}$$

where $L^2_{\mathrm{sym}}\Big(\underbrace{\mathbb{R}^3_{>\kappa}\times\cdots\times\mathbb{R}^3_{>\kappa}}_{n};\mathcal{H}_\kappa\Big)$ is the $\mathcal{H}_\kappa$-valued symmetric L^2-space on $\underbrace{\mathbb{R}^3_{>\kappa}\times\cdots\times\mathbb{R}^3_{>\kappa}}_{n}$. Under the natural identification (25), the Hamiltonian $H_\kappa(P)$ can be identified as

$$\begin{aligned} &V_\kappa H_\kappa(P)V_\kappa^* \\ &\quad= H_{\le\kappa}(P)\oplus\bigoplus_{n=1}^{\infty}\left[\int^{\oplus}_{|k_1|,\dots,|k_n|>\kappa}\left(H_{\le\kappa}\left(P-\sum_{j=1}^{n}k_j\right)+n\right)\mathrm{d}k_1\cdots\mathrm{d}k_n\right], \end{aligned} \tag{26}$$

where

$$\begin{aligned} H_{\le\kappa}(P) &= \frac{1}{4}(P-\mathbb{1}\otimes P_{\mathrm{f},\le\kappa})^2+\left(-\Delta_{x_\mathrm{r}}+\frac{\alpha U}{|x_\mathrm{r}|}\right)\otimes\mathbb{1}+\mathbb{1}\otimes N_{\le\kappa} \\ &\quad+2\sqrt{\alpha}\lambda_0\int_{|k|\le\kappa}\frac{\mathrm{d}k}{(2\pi)^{3/2}|k|}\cos\frac{k\cdot x_\mathrm{r}}{2}\otimes\big[a(k)+a(k)^*\big] \end{aligned}$$

which is acting in $\mathcal{H}_\kappa$ and $P_{\mathrm{f},\le\kappa} = \int_{|k|\le\kappa}\mathrm{d}k\, k a(k)^*a(k)$. We note that, by the Kato–Rellich theorem, $H_{\le\kappa}(P)$ is self-adjoint on $\mathrm{dom}(-\Delta_{x_\mathrm{r}}\otimes\mathbb{1})\cap\mathrm{dom}(\mathbb{1}\otimes P^2_{\mathrm{f},\le\kappa})\cap\mathrm{dom}(\mathbb{1}\otimes N_{\le\kappa})$ for all P. Therefore, by the closed graph theorem, there exists a positive constant C such that

$$\big\|\big(-\Delta_{x_\mathrm{r}}\otimes\mathbb{1}+\mathbb{1}\otimes P^2_{\mathrm{f},\le\kappa}+\mathbb{1}\otimes N_{\le\kappa}\big)\varphi\big\|\le C\big(\|H_{\le\kappa}(P)\varphi\|+\|\varphi\|\big) \tag{27}$$

for $\varphi\in\mathrm{dom}(-\Delta_{x_\mathrm{r}}\otimes\mathbb{1})\cap\mathrm{dom}(\mathbb{1}\otimes P^2_{\mathrm{f},\le\kappa})\cap\mathrm{dom}(\mathbb{1}\otimes N_{\le\kappa})$.

Lemma 4.9. *Let* $C_\kappa(P) = E_\kappa(P)+\min\{1,E_{\mathrm{bin},\kappa}\}-P^2/4$.

$$\inf\operatorname{ess.spec}\big(H_{\le\kappa}(P)\big)\ge C_\kappa(P)\,.$$

Proof. By Lemma 4.8, we get

$$\begin{aligned} \big\langle\psi,H_{\le\kappa}(P)\psi\big\rangle &\ge C_\kappa(P)\|\psi\|^2-\Delta_\kappa(P)\|\phi_R\otimes\Gamma\big(j_1(-\mathrm{i}\nabla_k)\big)V_\kappa^*\psi\otimes\Omega_{>\kappa}\|^2 \\ &\quad+o(1)\|\psi\|^2_{H_{\le\kappa}(P)} \end{aligned} \tag{28}$$

for $\psi \in \mathrm{dom}(H_{\le\kappa}(P))$, where $\Omega_{>\kappa}$ is the Fock vacuum in $\mathfrak{F}(L^2(\mathbb{R}^3_{>\kappa}))$. By Weyl's criterion, for any $\lambda \in \mathrm{ess.\,spec}(H_{\le\kappa}(P))$, there is a normalized sequence $\{\psi_n\} \subset \mathrm{dom}(H_{\le\kappa}(P))$ such that $\text{w-lim}_{n\to\infty}\ \psi_n = 0$ and $\lim_{n\to\infty} \|(H_{\le\kappa}(P) - \lambda)\psi_n\| = 0$. Then, by (28),

$$\big\langle \psi_n, H_{\le\kappa}(P)\psi_n\big\rangle \ge C_\kappa(P) - \Delta_\kappa(P)\big\|\phi_R \otimes \Gamma\big(j_1(-\mathrm{i}\nabla_k)\big)V_\kappa^*\psi_n \otimes \Omega_{>\kappa}\big\|^2 + o(1)\|\psi_n\|^2_{H_{\le\kappa}(P)}\,. \tag{29}$$

We remark that, by (27),

$$\langle V_\kappa^*\psi_n \otimes \Omega_{>\kappa}, \mathbb{1} \otimes N_{\mathrm{f}} V_\kappa^*\psi_n \otimes \Omega_{>\kappa}\rangle = \langle \psi_n, \mathbb{1} \otimes N_{\le\kappa}\psi_n\rangle \le C < \infty\,,$$

where C is a positive constant independent of n. From this, it follows that

$$\big\|\phi_R \otimes \big(\mathbb{1} - \chi_M(N_{\mathrm{f}})\big)\Gamma\big(j_1(-\mathrm{i}\nabla_k)\big)V_\kappa^*\psi_n \otimes \Omega_{>\kappa}\big\| \le \frac{\mathrm{Const.}}{M}\,. \tag{30}$$

Let η be a continuous positive function on $\mathbb{R}^3$ that is identically one on the unit ball, and vanishing outside the ball of radius 2. Set $\eta_\kappa(k) = \eta(k/\kappa)$. We note that

$$V_\kappa^*\psi_n \otimes \Omega_{>\kappa} = \mathbb{1}_{L^2(\mathbb{R}^3)} \otimes \Gamma(\eta_\kappa)V_\kappa^*\psi_n \otimes \Omega_{>\kappa} \tag{31}$$

for all $n \in \mathbb{N}$. Hence, we obtain

$$\begin{aligned}&\big\|\phi_R \otimes \chi_M(N_{\mathrm{f}})\Gamma\big(j_1(-\mathrm{i}\nabla_k)\big)V_\kappa^*\psi_n \otimes \Omega\big\|^2 \\ &\quad = \Big\langle (-\Delta_{x_{\mathrm{r}}} + \mathbb{1})^{1/2} \otimes \chi_M(N_{\mathrm{f}})\Gamma\big(j_1(-\mathrm{i}\nabla_k)\big)V_\kappa^*\psi_n \otimes \Omega_>\kappa, \\ &\qquad (-\Delta_{x_{\mathrm{r}}} + \mathbb{1})^{-1/2}\phi_R^2 \otimes \chi_M(N_{\mathrm{f}})\Gamma\big(j_1(-\mathrm{i}\nabla_k)\big)\Gamma(\eta_\kappa)V_\kappa^*\psi_n \otimes \Omega_{>\kappa}\Big\rangle\,.\end{aligned}$$

It is not hard to check that, by (27),

$$\begin{aligned}&\big\|(-\Delta_{x_{\mathrm{r}}} + \mathbb{1})^{1/2} \otimes \chi_M(N_{\mathrm{f}})\Gamma\big(j_1(-\mathrm{i}\nabla_k)\big)V_\kappa^*\psi_n \otimes \Omega_{>\kappa}\big\|^2 \\ &\qquad \le \mathrm{Const.}\ \Big\langle \psi_n, \big(H_{\le\kappa}(P) + \mathbb{1}\big)\psi_n\Big\rangle\,.\end{aligned}$$

The right hand side of this inequality is uniformly bounded in n. Furthermore, $(-\Delta_{x_{\mathrm{r}}} + \mathbb{1})^{-1/2}\phi_R^2 \otimes \chi_M(N_{\mathrm{f}})\Gamma(j_1(-\mathrm{i}\nabla_k))\Gamma(\eta_\kappa)$ is a compact operator which implies

$$\text{s-}\lim_{n\to\infty}(-\Delta_{x_{\mathrm{r}}} + \mathbb{1})^{-1/2}\phi_R^2 \otimes \chi_M(N_{\mathrm{f}})\Gamma\big(j_1(-\mathrm{i}\nabla_k)\big)\Gamma(\eta_\kappa)V_\kappa^*\psi_n \otimes \Omega_{>\kappa} = 0\,.$$

From these facts, one concludes that

$$\lim_{n\to\infty}\big\|\phi_R \otimes \Gamma\big(j_1(-\mathrm{i}\nabla_k)\big)V_\kappa^*\psi_n \otimes \Omega_{>\kappa}\big\| = 0$$

and, by (29),

$$\lambda \ge C_\kappa(P) + o(1)(\lambda^2 + 1)\,. \tag{32}$$

Taking $L \to \infty$ and $R \to \infty$, we obtain the desired result. □

Proof of Proposition 4.5. By (26), we have

$$\inf \mathrm{ess.\,spec}\big(H_\kappa(P)\big) = \min\Big\{\inf \mathrm{ess.\,spec}\big(H_{\le\kappa}(P)\big), \tau(P)\Big\}\,, \tag{33}$$

where

$$\tau(P) = \inf_{n\ge 1} \inf_{k_1,\dots,k_n\in\mathbb{R}^3_{>\kappa}} \left[\inf\mathrm{spec}\left(H_{\le\kappa}\left(P-\sum_{j=1}^n k_j\right)\right)+n\right].$$

First, we show that

$$\tau(P) \ge E_\kappa(0) + 1\,. \tag{34}$$

Since

$$\big\langle V_\kappa^* f\otimes\Omega_{>\kappa}, H_\kappa(P)V_\kappa^* f\otimes\Omega_{>\kappa}\big\rangle = \big\langle f, H_{\le\kappa}(P)f\big\rangle\,,$$

we have that

$$E_\kappa(P) \le \inf\mathrm{spec}\big(H_{\le\kappa}(P)\big)$$

for all P. Combining this with Proposition 4.1 (iii), we can check (34).

From Proposition 4.1 (i), Lemma 4.9 and (34), it follows that

$$\begin{aligned}\inf \mathrm{ess.\,spec}\big(H_\kappa(P)\big) - E_\kappa(P) &\ge \min\Big\{\min\big\{1, E_{\mathrm{bin},\kappa}\big\} - \frac{P^2}{4}\,, E_\kappa(0) - E_\kappa(P) + 1\Big\}\\ &\ge \min\Big\{\min\{1, E_{\mathrm{bin},\kappa}\} - \frac{P^2}{4}, 1 - \frac{P^2}{4}\Big\}\\ &= \min\big\{1, E_{\mathrm{bin},\kappa}\big\} - \frac{P^2}{4}\,.\end{aligned}$$

□

Appendix A. Self-adjointness, fiber decomposition

A.1. Proof of Theorem 2.1 (i)

The basic idea of the proof is due to Nelson [21]. Let $K < \kappa$, and let the linear operator $T_{\kappa,K}$ be given by

$$T_{\kappa,K} = \sum_{j=1,2}\int_{|k|\le\kappa} \mathrm{d}k\,\beta_K(k)\left[\mathrm{e}^{\mathrm{i}k\cdot x_j}\otimes a(k) - \mathrm{e}^{-\mathrm{i}k\cdot x_j}\otimes a(k)^*\right]$$

with

$$\beta_K(k) = -\frac{\sqrt{\alpha}\lambda_0}{(2\pi)^{3/2}|k|(1+k^2/2)}\big(1-\chi_K(k)\big)\,,$$

where $\chi_K(k) = 1$ for $|k|\le K$, $\chi_K(k) = 0$ otherwise. $T_{\kappa,K}$ is a skew symmetric operator. We denote the closure of $T_{\kappa,K}$ by the same symbol. Then $T_{\kappa,K}$ is a skew-adjoint operator: $T^*_{\kappa,K} = -T_{\kappa,K}$. The unitary operator $U_{\kappa,K} = \mathrm{e}^{T_{\kappa,K}}$ is called the *Gross transformation*. We can easily observe that

$$U_{\kappa,K}p_j\otimes 1\!\!1 U^*_{\kappa,K} = p_j\otimes 1\!\!1 - A_{\kappa,K}(x_j) - A_{\kappa,K}(x_j)^*\,, \tag{35}$$

$$U_{\kappa,K}1\!\!1\otimes a(k)U^*_{\kappa,K} = 1\!\!1\otimes a(k) + \sum_{j=1,2}\beta_K(k)\chi_\kappa(k)\mathrm{e}^{-\mathrm{i}k\cdot x_j}\otimes 1\!\!1\,, \tag{36}$$

where

$$A_{\kappa,K}(x) = \int_{|k|\le\kappa} \mathrm{d}k\, k\beta_K(k)\mathrm{e}^{\mathrm{i}k\cdot x} \otimes a(k)$$

and we use the symbol $p_j = -\mathrm{i}\nabla_{x_j}$ $(j = 1, 2)$. Using these formulae one gets

$$U_{\kappa,K} H_{\mathrm{bp},\kappa} U_{\kappa,K}^* = H_{\kappa,K}^{\mathrm{bp}} \tag{37}$$

on $C_0^\infty(\mathbb{R}^6)\hat{\otimes}\mathfrak{F}_{\mathrm{fin}}(L^2(\mathbb{R}^3))$, where

$$\begin{aligned} H_{\kappa,K}^{\mathrm{bp}} = \sum_{j=1,2} \Big\{ &- \frac{1}{2}\Delta_j \otimes 1\!\!1 + \frac{1}{2}\big(- 2p_j \cdot A_{\kappa,K}(x_j) - 2A_{\kappa,K}(x_j)^* \cdot p_j \\ &+ A_{\kappa,K}(x_j)^2 + A_{\kappa,K}(x_j)^{*2} + 2A_{\kappa,K}(x_j)^* \cdot A_{\kappa,K}(x_j)\big) \\ &+ \sqrt{\alpha}\lambda_0 \int_{|k|\le K} \mathrm{d}k\, \frac{1}{(2\pi)^{3/2}|k|} \big(\mathrm{e}^{\mathrm{i}k\cdot x_j} \otimes a(k) + \mathrm{e}^{-\mathrm{i}k\cdot x_j} \otimes a(k)^*\big) \Big\} \\ &+ 1\!\!1 \otimes N_{\mathrm{f}} + V_{\kappa,K}(x_1 - x_2) \otimes 1\!\!1 + \frac{\alpha U}{|x_1 - x_2|} \otimes 1\!\!1 + E_{\kappa,K}\,, \end{aligned} \tag{38}$$

$$V_{\kappa,K}(x_1 - x_2) = \sum_{i\ne j} \int_{|k|\le\kappa} \mathrm{d}k \left\{ \beta_K(k)^2 + \frac{2\sqrt{\alpha}\lambda_0}{(2\pi)^{3/2}|k|}\beta_K(k) \right\} \mathrm{e}^{-\mathrm{i}k\cdot(x_i - x_j)}\,,$$

$$E_{\kappa,K} = -2\alpha\lambda_0^2 \int_{K\le|k|\le\kappa} \mathrm{d}k\, \frac{1}{(2\pi)^3(1 + k^2/2)|k|^2}\,.$$

Notice that $E_{\kappa,K}$ is finite even for $\kappa = \infty$. $H_{\kappa,K}^{\mathrm{bp}}$ is closable and we denote its closure by the same symbol.

Proposition A.1. *For any $\alpha < \infty, U < \infty, \kappa < \infty$ and K, $H_{\kappa,K}^{\mathrm{bp}}$ is self-adjoint on* $\mathrm{dom}(L_{\mathrm{bp}})$*, essentially self-adjoint on any core for L_{bp} and bounded from below. Moreover*

$$U_{\kappa,K} H_{\mathrm{bp},\kappa} U_{\kappa,K}^* = H_{\kappa,K}^{\mathrm{bp}}\,.$$

Proof. By the inequality (1), and

$$\|a(f)^\# a(g)^\# \varphi\| \le 8\|f\|\|g\|\|(N_{\mathrm{f}} + 1\!\!1)\varphi\|\,,$$

one can check that

$$\|H_{\kappa,K}^{\mathrm{bp}}\varphi\| \le C(\|L_{\mathrm{bp}}\varphi\| + \|\varphi\|)\,, \quad \varphi \in \mathrm{dom}(L_{\mathrm{bp}})$$

with some positive constant $C < \infty$. (Note that the finiteness of κ is crucial here.) From this we have

$$\|H_{\mathrm{bp},\kappa} U_{\kappa,K}\varphi\| = \|U_{\kappa,K}^* H_{\mathrm{bp},\kappa} U_{\kappa,K}\varphi\| \le C(\|L_{\mathrm{bp}}\varphi\| + \|\varphi\|) \tag{39}$$

for $\varphi \in C_0^\infty(\mathbb{R}^6)\hat{\otimes}\mathfrak{F}_{\mathrm{fin}}(C_0^\infty(\mathbb{R}^3))$. Since $\mathrm{dom}(H_{\mathrm{bp},\kappa}) = \mathrm{dom}(L_{\mathrm{bp}})$, we have

$$\|L_{\mathrm{bp}} U_{\kappa,K}\varphi\| \le C'(\|L_{\mathrm{bp}}\varphi\| + \|\varphi\|)\,, \quad \varphi \in C_0^\infty(\mathbb{R}^6)\hat{\otimes}\mathfrak{F}_{\mathrm{fin}}\big(C_0^\infty(\mathbb{R}^3)\big)$$

by the closed graph theorem and (39). Thus we conclude that $U_{\kappa,K}\mathrm{dom}(L_{\mathrm{bp}}) \subseteq \mathrm{dom}(L_{\mathrm{bp}})$. Similarly $U^*_{\kappa,K}\mathrm{dom}(L_{\mathrm{bp}}) \subseteq \mathrm{dom}(L_{\mathrm{bp}})$ and hence $\mathrm{dom}(U_{\kappa,K}H_{\mathrm{bp},\kappa}U^*_{\kappa,K}) = \mathrm{dom}(U_{\kappa,K}L_{\mathrm{bp}}U^*_{\kappa,K}) = \mathrm{dom}(L_{\mathrm{bp}}) = \mathrm{dom}(H_{\mathrm{bp},\kappa})$. Since

$$U_{\kappa,K}H_{\mathrm{bp},\kappa}U^*_{\kappa,K}\varphi = H^{\mathrm{bp}}_{\kappa,K}\varphi$$

for all $\varphi \in C_0^\infty(\mathbb{R}^6)\hat{\otimes}\mathfrak{F}_{\mathrm{fin}}(C_0^\infty(\mathbb{R}^3))$, we conclude that $U^*_{\kappa,K}H_{\mathrm{bp},\kappa}U_{\kappa,K} = H^{\mathrm{bp}}_{\kappa,K}$ as an operator equality. □

The quadratic form

$$\begin{aligned} B_{\kappa,K}(\varphi,\psi) = \sum_{j=1,2}\Big\{ &-\big\langle p_j\otimes 1\!\!1\varphi, A_{\kappa,K}(x_j)\psi\big\rangle - \big\langle A_{\kappa,K}(x_j)\varphi, p_j\otimes 1\!\!1\psi\big\rangle \\ &+ \frac{1}{2}\big\langle \varphi, A_{\kappa,K}(x_j)^2\psi\big\rangle + \frac{1}{2}\big\langle A_{\kappa,K}(x_j)^2\varphi,\psi\big\rangle \\ &+ \big\langle A_{\kappa,K}(x_j)\varphi, A_{\kappa,K}(x_j)\psi\big\rangle\Big\} \\ &+ \langle\varphi, H_{IK}\psi\rangle + \big\langle\varphi, V_{\kappa,K}(x_1-x_2)\otimes 1\!\!1\psi\big\rangle \\ &+ \left\langle\varphi, \frac{\alpha U}{|x_1-x_2|}\otimes 1\!\!1\psi\right\rangle + E_{\kappa,K}\langle\varphi,\psi\rangle \end{aligned} \tag{40}$$

is well defined on $\mathrm{dom}(L_{\mathrm{bp}}^{1/2}) \times \mathrm{dom}(L_{\mathrm{bp}}^{1/2})$ for all $\kappa \le \infty$ and K, where

$$H_{IK} = \sqrt{\alpha}\lambda_0 \sum_{j=1,2}\int_{|k|\le K}\frac{\mathrm{d}k}{(2\pi)^{3/2}|k|}\Big[\mathrm{e}^{\mathrm{i}k\cdot x_j}\otimes a(k) + \mathrm{e}^{-\mathrm{i}k\cdot x_j}\otimes a(k)^*\Big]\,.$$

Lemma A.2. *For all $\varepsilon > 0$, there is a $0 < C_{\varepsilon,K} < \infty$ such that*

$$|B_{\kappa,K}(\varphi,\varphi)| \le \big(4C(K)^2 + 4C(K) + \varepsilon\big)\big\|L_{\mathrm{bp}}^{1/2}\varphi\big\|^2 + C_{\varepsilon,K}\|\varphi\|^2 \tag{41}$$

for all $\kappa \le \infty$, where

$$C(K)^2 = \int \mathrm{d}k\, k^2\beta_K(k)^2 = \int_{|k|>K}\mathrm{d}k\,\frac{\alpha\lambda_0^2}{(2\pi)^3(1+k^2/2)^2}\,.$$

Proof. First we note that, for $\varphi \in \mathrm{dom}(L_{\mathrm{bp}})$,

$$\|p_j\otimes 1\!\!1\varphi\| \le \|(L_{\mathrm{bp}}+1\!\!1)^{1/2}\varphi\|\,, \tag{42}$$

$$\|A_{\kappa,K}(x_j)^{\#}\varphi\| \le C(K)\|(L_{\mathrm{bp}}+1\!\!1)^{1/2}\varphi\| \tag{43}$$

by (1). From these inequalities, it follows that

$$\big|\big\langle p_j\varphi, A_{\kappa,K}(x_j)\varphi\big\rangle\big| \le C(K)\|(L_{\mathrm{bp}}+1\!\!1)^{1/2}\varphi\|^2\,,$$

$$\big|\big\langle \varphi, A_{\kappa,K}(x_j)^2\varphi\big\rangle\big| \le C(K)^2\|(L_{\mathrm{bp}}+1\!\!1)^{1/2}\varphi\|^2\,.$$

On the other hand, for any $\varepsilon_1 > 0$, we have

$$|\langle\varphi, H_{IK}\varphi\rangle| \le \varepsilon_1\|(L_{\mathrm{bp}}+1\!\!1)^{1/2}\varphi\|^2 + \frac{4}{\varepsilon_1}C_2(K)\|\varphi\|^2$$

by (1), where $C_2(K)=\alpha\lambda_0^2\int_{|k|\le K}\mathrm{d}k/(2\pi)^3|k|^2$. Moreover,

$$\begin{aligned}\big|\big\langle\varphi, V_{\kappa,K}(x_1-x_2)\otimes \mathbb{1}\varphi\big\rangle\big| &\le 2\int \mathrm{d}k\, \left\{\beta_K(k)^2+\frac{2\sqrt{\alpha}\lambda_0}{(2\pi)^{3/2}|k|}|\beta_K(k)|\right\}\|\varphi\|^2\\ &=: 2C_3(K)\|\varphi\|^2\end{aligned}$$

and, for any $\varepsilon_2>0$, there exists $b_{\varepsilon_2}>0$ such that

$$\left|\left\langle\varphi, \frac{U\alpha}{|x_1-x_2|}\otimes\mathbb{1}\varphi\right\rangle\right|\le \varepsilon_2\|L_{\mathrm{bp}}^{1/2}\varphi\|^2+b_{\varepsilon_2}\|\varphi\|^2\,.$$

Combining these results, we obtain the desired assertion. □

Choose K sufficiently large as $4C(K)^2+4C(K)<1$. Then, by Lemma A.2 and the KLMN theorem (see, e.g., [23]), for $\kappa\le\infty$, there exists a unique self-adjoint operator $H^{\mathrm{bp}'}_{\kappa,K}$ such that

$$\left\langle\varphi, H^{\mathrm{bp}'}_{\kappa,K}\varphi\right\rangle=\left\langle L_{\mathrm{bp}}^{1/2}\varphi, L_{\mathrm{bp}}^{1/2}\varphi\right\rangle+B_{\kappa,K}(\varphi,\varphi)\,.$$

For $\kappa<\infty$, by Proposition A.1, we have

$$H^{\mathrm{bp}'}_{\kappa,K}=H^{\mathrm{bp}}_{\kappa,K}=U_{\kappa,K}H_{\mathrm{bp},\kappa}U^*_{\kappa,K}\,.$$

From this fact, it is natural to denote $H^{\mathrm{bp}'}_{\infty,K}$ as $H^{\mathrm{bp}}_{\infty,K}$.

Lemma A.3.

$$\lim_{\kappa\to\infty}B_{\kappa,K}(\varphi,\varphi)=B_{\infty,K}(\varphi,\varphi)$$

uniformly on any set of φ *in* $\mathrm{dom}(L_{\mathrm{bp}}^{1/2})$ *for which* $\|L_{\mathrm{bp}}^{1/2}\varphi\|+\|\varphi\|$ *is bounded.*

Proof. By the similar argument in the proof of Lemma A.2, we have

$$\begin{aligned}|B_{\kappa,K}(\varphi,\varphi)-B_{\infty,K}(\varphi,\varphi)| &\le 4\big(C(\kappa)+2C(K)C(\kappa)\big)\|(L_{\mathrm{bp}}+\mathbb{1})^{1/2}\varphi\|^2\\ &\quad+\big(2C_3(\kappa)+|E_{\infty,K}-E_{\kappa,K}|\big)\|\varphi\|^2\,,\end{aligned}\tag{44}$$

where $C(\kappa)$ (resp. $C_3(\kappa)$) is $C(K)$ (resp. $C_3(K)$) with K replaced by κ. □

Applying [23, Theorem VIII. 25], we immediately obtain the following.

Proposition A.4. *For* K *satisfying* $4C(K)^2+4C(K)<1$, $H^{\mathrm{bp}}_{\kappa,K}$ *converges to* $H^{\mathrm{bp}}_{\infty,K}$ *as* $\kappa\to\infty$ *in the norm resolvent sense.*

Proof of Theorem 2.1 (i). Since $U_{\kappa,K}$ converges to $U_{\infty,K}$ strongly, we have the desired assertion by Proposition A.4. □

A.2. Proof of Theorem 2.1 (ii) and (iii)

Let $H^{\mathrm{bp}}_{\kappa,K}$ be the Hamiltonian given by (38). It is not hard to see that $\mathcal{U}H^{\mathrm{bp}}_{\kappa,K}\mathcal{U}^*$ is also decomposable and

$$\mathcal{U}H^{\mathrm{bp}}_{\kappa,K}\mathcal{U}^* = \int_{\mathbb{R}^3}^{\oplus} \mathcal{H}^{\mathrm{bp}}_{\kappa,K}(P)\,\mathrm{d}P\,.$$

On $C_0^\infty(\mathbb{R}^3)\hat{\otimes}\mathfrak{F}_{\mathrm{fin}}(C_0^\infty(\mathbb{R}^3))$, we can represent $\mathcal{H}^{\mathrm{bp}}_{\kappa,K}(P)$ as follows,

$$\begin{aligned}
\mathcal{H}^{\mathrm{bp}}_{\kappa,K}(P) = {} & \frac{1}{4}(P - \mathbb{1}\otimes P_{\mathrm{f}})^2 \\
& - \Delta_{x_{\mathrm{r}}}\otimes\mathbb{1} + \frac{\alpha U}{|x_{\mathrm{r}}|}\otimes\mathbb{1} + \mathbb{1}\otimes N_{\mathrm{f}} \\
& + \sum_{j=1,2}\Bigg\{ - \left[(-1)^{j-1}(-\mathrm{i}\nabla_{x_{\mathrm{r}}})\otimes\mathbb{1} + \frac{1}{2}(P - \mathbb{1}\otimes P_{\mathrm{f}})\right]\cdot A_{\kappa,K}\left((-1)^{j-1}\frac{x_{\mathrm{r}}}{2}\right) \\
& - A_{\kappa,K}\left((-1)^{j-1}\frac{x_{\mathrm{r}}}{2}\right)^*\cdot\left[(-1)^{j-1}(-\mathrm{i}\nabla_{x_{\mathrm{r}}})\otimes\mathbb{1} + \frac{1}{2}(P - \mathbb{1}\otimes P_{\mathrm{f}})\right] \\
& + \frac{1}{2}A_{\kappa,K}\left((-1)^{j-1}\frac{x_{\mathrm{r}}}{2}\right)^2 + \frac{1}{2}A_{\kappa,K}\left((-1)^{j-1}\frac{x_{\mathrm{r}}}{2}\right)^{*2} \\
& + A_{\kappa,K}\left((-1)^{j-1}\frac{x_{\mathrm{r}}}{2}\right)^*\cdot A_{\kappa,K}\left((-1)^{j-1}\frac{x_{\mathrm{r}}}{2}\right)\Bigg\} \\
& + 2\sqrt{\alpha}\lambda_0\int_{|k|\le K}\frac{\mathrm{d}k}{(2\pi)^{3/2}|k|}\cos\frac{k\cdot x_{\mathrm{r}}}{2}\otimes\left[a(k)+a(k)^*\right] \\
& + V_{\kappa,K}(x_{\mathrm{r}})\otimes\mathbb{1} + E_{\kappa,K}\,.
\end{aligned} \tag{45}$$

The symmetric operator $H^{\mathrm{bp}}_{\kappa,K}(P)$ is now defined by the right hand side of (45). Clearly this operator is closable and we denote its closure by the same symbol.

Proposition A.5. *For all $\kappa < \infty$, $K < \infty$, $\alpha < \infty$ and $P \in \mathbb{R}^3$, $H^{\mathrm{bp}}_{\kappa,K}(P)$ is self-adjoint on* $\mathrm{dom}(-\Delta_{x_{\mathrm{r}}}\otimes\mathbb{1})\cap\mathrm{dom}(\mathbb{1}\otimes P_{\mathrm{f}}^2)\cap\mathrm{dom}(\mathbb{1}\otimes N_{\mathrm{f}})$, *essentially self-adjoint on any core for the self-adjoint operator L defined by* (4). *Moreover,*

$$\mathcal{U}H^{\mathrm{bp}}_{\kappa,K}\mathcal{U}^* = \int_{\mathbb{R}^3}^{\oplus} H^{\mathrm{bp}}_{\kappa,K}(P)\,\mathrm{d}P\,. \tag{46}$$

Proof. In the proof of Propsotion A.1, we have proved that $\mathrm{dom}(U_{\kappa,K}L_{\mathrm{bp}}U^*_{\kappa,K}) = \mathrm{dom}(L_{\mathrm{bp}})$. Thus, by the closed graph theorem, there is a constant C such that

$$\|U_{\kappa,K}L_{\mathrm{bp}}U^*_{\kappa,K}\varphi\|^2 + \|\varphi\|^2 \le C\left(\|L_{\mathrm{bp}}\varphi\|^2 + \|\varphi\|^2\right)$$

for all $\varphi\in\mathrm{dom}(L_{\mathrm{bp}})$. Choose φ as $\mathcal{U}\varphi = \eta_n\otimes\psi$ with $\psi\in C_0^\infty(\mathbb{R}^3)\hat{\otimes}\mathfrak{F}_{\mathrm{fin}}(C_0^\infty(\mathbb{R}^3))$ and

$$\eta_n = n^{3/2}\chi_{M_n(P)}\,, \tag{47}$$

with $M_n(P) = \{k \in \mathbb{R}^3 \,\big|\, |k_j - P_j| \le \frac{1}{2n},\, j = 1,2,3\}$, where χ_S is the characteristic function for the set S. Then, we get that

$$\int_{\mathbb{R}^3} \mathrm{d}k\, \eta_n(k)^2 \|W_{\kappa,K} L(k) W_{\kappa,K}^* \psi\|^2 \le C \left(\int_{\mathbb{R}^3} \mathrm{d}k\, \eta_n(k)^2 \|L(k)\psi\|^2 + \|\psi\|^2 \right),$$

where

$$L(P) = \frac{1}{4}(P - \mathbb{1} \otimes P_{\mathrm{f}})^2 - \Delta_{x_{\mathrm{r}}} \otimes \mathbb{1} + \mathbb{1} \otimes N_{\mathrm{f}}$$

and

$$W_{\kappa,K} = \exp\left\{ \sum_{j=1,2} \int \mathrm{d}k\, \beta_K(k) \Big[\mathrm{e}^{\mathrm{i}k\cdot(-1)^{j-1}x_{\mathrm{r}}/2} \otimes a(k) - \mathrm{e}^{-\mathrm{i}k\cdot(-1)^{j-1}x_{\mathrm{r}}/2} \otimes a(k^*) \Big] \right\}.$$

Note here that we have used the following facts:

$$\mathcal{U} U_{\kappa,K} \mathcal{U}^* = \int_{\mathbb{R}^3}^{\oplus} W_{\kappa,K}\, \mathrm{d}P\,, \tag{48}$$

$$\mathcal{U} L_{\mathrm{bp}} \mathcal{U}^* = \int_{\mathbb{R}^3}^{\oplus} L(P)\, \mathrm{d}P\,.$$

Taking the limit $n \to \infty$, we get

$$\|W_{\kappa,K}^* L(P) W_{\kappa,K} \psi\|^2 + \|\psi\|^2 \le C\big(\big\|L(P)\psi\big\|^2 + \|\psi\|^2 \big)\,.$$

Since $C_0^\infty(\mathbb{R}^3) \hat{\otimes} \mathfrak{F}_{\mathrm{fin}}(C_0^\infty(\mathbb{R}^3))$ is a core for $L(P)$, we can extend this inequality to $\mathrm{dom}(L(P)) = \mathrm{dom}(-\Delta_{x_{\mathrm{r}}} \otimes \mathbb{1}) \cap \mathrm{dom}(\mathbb{1} \otimes P_{\mathrm{f}}^2) \cap \mathrm{dom}(\mathbb{1} \otimes N_{\mathrm{f}})$. Thus, we have $W_{\kappa,K} \mathrm{dom}(L(P)) \subseteq \mathrm{dom}(L(P))$ for all P. Similarly $W_{\kappa,K}^* \mathrm{dom}(L(P)) \subseteq \mathrm{dom}(L(P))$ and we conclude that

$$\mathrm{dom}\big(W_{\kappa,K} H_\kappa(P) W_{\kappa,K}^*\big) = \mathrm{dom}\big(W_{\kappa,K} L(P) W_{\kappa,K}^*\big) = \mathrm{dom}\big(L(P)\big)\,.$$

Since

$$W_{\kappa,K} H_\kappa(P) W_{\kappa,K}^* = H_{\kappa,K}^{\mathrm{bp}}(P) \tag{49}$$

on $C_0^\infty(\mathbb{R}^3) \hat{\otimes} \mathfrak{F}_{\mathrm{fin}}(C_0^\infty(\mathbb{R}^3))$, we arrive at $W_{\kappa,K} H_\kappa(P) W_{\kappa,K}^* = H_{\kappa,K}^{\mathrm{bp}}(P)$ as an operator equality. Thus, $H_{\kappa,K}^{\mathrm{bp}}(P)$ is self-adjoint on $\mathrm{dom}(L(P))$. To show (46) is an easy exercise. □

Lemma A.6. *$\mathcal{U} H_{\infty,K}^{\mathrm{bp}} \mathcal{U}^*$ is decomposable and can be represented as*

$$\mathcal{U} H_{\infty,K}^{\mathrm{bp}} \mathcal{U}^* = \int_{\mathbb{R}^3}^{\oplus} \tilde{H}_{\infty,K}^{\mathrm{bp}}(P)\, \mathrm{d}P\,.$$

Moreover, for a.e. P, $H_{\kappa,K}^{\mathrm{bp}}(P)$ converges to $\tilde{H}_{\infty,K}^{\mathrm{bp}}(P)$ in the norm resolvent sense as $\kappa \to \infty$.

This is a direct consequence of the following abstract theory.

Lemma A.7. *Let A_n $(n \in \mathbb{N})$ and A be self-adjoint operators on a Hilbert space $\int_M^{\oplus} \mathfrak{h}\, \mathrm{d}\mu(m)$. Suppose that A_n is decomposable for all $n \in \mathbb{N}$, i.e., $A_n = \int_M^{\oplus} A_n(m)\, \mathrm{d}\mu(m)$. Suppose that A_n converges to A in the norm resolvent sense as $n \to \infty$. Then,*

(i) *A is also decomposable. Hence we can represent A as the fiber direct integral $A = \int_M^{\oplus} A(m)\, \mathrm{d}\mu(m)$,*
(ii) *For μ-a.e. m, $A_n(m)$ converges to $A(m)$ in the norm resolvent sense as $n \to \infty$.*

Proof. (i) A_n is decomposable if and only if $\mathrm{e}^{\mathrm{i}tA_n}F = F\mathrm{e}^{\mathrm{i}tA_n}$ for all $t \in \mathbb{R}$ and $F \in L^\infty(M, \mathrm{d}\mu)$. Taking $n \to \infty$, we arrive at $\mathrm{e}^{\mathrm{i}tA}F = F\mathrm{e}^{\mathrm{i}tA}$ which means that A is decomposable and can be written as $A = \int_M^{\oplus} A(m)\, \mathrm{d}\mu(m)$.

(ii) For μ-a.e. m, we obtain that

$$\big\| \big(A_n(m) + \mathrm{i}\big)^{-1} - \big(A(m) + \mathrm{i}\big)^{-1} \big\| \le \|(A_n + \mathrm{i})^{-1} - (A + \mathrm{i})^{-1}\| \to 0 \quad (n \to \infty)\,. \square$$

We note that Lemma A.6 guarantees the existence of the limiting Hamiltonian $\tilde{H}^{\mathrm{bp}}_{\infty,K}(P)$ only for a.e. P. To prove the existence of the limiting Hamiltonian for *all* P, we need more technical preparations.

Let $\tilde{B}^P_{\kappa,K}(\varphi, \psi)$ be the quadratic form on $\mathrm{dom}(L(P)^{1/2}) \times \mathrm{dom}(L(P)^{1/2})$ defined by

$$\begin{aligned}
\tilde{B}^P_{\kappa,K}(\varphi,\psi) = \sum_{j=1,2} \bigg\{ &- \Big\langle \Big[(-1)^{j-1}(-\mathrm{i}\nabla_{x_\mathrm{r}}) \otimes \mathbb{1} \\
&+ \frac{1}{2}(P - \mathbb{1} \otimes P_\mathrm{f}) \Big] \varphi, A_{\kappa,K}\Big((-1)^{j-1} \frac{x_\mathrm{r}}{2} \Big) \psi \Big\rangle \\
&- \Big\langle A_{\kappa,K}\Big((-1)^{j-1} \frac{x_\mathrm{r}}{2} \Big) \varphi, \Big[(-1)^{j-1}(-\mathrm{i}\nabla_{x_\mathrm{r}}) \otimes \mathbb{1} + \frac{1}{2}(P - \mathbb{1} \otimes P_\mathrm{f}) \Big] \psi \Big\rangle \\
&+ \frac{1}{2} \Big\langle \varphi, A_{\kappa,K}\Big((-1)^{j-1} \frac{x_\mathrm{r}}{2} \Big)^2 \psi \Big\rangle + \frac{1}{2} \Big\langle A_{\kappa,K}\Big((-1)^{j-1} \frac{x_\mathrm{r}}{2} \Big)^2 \varphi, \psi \Big\rangle \\
&+ \Big\langle A_{\kappa,K}\Big((-1)^{j-1} \frac{x_\mathrm{r}}{2} \Big) \varphi, A_{\kappa,K}\Big((-1)^{j-1} \frac{x_\mathrm{r}}{2} \Big) \psi \Big\rangle \bigg\} \\
&+ \Big\langle \varphi, 2\sqrt{\alpha}\lambda_0 \int_{|k| \le K} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|} \cos \frac{k \cdot x_\mathrm{r}}{2} \otimes \big[a(k) + a(k)^*\big] \psi \Big\rangle \\
&+ \langle \varphi, V_{\kappa,K}(x_\mathrm{r}) \otimes \mathbb{1}\psi \rangle + \Big\langle \varphi, \frac{\alpha U}{|x_\mathrm{r}|} \otimes \mathbb{1}\psi \Big\rangle + E_{\kappa,K}\langle \varphi, \psi \rangle
\end{aligned} \tag{50}$$

for $K < \kappa \le \infty$.

Lemma A.8. (i) *For all $\varepsilon > 0$, there is a $C_{\varepsilon,K} > 0$ such that*

$$|\tilde{B}^P_{\kappa,K}(\varphi,\varphi)| \le \big(4C(K)^2 + 4C(K) + \varepsilon\big)\|L(P)^{1/2}\varphi\|^2 + C_{\varepsilon,K}\|\varphi\|^2\,.$$

(ii)

$$\lim_{\kappa\to\infty} \tilde{B}^P_{\kappa,K}(\varphi,\varphi) = \tilde{B}^P_{\infty,K}(\varphi,\varphi)$$

uniformly on any set of φ *in* $\mathrm{dom}(L(P)^{1/2})$ *for which* $\|L(P)^{1/2}\varphi\|^2 + \|\varphi\|^2$ *is bounded.*

Proof. (i) Let η_n be the vector defined by (47). Choose φ as $\mathcal{U}\varphi = \eta_n \otimes \psi$ with $\psi \in \mathrm{dom}(L(0)^{1/2})$. Then we have

$$B_{\kappa,K}(\varphi,\varphi) = \int_{\mathbb{R}^3} \mathrm{d}P\, \eta_n(P)^2 \tilde{B}^P_{\kappa,K}(\psi,\psi)$$

where $B_{\kappa,K}$ is the quadratic form given by (40). By Lemma A.2, we get

$$\begin{aligned}&\left|\int \mathrm{d}P\, \eta_n(P)^2 \tilde{B}^P_{\kappa,K}(\psi,\psi)\right| \\ &\qquad \le \big(4C(K)^2 + 4C(K) + \varepsilon\big) \int \mathrm{d}P\, \eta_n(P)^2 \|L(P)^{1/2}\psi\|^2 + C_{\varepsilon,K}\|\psi\|^2\,.\end{aligned}$$

Taking the limit $n\to\infty$, we conclude (i). (Here we use the fact $\mathrm{dom}(L(0)^{1/2}) = \mathrm{dom}(L(P)^{1/2})$ for all P.) Similarly we can prove

$$\begin{aligned}|\tilde{B}^P_{\kappa,K}(\psi,\psi) - \tilde{B}^P_{\infty,K}(\psi,\psi)| &\le 4\big(C(\kappa) + 2C(K)C(\kappa)\big)\big\|\big(L(P)+\mathbb{1}\big)^{1/2}\psi\big\|^2 \\ &\quad + \big(2C_3(\kappa) + |E_{\infty,K} - E_{\kappa,K}|\big)\|\psi\|^2 \end{aligned} \tag{51}$$

by (44). □

Proof of Theorem 2.1 (ii) *and* (iii). From Lemma A.8 and the KLMN theorem [24], it follows that, for sufficiently large K as $4C(K)^2 + 4C(K) < 1$, there exists a unique self-adjoint operator $H^{\mathrm{bp}'}_{\kappa,K}(P)$ such that

$$\big\langle \varphi, H^{\mathrm{bp}'}_{\kappa,K}(P)\varphi\big\rangle = \big\langle L(P)^{1/2}\varphi, L(P)^{1/2}\varphi\big\rangle + \tilde{B}^P_{\kappa,K}(\varphi,\varphi)\,.$$

For $\kappa < \infty$, it can be easily shown that $H^{\mathrm{bp}'}_{\kappa,K}(P) = H^{\mathrm{bp}}_{\kappa,K}(P)$. (From now on, we also denote $H^{\mathrm{bp}'}_{\infty,K}(P)$ by $H^{\mathrm{bp}}_{\infty,K}(P)$.) Moreover, by Lemma A.8, $H^{\mathrm{bp}}_{\kappa,K}(P)$ converges to $H^{\mathrm{bp}}_{\infty,K}(P)$ in the norm resolvent sense for all P. Since $W^*_{\kappa,K}$ converges to $W^*_{\infty,K}$ strongly, we conclude (ii) by (49)

Finally we show (iii) in Theorem 2.1. Since $\tilde{H}^{\mathrm{bp}}_{\infty,K}(P) = H^{\mathrm{bp}}_{\infty,K}(P)$ for a.e. P, we have that

$$\int^{\oplus}_{\mathbb{R}^3} \tilde{H}^{\mathrm{bp}}_{\infty,K}(P)\,\mathrm{d}P = \int^{\oplus}_{\mathbb{R}^3} H^{\mathrm{bp}}_{\infty,K}(P)\,\mathrm{d}P\,.$$

Noting that the operator equality (48) is valid for $\kappa = \infty$, we have the desired assertion. □

Appendix B. Convergence of the ground state energies and the bottom of the essential spectrum

Let $E_{\mathrm{bp},\kappa}$ and $E_{\mathrm{p},\kappa}$ be the ground state energy for $H_{\mathrm{bp},\kappa}$ and $H_{\mathrm{p},\kappa}$ respectively. Further we denote $\inf\operatorname{spec}(H_\kappa(P))$, resp. $\inf\operatorname{spec}(H(P))$, by $E_\kappa(P)$, resp. $E(P)$.

Proposition B.1. *For all $\alpha, U > 0$, the following holds.*

(i) $\lim_{\kappa\to\infty} E_{\mathrm{bp},\kappa} = E_{\mathrm{bp}}$.
(ii) $\lim_{\kappa\to\infty} E_{\mathrm{p},\kappa} = E_{\mathrm{p}}$.
(iii) $\lim_{\kappa\to\infty} E_\kappa(P) = E(P)$ *for all P.*

Proof. (i) and (iii) are direct consequences of Lemma A.3 and A.8. (Note that $E_{\mathrm{bp},\kappa} = \inf\operatorname{spec}(H^{\mathrm{bp}}_{\kappa,K})$ and $E_{\mathrm{bp}} = \inf\operatorname{spec}(H^{\mathrm{bp}}_{\infty,K})$. Also note that $E_\kappa(P) = \inf\operatorname{spec}(H^{\mathrm{bp}}_{\kappa,K}(P))$ and $E(P) = \inf\operatorname{spec}(H^{\mathrm{bp}}_{\infty,K}(P))$ for all P.) We can show (ii) in a similar way. □

Proposition B.2. *For all $\alpha, U > 0$,*

$$\lim_{\kappa\to\infty} \inf\operatorname{ess.spec}\big(H_\kappa(P)\big) = \inf\operatorname{ess.spec}\big(H(P)\big)\,. \tag{52}$$

Proof. Let $H^{\mathrm{bp}}_{\kappa,K}(P)$ be the Hamiltonian defined by the form sum $L(P) + \tilde{B}^P_{\kappa,K}$ for a sufficiently large K, see (50). Notice that (52) is equivalent to

$$\lim_{\kappa\to\infty} \inf\operatorname{ess.spec}\big(H^{\mathrm{bp}}_{\kappa,K}(P)\big) = \inf\operatorname{ess.spec}\big(H^{\mathrm{bp}}_{\infty,K}(P)\big) \tag{53}$$

because $W_{\kappa,K} H_\kappa(P) W^*_{\kappa,K} = H^{\mathrm{bp}}_{\kappa,K}(P)$ for all $\kappa \le \infty$. By Lemma A.8 (i), we have that, for all $\kappa \le \infty$ and large K,

$$L(P) + \mathbb{1} \le C\big(H^{\mathrm{bp}}_{\kappa,K}(P) + \mathbb{1}\big)$$

where C is independent of κ. Combining this with (51), we can conclude that

$$H^{\mathrm{bp}}_{\kappa,K}(P) \le \big(1 + D(\kappa)\big) H^{\mathrm{bp}}_{\infty,K}(P) + D(\kappa)$$

and

$$H^{\mathrm{bp}}_{\infty,K}(P) \le \big(1 + D(\kappa)\big) H^{\mathrm{bp}}_{\kappa,K}(P) + D(\kappa)\,,$$

where $D(\kappa)$ is a positive constant satisfying $\lim_{\kappa\to\infty} D(\kappa) = 0$. By the min-max principle, we have that

$$\inf\operatorname{ess.spec}\big(H^{\mathrm{bp}}_{\kappa,K}(P)\big) \le \big(1 + D(\kappa)\big) \inf\operatorname{ess.spec}\big(H^{\mathrm{bp}}_{\infty,K}(P)\big) + D(\kappa)$$

and

$$\inf\operatorname{ess.spec}\big(H^{\mathrm{bp}}_{\infty,K}(P)\big) \le \big(1 + D(\kappa)\big) \inf\operatorname{ess.spec}\big(H^{\mathrm{bp}}_{\kappa,K}(P)\big) + D(\kappa)\,.$$

Taking the limit $\kappa \to \infty$, we obtain the desired assertion (53). □

Appendix C. Lower energy bound

The proof of Lemma 3.5 (ii) is a modification of the single polaron case established in [15]. For more details we refer to [15, 16].

Step 1 (Elimination of the hard phonons). Let $\mathbf{Z}^{(1)} = (Z_1^{(1)}, Z_2^{(1)}, Z_3^{(1)})$ and $\mathbf{Z}^{(2)} = (Z_1^{(2)}, Z_2^{(2)}, Z_3^{(2)})$ be given by

$$Z_j^{(i)} = \sqrt{\alpha}\lambda_0 \int_{K \le |k| \le \kappa} \mathrm{d}k \, \frac{k_j \mathrm{e}^{\mathrm{i}k \cdot x_i}}{(2\pi)^{3/2}|k|^3} \otimes a(k) \,, \quad i = 1, 2 \,, \quad j = 1, 2, 3 \,.$$

Let D_y be the generalized partial differential operator in the variable y. By the standard calculation, one checks that

$$\sum_{i=1,2} \sum_{j=1,2,3} \left[-\mathrm{i}D_{x_{ij}}, Z_j^{(i)} - Z_j^{(i)*} \right] = H_{\mathrm{int}} \,, \tag{54}$$

where we use the symbols $x_1 = (x_{11}, x_{12}, x_{13}), x_2 = (x_{21}, x_{22}, x_{23})$, and

$$H_{\mathrm{int}} = \sqrt{\alpha}\lambda_0 \sum_{i=1,2} \int_{K \le |k| \le \kappa} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|} \left[\mathrm{e}^{\mathrm{i}k \cdot x_i} \otimes a(k) + \mathrm{e}^{-\mathrm{i}k \cdot x_i} \otimes a(k)^* \right] .$$

On the other hand, for arbitrary $\varepsilon > 0$

$$\begin{aligned}
&\Big| \sum_{j=1,2,3} \Big\langle \varphi, \Big[-\mathrm{i}D_{x_{ij}}, Z_j^{(i)} - Z_j^{(i)*} \Big] \varphi \Big\rangle \Big| \\
&\quad \le 2 \|(-\Delta_{x_i})^{1/2} \otimes \mathbb{1}\varphi\| \Big\| \Big(\mathbf{Z}^{(i)} - \mathbf{Z}^{(i)*} \Big) \varphi \Big\| \\
&\quad \le 2 \|(-\Delta_{x_i})^{1/2} \otimes \mathbb{1}\varphi\| \Big\{ 2 \Big\langle \varphi, \Big(\mathbf{Z}^{(i)*}\mathbf{Z}^{(i)} + \mathbf{Z}^{(i)}\mathbf{Z}^{(i)*} \Big) \varphi \Big\rangle \Big\}^{1/2} \\
&\quad \le \varepsilon \|(-\Delta_{x_i})^{1/2} \otimes \mathbb{1}\varphi\|^2 + \frac{2}{\varepsilon} \Big\langle \varphi, \Big(\mathbf{Z}^{(i)*}\mathbf{Z}^{(i)} + \mathbf{Z}^{(i)}\mathbf{Z}^{(i)*} \Big) \varphi \Big\rangle \\
&\quad \le \varepsilon \|(-\Delta_{x_i})^{1/2} \otimes \mathbb{1}\varphi\|^2 + \frac{4}{\varepsilon} \Big\langle \varphi, \mathbf{Z}^{(i)*}\mathbf{Z}^{(i)} \varphi \Big\rangle + \frac{1}{\varepsilon} \frac{\alpha\lambda_0^2}{\pi^2 K} \,.
\end{aligned}$$

In the last inequality we used that $\sum_{j=1,2,3} [Z_j^{(i)}, Z_j^{(i)*}] = \alpha\lambda_0^2 \int_{K \le |k| \le \kappa} \mathrm{d}k/(2\pi)^3|k|^4 \le \alpha\lambda_0^2/2\pi^2 K$. Moreover, by a standard number operator estimate, we have

$$\sum_{j=1,2,3} \Big\| Z_j^{(i)} \varphi \Big\|^2 \le \frac{\alpha\lambda_0^2}{2\pi^2 K} \|\mathbb{1} \otimes N_{\ge K} \varphi\| \,, \tag{55}$$

where $N_{\ge K} = \mathrm{d}\Gamma(1 - \chi_K) = \int_{K \le |k|} \mathrm{d}k \, a(k)^* a(k)$. Choose $\varepsilon = 4\alpha\lambda_0^2/\pi^2 K$. To summarize, combining (54) with (55), we obtain that

$$-\langle \varphi, H_{\mathrm{int}} \varphi \rangle \le \frac{8\alpha\lambda_0^2}{\pi^2 K} \Big\langle \varphi, \Big(-\frac{1}{2}\Delta_{x_1} - \frac{1}{2}\Delta_{x_2} \Big) \otimes \mathbb{1}\varphi \Big\rangle + \langle \varphi, \mathbb{1} \otimes N_{\ge K} \varphi \rangle + \frac{1}{4} \,. \tag{56}$$

Let

$$H_K = \left(1 - \frac{8\alpha\lambda_0^2}{\pi^2 K}\right)\left(-\frac{1}{2}\Delta_{x_1} - \frac{1}{2}\Delta_{x_2} + \frac{\alpha U}{|x_1 - x_2|}\right) \otimes \mathbb{1} + \mathbb{1} \otimes N_{<K}$$
$$+ \sum_{i=1,2} \sqrt{\alpha}\lambda_0 \int_{|k|<K} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|} \left[\mathrm{e}^{\mathrm{i}k\cdot x_i} \otimes a(k) + \mathrm{e}^{-\mathrm{i}k\cdot x_i} \otimes a(k)^*\right],$$

where $N_{<K} = \mathrm{d}\Gamma(\chi_K) = \int_{|k|<K} \mathrm{d}k\, a(k)^* a(k)$. Then, by (56),

$$H_{\mathrm{bp},\kappa} - H_K = \frac{8\alpha\lambda_0^2}{\pi^2 K}\left(-\frac{1}{2}\Delta_{x_1} - \frac{1}{2}\Delta_{x_2}\right) \otimes \mathbb{1} + \mathbb{1} \otimes N_{\geq K} + H_{\mathrm{int}} \geq -\frac{1}{4}\,,$$

that is, $H_{\mathrm{bp},\kappa} \geq H_K - 1/4$. From now on, we take $K = 8\alpha^{6/5}\lambda_0^2/\pi^2 c_1$ with some positive c_1 independent of α.

Step 2 (Localization of the electrons). Let $C_L(a) = (0, \pi(3/L)^{1/2})^6 + a \subset \mathbb{R}^6$ ($a \in \mathbb{R}^6$). For arbitrary $\varepsilon > 0$, take $\Psi \in C_0^\infty(\mathbb{R}^6)\hat{\otimes}\,\mathfrak{F}_{\mathrm{fin}}(C_0^\infty(\mathbb{R}^3))$ with $\|\Psi\| = 1$ and $\langle\Psi, H_K\Psi\rangle \leq \inf\mathrm{spec}(H_K) + \varepsilon/2$. For $\varphi \in C_0^\infty(C_L(0))$, set $\varphi_y(x) = \varphi(x - y)$. A direct calculation leads to

$$\int \mathrm{d}y\, \langle\varphi_y\Psi, H_K\varphi_y\Psi\rangle \leq \inf\mathrm{spec}(H_K) + \frac{\varepsilon}{2} + \frac{1}{2}\sum_{j=1,2} \|\nabla_{x_j}\varphi\|^2\,.$$

Consider the Dirichlet Laplacian $-\Delta_{\mathrm{D}}$ for $C_L(0)$ and let ϕ_0 be its ground state with ground state energy $2L$. At this point we would like to choose φ to be equal to ϕ_0. Unfortunately ϕ_0 does not belong to $C_0^\infty(C_L(0))$. However it can be approximated by $\varphi \in C_0^\infty(C_L(0))$ such that $\sum_{j=1,2} \|\nabla_{x_j}\varphi\|^2 \leq 2L + \varepsilon$. Hence

$$\int \mathrm{d}y \Big\langle \varphi_y\Psi,\ \big[H_K - \inf\mathrm{spec}(H_K) - L - \varepsilon\big]\varphi_y\Psi \Big\rangle \leq 0\,.$$

Accordingly there must be a point $y_0 \in \mathbb{R}^6$ such that $\langle\varphi_{y_0}\Psi, H_K\varphi_{y_0}\Psi\rangle/\|\varphi_{y_0}\Psi\|^2 \leq \inf\mathrm{spec}(H_K) + L + \varepsilon$ which implies

$$\inf_{\Psi\in\mathcal{D}_L,\, \|\Psi\|=1} \langle\Psi, H_K\Psi\rangle \leq \inf\mathrm{spec}(H_K) + L\,,$$

where $\mathcal{D}_L = C_0^\infty(C_L(y_0))\hat{\otimes}\,\mathfrak{F}_{\mathrm{fin}}(C_0^\infty(\mathbb{R}^3))$. (Here we have used the fact that $\varphi_{y_0}\Psi \in \mathcal{D}_L$.) Henceforth, we take $L = c_2\alpha^{9/5}$. Combining this choice with Step 1, we arrive at

$$E_{\mathrm{bp},\kappa} \geq \inf_{\Psi\in\mathcal{D}_L,\, \|\Psi\|=1} \langle\Psi, H_K\Psi\rangle - c_2\alpha^{9/5} - \frac{1}{4}\,. \tag{57}$$

Step 3 (Block decomposition of the phonons). Let $P = c_3\alpha^{3/5}$ and, for $n = (n_1, n_2, n_3) \in \mathbb{Z}^3$, let $D_P(n) = [n_1P - P/2, n_1P + P/2] \times [n_2P - P/2, n_2P + P/2] \times [n_3P - P/2, n_3P + P/2]$. We introduce $\Lambda_P = \{n \in \mathbb{Z}^3 \mid D_P(n) \cap B_K \neq \emptyset\}$, where $B_K = \{k \in \mathbb{R}^3 \,|\, |k| \leq K\}$. (Recall here that $K = 8\alpha^{6/5}\lambda_0^2/\pi^2 c_1$.) Then $\#\Lambda_P$ (the cardinality of Λ_P) $= \frac{4\pi}{3}K^3/P^3 +$ lower oder $= \mathcal{O}(\alpha^{9/5})$. For each $n \in \Lambda_P$, set

$$B(n) = \begin{cases} D_P(n)\,, & \text{if } D_P(n) \subset B_K \\ D_P(n) \cap B_K\,, & \text{if } D_P(n) \not\subseteq B_K \end{cases}$$

and let $k_{B(n)}$ be *any* fixed point in $B(n)$. Recall the definition of $C_L(a)$ and y_0 which are given in Step 2. We write y_0 as $y_0 = (y_{01}, y_{02})$ with $y_{0j} \in \mathbb{R}^3$ $(j = 1, 2)$. For $k \in B(n)$ and $x = (x_1, x_2) \in C_L(y_0)$, noting that $x_i - y_{0i} \in (0, \pi(3/L)^{1/2})^3$, we have

$$\left|\mathrm{e}^{\mathrm{i}k\cdot x_i} - \mathrm{e}^{\mathrm{i}k_{B(n)}\cdot x_i}\right| = \left|\mathrm{e}^{\mathrm{i}k\cdot(x_i - y_{0i})} - \mathrm{e}^{\mathrm{i}k_{B(n)}\cdot(x_i - y_{0i})}\right| \le |k - k_{B(n)}||x_i - y_{0i}|$$
$$\le \frac{3}{2} c_3 \left(\frac{6}{c_2}\right)^{1/2} \pi \alpha^{-3/10}\,.$$

Thus, for any $\delta > 0$, we obtain

$$\begin{aligned}
&\sum_{n\in\Lambda_P} \Bigg\{ \delta \mathbb{1} \otimes N_{B(n)} + \sqrt{\alpha}\lambda_0 \sum_{i=1,2} \int_{B(n)} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|} \Big[\left(\mathrm{e}^{\mathrm{i}k\cdot x_i} - \mathrm{e}^{\mathrm{i}k_{B(n)}\cdot x_i}\right) \otimes a(k) \\
&\qquad + \left(\mathrm{e}^{-\mathrm{i}k\cdot x_i} - \mathrm{e}^{-\mathrm{i}k_{B(n)}\cdot x_i}\right) \otimes a(k)^* \Big] \Bigg\} \\
&\qquad \ge -\frac{\alpha\lambda_0^2}{2\delta} \sum_{n\in\Lambda_P} \int_{B(n)} \frac{\mathrm{d}k}{(2\pi)^3|k|^2} \left| \sum_{i=1,2} \left(\mathrm{e}^{\mathrm{i}k\cdot x_i} - \mathrm{e}^{\mathrm{i}k_{B(n)}\cdot x_i}\right) \right|^2 \\
&\qquad \ge -\frac{12 c_3^2}{\delta c_1 c_2} \alpha^{8/5}\,,
\end{aligned}$$

where $N_{B(n)} = \mathrm{d}\Gamma(\chi_{B(n)}) = \int_{B(n)} \mathrm{d}k\, a(k)^* a(k)$. Take $\delta = c_4 \alpha^{-1/5}$. From the above inequality, it follows that, for any $\Psi \in \mathcal{D}_L$,

$$\langle \Psi, H_K \Psi \rangle \ge \left\langle \Psi, \tilde{H}_K\left(\{k_{B(n)}\}\right)\Psi \right\rangle - 12 c_3^2 \alpha^{9/5} / c_1 c_2 c_4 \tag{58}$$

with

$$\begin{aligned}
\tilde{H}_K\left(\{k_{B(n)}\}\right) &= (1 - c_1\alpha^{-1/5}) \left(-\frac{1}{2}\Delta_{x_1} - \frac{1}{2}\Delta_{x_2} + \frac{\alpha U}{|x_1 - x_2|}\right) \otimes \mathbb{1} \\
&\quad + \sum_{n\in\Lambda_P} \Bigg\{ (1-\delta)\mathbb{1} \otimes N_{B(n)} \\
&\quad + \sqrt{\alpha}\lambda_0 \sum_{i=1,2} \int_{B(n)} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|} \Big[\mathrm{e}^{\mathrm{i}k_{B(n)}\cdot x_i} \otimes a(k) \\
&\quad + \mathrm{e}^{-\mathrm{i}k_{B(n)}\cdot x_i} \otimes a(k)^* \Big] \Bigg\}\,.
\end{aligned}$$

An important point here is that the exponential factors $\mathrm{e}^{\pm\mathrm{i}x_i\cdot k_{B(n)}}$ in the electron-phonon interaction term contained in $\tilde{H}_K(\{k_{B(n)}\})$ are independent of k within $B(n)$, because $k_{B(n)}$ is fixed. Next we introduce a block annihilation operator A_n $(n \in \Lambda_P)$ by

$$A_n = \left(\int_{B(n)} \frac{\mathrm{d}k}{(2\pi)^3|k|^2} \right)^{-1/2} \int_{B(n)} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|} a(k)\,.$$

Each A_n is a normalized boson mode satisfying $[A_n, A^*_{n'}] = \delta_{n,n'}$. Moreover it satisfies that $A^*_n A_n \le N_{B(n)}$. By this fact, we conclude that, for each $\Psi \in \mathcal{D}_L$, $\langle \Psi, \tilde{H}_K(\{k_{B(n)}\})\Psi\rangle \ge \langle \Psi, H_K^{\rm Block}(\{k_{B(n)}\})\Psi\rangle$ with

$$\begin{aligned}\tilde{H}_K\big(\{k_{B(n)}\}\big) &= (1-c_1\alpha^{-1/5})\left(-\frac{1}{2}\Delta_{x_1} - \frac{1}{2}\Delta_{x_2} + \frac{\alpha U}{|x_1-x_2|}\right)\otimes \mathbb{1} \\ &\quad + \sum_{n\in\Lambda_P}\Bigg\{(1-c_4\alpha^{-1/5})\mathbb{1}\otimes A^*_n A_n \\ &\quad + \sqrt{\alpha}\lambda_0\left(\int_{B(n)}\frac{\mathrm{d}k}{(2\pi)^3|k|^2}\right)^{1/2}\sum_{i=1,2}\Big[\mathrm{e}^{\mathrm{i}k_{B(n)}\cdot x_i}\otimes A_n \\ &\quad + \mathrm{e}^{-\mathrm{i}k_{B(n)}\cdot x_i}\otimes A^*_n\Big]\Bigg\}.\end{aligned}$$

Therefore, by (58),

$$\langle \Psi, H_K\Psi\rangle \ge \Big\langle \Psi, H_K^{\rm Block}\big(\{k_{B(n)}\}\big)\Psi\Big\rangle - 12c_3^2\alpha^{9/5}/c_1c_2c_4\,.$$

Summarizing the results obtained in Step 2 and 3, we get

$$E_{\mathrm{bp},\kappa} \ge \inf_{\Psi\in\mathcal{D}_L,\,\|\Psi\|=1}\ \sup_{\{k_{B(n)}\}}\Big\langle \Psi, H_K^{\rm Block}\big(\{k_{B(n)}\}\big)\Psi\Big\rangle + \mathcal{O}(\alpha^{9/5})\,. \tag{59}$$

Step 4.

Proof of Lemma 3.5 (ii). As preliminary, we recall some fundamental properties of coherent states. Let a and a^* be the annihilation and creation operators in $L^2(\mathbb{R})$, and $|0\rangle$ be the ground state of the harmonic oscillator: $a|0\rangle = 0$. For $\xi\in\mathbb{C}$, a normalized coherent state for a single oscillator is given by $|\xi\rangle = \pi^{-1/2}\exp[-\frac{1}{2}|\xi|^2 + \xi a^*]|0\rangle$. We denote the orthogonal projection onto the coherent state $|\xi\rangle$ by $|\xi\rangle\langle\xi|$. Then

$$\int \mathrm{d}\xi\mathrm{d}\xi^*\,|\xi\rangle\langle\xi| = \mathbb{1}\,,\quad \int \mathrm{d}\xi\mathrm{d}\xi^*\,\xi|\xi\rangle\langle\xi| = a\,,\quad \int\mathrm{d}\xi\mathrm{d}\xi^*\,(|\xi|^2-1)|\xi\rangle\langle\xi| = a^*a\,, \tag{60}$$

where the above integral is understood as a weak integral.

For $\xi = \{\xi_n\}_{n\in\Lambda_P}$, $\xi_n\in\mathbb{C}$, let $|\xi\rangle = \Pi_{n\in\Lambda_P}\pi^{-1/2}\exp[-\frac{1}{2}|\xi_n|^2 + \xi_n A^*_n]\Omega$ be a normalized coherent state for block oscillators introduced in Step 3. For any normalized $\Psi\in\mathcal{D}_L$, set $\Psi_\xi(x) = \langle \xi, \Psi(x)\rangle_{\mathfrak{F}(L^2(\mathbb{R}^3))}$. Note that, since $\Psi\in\mathcal{D}_L$, Ψ_ξ is in $C_0^\infty(C_L(y_0))$. Using (60) for each block oscillator, we have

$$\Big\langle \Psi, H_K^{\rm Block}\big(\{k_{B(n)}\}\big)\Psi\Big\rangle = \int \Pi_{n\in\Lambda_P}\mathrm{d}\xi_n\mathrm{d}\xi_n^*\,\Big\langle \Psi_\xi, h_\xi\big(\{k_{B(n)}\}\big)\Psi_\xi\Big\rangle_{L^2(\mathbb{R}^6)}\,,$$

where $h_\xi(\{k_{B(n)}\})$ is the Schrödinger operator given by

$$h_\xi\big(\{k_{B(n)}\}\big) = (1 - c_1\alpha^{-1/5})h_{\rm el} + \sum_{n\in\Lambda_P}\Bigg\{(1 - c_4\alpha^{-1/5})(|\xi_n|^2 - 1) + \left(\int_{B(n)} \frac{\mathrm{d}k}{(2\pi)^3|k|^2}\right)^{1/2} \sqrt{\alpha}\lambda_0 \sum_{i=1,2}\Big[\xi_n \mathrm{e}^{\mathrm{i}k_{B(n)}\cdot x_i} + \xi_n^* \mathrm{e}^{\mathrm{i}k_{B(n)}\cdot x_i}\Big]\Bigg\}$$

with $h_{\rm el} = -\Delta_{x_1}/2 - \Delta_{x_2}/2 + \alpha U|x_1 - x_2|^{-1}$. By completing the square and taking the supremum over $\{k_{B(n)}\}$,

$$\begin{aligned}\sup_{\{k_{B(n)}\}}&\Big\langle \Psi, h_\xi\big(\{k_{B(n)}\}\big)\Psi\Big\rangle_{L^2(\mathbb{R}^6)}\\ &\ge (1 - c_1\alpha^{-1/5})\langle\Psi_\xi, h_{\rm el}\Psi_\xi\rangle\\ &\quad - \inf_{\{k_{B(n)}\}}\sum_{n\in\Lambda_P}\frac{\alpha\lambda_0^2}{(1 - c_4\alpha^{-1/5})}\int_{B(n)}\mathrm{d}k\,\frac{|\hat\rho_\xi(k_{B(n)})|^2}{|k|^2\|\Psi_\xi\|^2_{L^2(\mathbb{R}^6)}}\\ &\quad - (1 - c_4\alpha^{-1/5})\|\Psi_\xi\|^2_{L^2(\mathbb{R}^6)}\#\Lambda_P\,,\end{aligned}$$

where $\hat\rho_\xi(k) = (2\pi)^{-3/2}\int_{\mathbb{R}^3}\mathrm{d}x\,\mathrm{e}^{-\mathrm{i}k\cdot x}\rho_\xi(x)$ with $\rho_\xi(x) = \int_{\mathbb{R}^3}\mathrm{d}x_1\,|\Psi_\xi(x_1,x)|^2 + \int_{\mathbb{R}^3}\mathrm{d}x_2\,|\Psi_\xi(x,x_2)|^2$. We remark that

$$\begin{aligned}\inf_{\{k_{B(n)}\}}&\sum_{n\in\Lambda_P}\int_{B(n)}\mathrm{d}k\,\frac{|\hat\rho_\xi(k_{\{B(n)\}})|^2}{|k^2|}\\ &\le \int_{|k|\le K}\mathrm{d}k\,\frac{|\hat\rho_\xi(k)|^2}{|k^2|} \le \int_{\mathbb{R}^3}\mathrm{d}k\,\frac{|\hat\rho_\xi(k)|^2}{|k^2|}\\ &= \frac{1}{4\pi}\sum_{i,j=1,2}\int \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}y_1\mathrm{d}y_2\,\frac{|\Psi_\xi(x_1,x_2)|^2|\Psi_\xi(y_1,y_2)|^2}{|x_i - y_j|}\end{aligned}$$

by (10). Taking the fact that $\#\Lambda_P = \mathcal{O}(\alpha^{9/5})$ and the above remark into consideration, we have

$$\begin{aligned}\sup_{\{k_{B(n)}\}}&\Big\langle\Psi, H_K^{\rm Block}\big(\{k_{B(n)}\}\big)\Psi\Big\rangle\\ &\ge \int \Pi_{n\in\Lambda_P}\mathrm{d}\xi_n\mathrm{d}\xi_n^*\,\|\Psi_\xi\|^2_{L^2(\mathbb{R}^6)}\bigg[(1 - c_1\alpha^{-1/5})\langle\tilde\Psi_\xi, h_{\rm el}\tilde\Psi_\xi\rangle\\ &\quad - \frac{\alpha}{\sqrt{2}(1 - c_4\alpha^{-1/5})}\sum_{i,j=1,2}\int\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}y_1\mathrm{d}y_2\,\frac{|\tilde\Psi_\xi(x_1,x_2)|^2|\tilde\Psi_\xi(y_1,y_2)|^2}{|x_i - y_j|}\bigg]\\ &\quad + \mathcal{O}(\alpha^{9/5})\,,\end{aligned} \tag{61}$$

where $\tilde{\Psi}_\xi = \Psi_\xi / \|\Psi_\xi\|_{L^2(\mathbb{R}^6)}$. The integrand of the right hand side of the above inequality is the Pekar–Tomasevich energy functional. Thus

$$\begin{aligned}\text{RHS of (61)} &\geq \int \Pi_{n\in\Lambda_P} \mathrm{d}\xi_n \mathrm{d}\xi_n^* \, \|\Psi_\xi\|^2_{L^2(\mathbb{R}^6)} (1 - c_1\alpha^{-1/5}) \\ &\quad \times c_{\mathrm{bp}}\Big((1 - c_1\alpha^{-1/5})(1 - c_4\alpha^{-1/5})U\Big)\alpha^2 + \mathcal{O}(\alpha^{9/5}) \\ &= (1 - c_1\alpha^{-1/5}) c_{\mathrm{bp}}\Big((1 - c_1\alpha^{-1/5})(1 - c_4\alpha^{-1/5})U\Big)\alpha^2 + \mathcal{O}(\alpha^{9/5})\,.\end{aligned}$$

Combining this result with (59), we have that

$$E_{\mathrm{bp},\kappa} \geq c_{\mathrm{bp}}\Big((1 - c_1\alpha^{-1/5})(1 - c_4\alpha^{-1/5})U\Big)\alpha^2 + \mathcal{O}(\alpha^{9/5})$$

for any $\kappa > K$. (Note that the error term $\mathcal{O}(\alpha^{9/5})$ does not depend on κ.) Taking $\kappa \to \infty$, we obtain the desired result. □

Appendix D. Localization formula

In this appendix, we consider the Hamiltonian in configuration space. Namely let $\check{a}(x)$ and $\check{a}(x)^*$ be the creation and annihilation operators in configuration space. In this representation, the Hamiltonian $H_{\mathrm{bp},\kappa}$ is written as

$$\begin{aligned}H_{\mathrm{bp},\kappa} = &\sum_{j=1,2} \left\{ -\frac{1}{2}\Delta_{x_j} \otimes \mathbb{1} + \sqrt{\alpha}\lambda_0 \int_{\mathbb{R}^3} \mathrm{d}y \left[h_{x_j}(y) \otimes \check{a}(y) + h_{x_j}(y) \otimes \check{a}(y)^* \right] \right\} \\ &+ \frac{\alpha U}{|x_1 - x_2|} \otimes \mathbb{1} + \mathbb{1} \otimes N_{\mathrm{f}}\,,\end{aligned}$$

where

$$h_x(y) = (2\pi)^{-3} \int_{|k|\leq\kappa} \mathrm{d}k \, \frac{\mathrm{e}^{-\mathrm{i}k\cdot(x-y)}}{|k|}\,.$$

Clearly $h_x(y)$ is real and $h_x(y) = h_0(y - x)$.

Let χ be the smooth nonnegative function on $\mathbb{R}^3$, identically one on the unit ball, and vanishing outside the ball of radius 2. Set

$$g_1(y;x) = 1 - \chi\left(\frac{y-x}{L}\right), \quad g_2(y;x) = \chi\left(\frac{y-x}{L}\right)$$

and introduce

$$j_{1,L}(y;x) = \frac{g_1(y;x)}{\sqrt{g_1(y;x)^2 + g_2(y;x)^2}}\,, \quad j_{2,L}(y;x) = \frac{g_2(y;x)}{\sqrt{g_1(y;x)^2 + g_2(y;x)^2}}\,.$$

Remark that

$$j_{1,L}(\cdot\,;x)^2 + j_{2,L}(\cdot\,;x)^2 = 1 \tag{62}$$

for each $x \in \mathbb{R}^3$. For each $x_2 \in \mathbb{R}^3$, we define a linear operator $j_{x_2}^{(L)}$ from $L^2(\mathbb{R}_y^3)$ to $L^2(\mathbb{R}_y^3) \oplus L^2(\mathbb{R}_y^3)$ by

$$\left(j_{x_2}^{(L)} f\right)(y) = j_{1,L}(y;x_2)f(y) \oplus j_{2,L}(y;x_2)f(y)\,.$$

It is easy to check that $j_{x_2}^{(L)}$ is an isometry by (62). Let U be the unitary operator from $\mathfrak{F}(L^2(\mathbb{R}_y^3) \oplus L^2(\mathbb{R}_y^3))$ to $\mathfrak{F}(L^2(\mathbb{R}_y^3))$ given by the relation

$$\mathsf{U}\check{a}(f \oplus g)^{\#}\mathsf{U}^* = \check{a}(f)^{\#} \otimes \mathbb{1} + \mathbb{1} \otimes \check{a}(g)^{\#}\,.$$

Now we introduce an isometry operator from $L^2(\mathbb{R}^6) \otimes \mathfrak{F}(L^2(\mathbb{R}_y^3))$ to $L^2(\mathbb{R}^6) \otimes \mathfrak{F}(L^2(\mathbb{R}_y^3)) \otimes \mathfrak{F}(L^2(\mathbb{R}_y^3))$ by

$$U_L(x) = \mathsf{U}\Gamma\left(j_{x_2}^{(L)}\right),$$

where $x = (x_1, x_2) \in \mathbb{R}^6$ are the electron coordinates.

Let $H_{\mathrm{bp},\kappa}^{\otimes}$ be the Hamiltonian acting in $L^2(\mathbb{R}^6) \otimes \mathfrak{F}(L^2(\mathbb{R}_y^3)) \otimes \mathfrak{F}(L^2(\mathbb{R}_y^3))$ defined by

$$\begin{aligned} H_{\mathrm{bp},\kappa}^{\otimes} &= \left(-\frac{1}{2}\Delta_{x_1} - \frac{1}{2}\Delta_{x_2}\right) \otimes \mathbb{1}_{\mathfrak{F}} \otimes \mathbb{1}_{\mathfrak{F}} + \mathbb{1}_{L^2} \otimes N_{\mathrm{f}} \otimes \mathbb{1}_{\mathfrak{F}} + \mathbb{1}_{L^2} \otimes \mathbb{1}_{\mathfrak{F}} \otimes N_{\mathrm{f}} \\ &\quad + \sqrt{\alpha}\lambda_0 \int_{\mathbb{R}^3} \mathrm{d}y\, \left[h_{x_1}(y) \otimes \check{a}(y) \otimes \mathbb{1}_{\mathfrak{F}} + h_{x_1}(y) \otimes \check{a}(y)^* \otimes \mathbb{1}_{\mathfrak{F}}\right] \\ &\quad + \sqrt{\alpha}\lambda_0 \int_{\mathbb{R}^3} \mathrm{d}y\, \left[h_{x_2}(y) \otimes \mathbb{1}_{\mathfrak{F}} \otimes \check{a}(y) + h_{x_2}(y) \otimes \mathbb{1}_{\mathfrak{F}} \otimes \check{a}(y)^*\right]. \end{aligned}$$

Clearly $\inf \mathrm{spec}(H_{\mathrm{bp},\kappa}^{\otimes}) = 2E_{\mathrm{p},\kappa}$. Recall the definition of $\bar{\phi}_R(x_1, x_2)$ given in the proof of Proposition 4.2 (ii).

Lemma D.1. *For* $\varphi \in \mathrm{dom}(H_{\mathrm{bp},\kappa})$,

$$\langle \varphi, \bar{\phi}_R H_{\mathrm{bp},\kappa} \bar{\phi}_R \varphi \rangle = \left\langle \varphi, U_{R/4}(x)^* \bar{\phi}_R H_{\mathrm{bp},\kappa}^{\otimes} \bar{\phi}_R U_{R/4}(x)\varphi \right\rangle + O(1)\,,$$

where $O(1)$ *is the error term satisfying* $|O(1)| \le G(R)(\langle \varphi, H_{\mathrm{bp},\kappa}\varphi\rangle + b\|\varphi\|^2)$ *with* $G(R)$ *vanishing as* $R \to \infty$*, and some positive constant* $b > E_{\mathrm{bp},\kappa}$.

Proof. The proof is almost in parallel to that of [9, Lemma A.1]. However, for the convenience of the reader we provide a sketch of the proof. First we investigate the difference of the electron-phonon interaction terms, namely,

$$\begin{aligned} &\sum_{j=1,2} \bar{\phi}_R \int_{\mathbb{R}^3} \mathrm{d}y\, \left[h_{x_j}(y) \otimes \check{a}(y) + h_{x_j}(y) \otimes \check{a}(y)^*\right] \bar{\phi}_R \\ &\quad - U_{R/4}(x)^* \bar{\phi}_R \int_{\mathbb{R}^3} \mathrm{d}y\, \left[h_{x_1}(y) \otimes \check{a}(y) \otimes \mathbb{1}_{\mathfrak{F}} + h_{x_1}(y) \otimes \check{a}(y)^* \otimes \mathbb{1}_{\mathfrak{F}}\right] \bar{\phi}_R U_{R/4}(x) \\ &\quad - U_{R/4}(x)^* \bar{\phi}_R \int_{\mathbb{R}^3} \mathrm{d}y\, \left[h_{x_2}(y) \otimes \mathbb{1}_{\mathfrak{F}} \otimes \check{a}(y) + h_{x_2}(y) \otimes \mathbb{1}_{\mathfrak{F}} \otimes \check{a}(y)^*\right] \bar{\phi}_R U_{R/4}(x)\,. \end{aligned} \tag{63}$$

It suffices to show

$$\big\|\big[\bar\phi_R\check a(h_{x_1})^{\#}\bar\phi_R - U_{R/4}(x)^*\bar\phi_R\check a(h_{x_1})\otimes \mathbb{1}_{\mathfrak F}\bar\phi_R U_{R/4}(x)\big]\varphi\big\| = \tilde O(1) \tag{64}$$

and

$$\left\|\left[\bar\phi_R\check a(h_{x_2})^{\#}\bar\phi_R - U_{R/4}(x)^*\bar\phi_R\int_{\mathbb{R}^3}\mathrm{d}y\, h_{x_2}(y)\otimes \mathbb{1}_{\mathfrak F}\otimes \check a(y)^{\#}\bar\phi_R U_{R/4}(x)\right]\varphi\right\| = \tilde O(1)\,, \tag{65}$$

where $\tilde O(1)$ satisfies $\tilde O(1)\le G(R)'(\langle\varphi, H_{\mathrm{bp},\kappa}\varphi\rangle + b\|\varphi\|^2)^{1/2}$ with $G(R)'$ vanishing as $R\to\infty$. To show (64), note that

$$\begin{aligned}
&\bar\phi_R\,\check a(h_{x_1})^{\#}\bar\phi_R - U_{R/4}(x)^*\bar\phi_R\,\check a(h_{x_1})\otimes \mathbb{1}_{\mathfrak F}\,\bar\phi_R U_{R/4}(x)\\
&\quad = U_{R/4}(x)^*\bar\phi_R\int_{\mathbb{R}^3}\mathrm{d}y\,\big(j_{1,R/4}(y;x_2)-1\big)h_{x_1}(y)\otimes \check a(y)^{\#}\otimes \mathbb{1}_{\mathfrak F}\,\bar\phi_R U_{R/4}(x)\\
&\qquad + U_{R/4}(x)^*\bar\phi_R\int_{\mathbb{R}^3}\mathrm{d}y\, j_{2,R/4}(y;x_2)h_{x_1}(y)\otimes \mathbb{1}_{\mathfrak F}\otimes \check a(y)^{\#}\,\bar\phi_R U_{R/4}(x) =: I_1 + I_2\,.
\end{aligned}$$

The standard number operator estimate leads to

$$\|I_1\varphi\| \le \left\{\sup_{x_1,x_2}\bar\phi_R(x_1,x_2)^2\big\|\big[j_{1,R/4}(\cdot,x_2)-1\big]h_{x_1}\big\|\right\}\|\mathbb{1}_{L^2}\otimes (N_{\mathrm f}+1)^{1/2}\varphi\|\,.$$

Since the number operator $N_{\mathrm f}$ is relatively bounded with respect to the Hamiltonian $H_{\mathrm{bp},\kappa}$, we have that $N_{\mathrm f}\le c_1 H_{\mathrm{bp},\kappa}+c_2$ for some positive constant c_1 and c_2, and hence $\|\mathbb{1}_{L^2}\otimes (N_{\mathrm f}+\mathbb{1})^{1/2}\varphi\|^2 \le c_1\langle\varphi, H_{\mathrm{bp},\kappa}\varphi\rangle + c_2\|\varphi\|^2$. Noting the support properties $\mathrm{supp}(1-j_{1,R/4}(\cdot,x_2))\subseteq\{y\in\mathbb{R}^3\,|\,|y-x_2|\le R/2\}$ and $\mathrm{supp}\bar\phi_R\subseteq\{x=(x_1,x_2)\in\mathbb{R}^6\,|\,|x_1-x_2|\ge R\}$, we have that

$$\begin{aligned}
&\bar\phi_R(x_1,x_2)\big\|\big[j_{1,R/4}(\cdot\,;x_2)-1\big]h_{x_1}\big\|^2\\
&\quad\le 4\bar\phi_R(x_1,x_2)\int_{|y-x_2|\le R/2 \text{ and } |x_1-x_2|\ge R}\mathrm{d}y\,|h_{x_1}(y)|^2\\
&\quad\le 4\bar\phi_R(x_1,x_2)\int_{|y-x_1|\ge R/2}\mathrm{d}y\,|h_{x_1}(y)|^2\\
&\quad= 4\bar\phi_R(x_1,x_2)\int_{|Y|\ge R/2}\mathrm{d}Y\,|h_0(Y)|^2\,.
\end{aligned}$$

Therefore we can conclude that $\|I_1\varphi\| = \tilde O(1)$. Similarly,

$$\|I_2\varphi\| \le \left\{\sup_{x_1,x_2}\bar\phi_R(x_1,x_2)^2\|j_{2,R/4}(\cdot;x_2)h_{x_1}\|\right\}\|\mathbb{1}_{L^2}\otimes (N_{\mathrm f}+\mathbb{1})^{1/2}\|$$

and

$$\bar\phi_R(x_1,x_2)\|j_{2,R/4}(\cdot;x_2)h_{x_1}\|^2 \le \bar\phi_R(x_1,x_2)\int_{|Y|\ge R/2}\mathrm{d}Y\,|h_0(Y)|^2$$

which imply $\|I_2\varphi\| = \tilde{O}(1)$. To show (65), we apply a similar reasoning and only remark that

$$\bar{\phi}_R(x_1,x_2)\|j_{1,R/4}(\cdot;x_2)h_{x_2}\|^2 \le \bar{\phi}_R(x_1,x_2)\int_{|Y|>R/4}\mathrm{d}Y\,|h_0(Y)|^2$$

and

$$\bar{\phi}_R(x_1,x_2)\big\|\big[j_{2,R/4}(\cdot;x_2)-1\big]h_{x_2}\big\|^2 \le 4\bar{\phi}_R(x_1,x_2)\int_{|Y|>R/4}\mathrm{d}Y\,|h_0(Y)|^2\,.$$

It is clear that

$$U_{R/4}(x)^*(\mathbb{1}_{L^2}\otimes N_{\mathrm{f}}\otimes\mathbb{1}_{\mathfrak{F}}+\mathbb{1}_{L^2}\otimes\mathbb{1}_{\mathfrak{F}}\otimes N_{\mathrm{f}})U_{R/4}(x)=\mathbb{1}_{L^2}\otimes N_{\mathrm{f}}\,.$$

To show that

$$\Big\langle\varphi,\bar{\phi}_R\sum_{j=1,2}(-\Delta_{x_j})\otimes\mathbb{1}_{\mathfrak{F}}\bar{\phi}_R\,\varphi\Big\rangle - \Big\langle\varphi,U_{R/4}(x)^*\bar{\phi}_R\sum_{j=1,2}(-\Delta_{x_j})\otimes\mathbb{1}_{\mathfrak{F}}\otimes\mathbb{1}_{\mathfrak{F}}\bar{\phi}_R U_{R/4}(x)\varphi\Big\rangle = O(1)\,,$$

one follows the proof of [9, Lemma A.1]. □

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