On Polarons and Multipolarons in Electromagnetic Fields

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Dipl. Phys. David Wellig

aus Fieschertal (Schweiz)

Hauptberichter: Prof. Dr. Marcel Griesemer
Mitberichter: Prof. Dr. Jacob Schach Møller

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Zusammenfassung

Diese Dissertation handelt von Systemen von sogenannten großen Polaronen in elektromagnetischen Feldern. Wir interessieren uns insbesondere für die Grundzustandsenergie im Fall starker Wechselwirkung, $\alpha \gg 1$, zwischen Elektronen und Phononen und für die Existenz von Bindungszuständen zwischen mehreren Polaronen. Zur Beschreibung der Polaronen verwenden wir das Modell von H. Fröhlich, sowie die approximativen Modelle von Pekar, und Pekar und Tomasevich. Die Vermutung, dass die Grundzustandsenergie dieser Modelle asymptotisch, für $\alpha \to \infty$, in führender Ordnung übereinstimmen, war der Ausgangspunkt dieser Arbeit. Wir beweisen diese Vermutung für eine große Klasse äußerer elektromagnetischer Felder. Eine geeignete Skalierung der Felder sorgt dafür, dass sie bereits in führender Ordnung eine nicht-triviale Rolle spielen. Die asymptotische Übereinstimmung der Grundzustandsenergien erlaubt es uns, die Frage nach der Bindung von Fröhlich Polaronen im Fall großer α auf die entsprechende Frage im Modell von Pekar und Tomasevich zurückzuführen.

Die Niederschrift dieser Dissertation ist unterteil in vier Kapitel, wobei das erste die Einleitung ist. Die Kapitel 2, 3 und 4 stellen drei unabhängige Publikationen dar.

Das Kapitel 2 ist dem Pekarfunktional mit elektromagnetischen Feldern gewidmet. Wir beweisen die Existenz eines Minimierers im Fall wo das Magnetfeld konstant ist und das elektrische Feld verschwindet. Der Minimierer existiert aber auch dann, wenn diese Feldkonfiguration lokal so gestört wird, dass die minimale Energie dabei reduziert wird. Aus der Existenz eines Minimierers des Pekarfunktionals leiten wir die Bindung von zwei Polaronen im Modell von Pekar und Tomasevich her.

In Kapitel 3 vergleichen wir die Grundzustandsenergie des 1-Teilchen Fröhlich Modells im Limes $\alpha \to \infty$ mit dem Minimum des entsprechenden Pekarfunktionals. Wir beweisen die oben erwähnte Vermutung im Fall eines einzigen Polarons. Dieses Resultat, in Verbindung mit den Ergebnissen aus Kapitel 2, erlaubt es uns die Bindung zweier Fröhlich Polaronen in starken elektromagnetischen Feldern zu beweisen.

In Kapitel 4 wird die Analyse aus dem vorherigen Kapitel auf N-Polaronen ausgeweitet. Es wird eine Abschätzung der Wechselwirkungsenergie räumlich getrennter Gruppen von Po-

laronen in elektromagnetischen Feldern hergeleitet. Diese erlaubt es uns die asymptotische Exaktheit der Minimalenergie des Pekar-Tomasevichfunktionals für starke Kopplungen zu beweisen, wobei, wie in Kapitel 3, die externen Felder geeignet skaliert werden. Als Anwendung wird Bindung von N Polaronen in konstanten starken Magnetfeldern bewiesen.

Abstract

This dissertation is concerned with a system of so-called large polarons in electromagnetic fields. We are especially interested in the ground state energy in the case of strong interactions, $\alpha \gg 1$, between electrons and phonons and in the existence of bound states of several polarons. For the description of the polarons we use the model of H. Fröhlich, as well as the approximative models of Pekar, and Pekar and Tomasevich. The conjecture, that the ground state energy asymptotically coincides in the leading order, $\alpha \to \infty$, was the starting point of this work. We prove this conjecture for a large class of external electromagnetic fields. A suitable scaling of the fields makes sure, that they already play a non-trivial role in the leading order. The asymptotic coincidence of the ground state energies allows us to trace back the question of binding of Fröhlich polarons in the case of large α to the corresponding question in the model of Pekar and Tomasevich.

The transcription of this dissertation is divided into four chapters, of which the introduction is the first one. The Chapters 2, 3 and 4 constitute three independent publications.

The Chapter 2 is dedicated to the Pekar functional with electromagnetic fields. We proof the existence of a minimizer in the case of a constant magnetic field and a vanishing electric field. The minimizer exists as well, if this field configuration is locally perturbed such that the minimal energy is lowered. From the existence of the minimizer of the Pekar functional we derive binding of two polarons in the model of Pekar and Tomasevich.

In Chapter 3, we compare the ground state energy of the 1-particle Fröhlich model in the limit $\alpha \to \infty$ with the minimum of the corresponding Pekar functional. We prove the above mentioned conjecture in the case of a single polaron. This result, in connection with the results of Chapter 2, allows us to prove binding of two Fröhlich polarons in strong electromagnetic fields.

In Chapter 4 the analysis of the previous chapter is extended to N-polaron systems. To do so, an estimate of the interaction energy of spatially divided clusters of polarons in electromagnetic fields is derived. This allows us to proof the asymptotic exactness of the minimal energy of the Pekar-Tomasevich functional for strong couplings, whereas, as in Chapter 3, the external fields are suitably rescaled. As an application binding for N polarons in constant strong magnetic fields is proved.

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Chapter 1

Introduction

This introductory chapter interconnects the individual results of the present thesis and puts them into a more general context.

In this dissertation we are interested in polarons and multipolarons in magnetic and electric fields. We want to know how they affect the properties of the Fröhlich model and the Pekar functional. Especially, we examine the existence of a minimizer of the electromagnetic Pekar functional. Furthermore, in the case of electromagnetic fields we prove that in the leading order for $\alpha \to \infty$ the minimal energy of the Pekar functional and the Pekar-Tomasevich functional for N particles exactly describe the ground state energy of the Fröhlich model. We also study conditions of binding for bipolarons and multipolarons in electromagnetic fields.

The presence of an excess electron in a ionic crystal generates a polarization of the crystal lattice. The potential well, that is generated this way, was supposed to trap the electron, which was already long ago assumed by Landau [20]. The system of an electron with the induced deformation of the lattice is called a polaron. A N-polaron or a multipolaron is a system of N electrons with its corresponding deformations of the lattice. Since energetically it is more favorable to distort the lattice in a small region, the electrons tend to stay near to each other and hence there acts an attractive force between the electrons which competes with the repulsive electron-electron interaction. The question which force is stronger or in other words whether there exist bound states, is discussed in the context of the Fröhlich model in the subsequent chapters.

A hamilton operator for the description of a polaron was introduced by H. Fröhlich [16]. The polarons in this model are called 'large polarons', since the spatial extension of the polarons is assumed to be big in comparison to the lattice spacing. Further, it is supposed that the electron only interacts with the optical, longitudinal modes of the phonon field. Relativistic effects and spin are not taken into account. The Fröhlich hamiltonian acts on

$L^2(\mathbb{R}^3) \otimes \mathcal{F}$, where $\mathcal{F}$ is the symmetric Fock space over $L^2(\mathbb{R}^3)$, and it is defined by

$$-\Delta + \frac{\sqrt{\alpha}}{\sqrt{2}\pi} \int \frac{1}{|k|} \left(a(k) e^{ikx} + h.c. \right) dk + \int a^*(k) a(k) dk. \tag{1.1}$$

The coupling constant α describes the strenght of the interaction between electron and phonons. The coupling constant α has to be bounded from above in terms of the electron-electron repulsion strenght U in the physical regime, intuitively because the polarization of the lattice is a response to the presence of the electron [30]. For general information about polarons see [1, 8] and references therein.

If the Fröhlich hamilton operator (1.1) is evaluated on the product ansatz $\varphi \otimes \eta \in L^2(\mathbb{R}^3) \otimes \mathcal{F}$ for $\|\varphi\| = 1$ and if it is minimized over all normalized η, then one finds the Pekar functional after scaling out α

$$\int |\nabla \varphi(x)|^2 dx - \int \frac{|\varphi(x)|^2 |\varphi(y)|^2}{|x-y|} dx dy. \tag{1.2}$$

The product ansatz can be understood as an adiabatic approximation, i.e. the electron follows adiabaticly the deformation of the lattice that was generated by itself [24].

Lieb [23] proved the existence of a minimizer of (1.2) subject to $\int |\varphi|^2 dx = 1$ by an application of the symmetric decreasing rearrangement inequalities. Furthermore, he showed that the minimizer is sperically symmetric, unique up to translations and that it can be chosen pointwise positive. If a constant magnetic field with corresponding vector potential A is turned on in (1.2), i. e. $-i\nabla$ is replaced by $-i\nabla + A$, there still exists a normalized minimizer. This is proved in Chapter 2 with the help of Lions' concentration compactness lemma [25].

Since the minimizer of (1.2) constrained by $\int |\varphi|^2 dx = 1$ is a radial function, it is likely that in the case of constant magnetic fields there exists a minimizer that is rotational symmetric about the direction of the magnetic field. This remains an open problem. For bipolarons without external fields it is known by [13], that for small values of the Coulomb constant U the minimizer of the Pekar-Tomasevich functional is rotation invariant after some translation.

If general electric V and magnetic potentials A are imposed, i.e. $-\Delta$ is substituted by $(-i\nabla + A)^2 + V$ in (1.1), and if they locally lower the energy of the corresponding generalized Pekar functional, then there also exists a normalized minimizer. The existence of a minimizer is proved in Chapter 2. The presence of locally perturbed electric and magnetic fields break up the translation invariance of the Pekar functional, thus a minimizer can be catched in the low energy region. Furthermore, in Chapter 2, in the model of Pekar in electromagnetic fields we show an easy variational argument to derive binding of two polarons from the existence of the minimizer. This argument can be generalized to N-polaron systems [3].

It is well-known from Donsker and Varadhan [9] that the ground state energy of (1.1) times α^{-2} converges for $\alpha \to \infty$ to the minimal energy of (1.2) constrained by $\|\varphi\| = 1$. Lieb and Thomas presented another proof for the asymptotic exactness of the Pekar minimal energy [24], but in addition they found an error bound of the order $\alpha^{-9/5}$. The asymptotic exactness implies that the Pekar functional has a certain physical relevance since it describes polarons for strong couplings. In return, this motivates us, from the physical point of view, to study the Pekar functional.

In Chapter 3, we prove that the ground state energy of the Fröhlich model for $N = 1$ subject to electromagnetic fields in the leading order for $\alpha \to \infty$ is exactly described by the minimal energy of the Pekar functional. In our proof we make use of the operator theoretical methods developed in [24]. For the external fields not to be negligible for strong couplings, they have to grow with α, which is done by a suitable rescaling of the fields. However, the translation invariance, that is used in the proof in [24], breaks up in the presence of general electric and magnetic fields. By a modification, we show that this feature is not needed for our proof to work.

In Chapter 3, in the case of electromagnetic fields we show that binding for two polarons in the Pekar model, proved in Chapter 2, leads to binding for Fröhlich polarons in the strong coupling regime. A question arises: Does the presence of a magnetic field increase the binding energy of bipolarons or not? For fixed $\alpha > 0$, in the recently developed paper [12], Frank and Geisinger explicitly specify the dependence of the Fröhlich and Pekar ground state energies on large constant magnetic fields. Maybe a generalization of their work to bipolarons gives an answer to the above question.

Systems of large N-polarons are described by a generalization of (1.1). Here, additionally the electron-electron interaction has to be taken into account, see (4.1). Similarly the Pekar functional is generalized to the N-Pekar-Tomasevich functional, see (4.31).

The Fröhlich ground state energy for N-polarons in electromagnetic fields is described by the Pekar-Tomasevich minimal energy plus a higher order error term that is proportional to $\alpha^{42/23}N^3$. We prove this statement in Chapter 4 with the help of a generalization of the techniques developed in [24]. However they have to be modified, since they only work for polarons that are in a neighborhood of each other. On account of this, all polarons that are close to one another are grouped into the same ball and then the inter-ball interaction energies are estimated from above. Like in Chapter 3 the translation invariance is not needed for the proof to work. A similar analysis was done in [2] in order to examine the Fröhlich ground state energy for N-polarons without external fields in the strong coupling limit.

As a corollary, in Chapter 4, if U/α takes values in the lower physical admissible range, binding for N-polarons subject to strong constant magnetic fields is proved. On the other hand, by [15] we know that in the case without external fields binding does not occur for U/α sufficiently large. It would be interesting to know where the binding non-binding transition occurs and if there is binding for small values of α. At least numerical calculations suggest that there is no bipolaron formation in the case without external fields for small α [31, 32].

This dissertation is based on the articles

1. M. Griesemer, F. Hantsch and D. Wellig. *On the Magnetic Pekar Functional and the Existence of Bipolarons.*

2. M. Griesemer and D. Wellig. *The Strong-Coupling Polaron in Electromagnetic Fields.*

3. D. Wellig. *On the Strong Coupling Limit of Many-Polaron Systems in Electromagnetic Fields.*

Remark. For simplicity and clarity, the notation may partly differ in distinct chapters. Since the notation is introduced in every chapter no misunderstandings should occur.

Chapter 2

On the Magnetic Pekar Functional and the Existence of Bipolarons

M. Griesemer, F. Hantsch and D. Wellig

Abstract

First, this paper proves the existence of a minimizer for the Pekar functional including a constant magnetic field and possibly some additional local fields that are energy reducing. Second, the existence of the aforementioned minimizer is used to establish the binding of polarons in the model of Pekar-Tomasevich including external fields.

2.1 Introduction

The Pekar functional including external electric and magnetic potentials is given by

$$\int \left(|D_A\varphi|^2 + V|\varphi|^2 \right) dx - \int \frac{|\varphi(x)|^2|\varphi(y)|^2}{|x-y|} dxdy \tag{2.1}$$

where $D_A := -i\nabla + A$ and $\varphi \in H^1_A(\mathbb{R}^3)$. The letters V and A denote (real-valued) scalar and vector potentials associated with the external electric and magnetic fields $-\nabla V$ and $\operatorname{curl} A$. Since φ denotes the wave function of a quantum particle (electron) we impose the constraint that

$$\int |\varphi|^2 \, dx = 1. \tag{2.2}$$

The functional (2.1) arises e.g. in the study of the ground state energy of the polaron [9, 24] and in the analysis of a self-gravitating quantum particle [27]. Depending on the context, the Euler-Lagrange equation associated with (2.1), (2.2) is called Choquard equation or Schrödinger-Newton equation. The time-dependent version of the Euler-Lagrange equation describes the dynamics of interacting many-boson systems in the mean field limit [10]. We are interested in the question whether the functional (2.1) subject to (2.2) has a minimizer, and we shall give a positive answer for a class of potentials including all previously considered cases. Second, we shall use the existence of a minimizer to prove binding of polarons in the model of Pekar and Tomasevich with an external magnetic field.

In the case $A = 0$ and $V = 0$ it is a well-known result, due to Lieb [23], that the Pekar functional (2.1), (2.2) possesses a unique, rotationally symmetric minimizer, which moreover can be chosen pointwise positive. For the existence part a second proof has been given by Lions as an application of his concentration compactness principle [25]. Lions also considered the case of non-vanishing $V \leq 0$. In this paper we establish existence of a minimizer for constant magnetic fields and vanishing V, as well as for certain local perturbations of this field configuration. For example, if $\operatorname{curl} A$ is constant, $V(x) = -|x|^{-1}$, then (2.1) has a minimizer as well. More generally, the Pekar functional has a minimizer for any local perturbation of the fields $A(x) = (B \wedge x)/2$, $V = 0$ that leads to a reduction of the energy. We give examples of non-linear vector potentials for which this trapping assumption is satisfied.

In the second part of the paper we address the question of binding of two polarons subject to given electromagnetic fields A, V in the model of Pekar and Tomasevich. For $A = 0, V = 0$ this question has been studied by Miyao, Spohn and by Lewin and answered in the affirmative for admissible values of the electron-electron repulsion close to the critical one [26, 21]. In fact, Lewin proved the binding of any given number of polarons by establishing a Van der Waals type interaction between two polaron clusters. This method makes use of a spherical invariance which is broken by the presence of a magnetic field. We here describe a much softer argument to explain the binding of two polarons that works for any given A, V and requires nothing but the existence of a minimizer for (2.1), (2.2). This argument is based on the observation that the product $\psi \otimes \psi$ of two copies of a minimizer ψ of (2.1), (2.2) does not solve the Euler-Lagrange equation of the Pekar-Tomasevich functional and hence cannot be a minimizer of this functional. This argument does not depend on the presence of external fields and seems to be novel. It can be extended to multipolaron systems, and this will be done in subsequent work.

In a companion paper we derive estimates on the ground state energy of the Fröhlich polaron subject to electromagnetic fields A, V in the limit of strong electron-phonon coupling,

$\alpha \to \infty$. For fields A, V that are suitably rescaled with α, it turns out that this ground state energy is correctly given by α^2 times the minimum of (2.1), (2.2) up to errors of smaller order. In view of the results of the present paper the binding of Fröhlich polarons subject to strong external fields and large α will follow. In the case $A = 0$, $V = 0$ a similar result has previously been established by Miyao and Spohn on the bases of [9, 24, 23]. In the physical literature the existence of Fröhlich bipolarons in the presence of magnetic fields is studied e.g. in [5].

Solutions to the Choquard equation with magnetic field have very recently been studied in [7, 6]. In [6] infinitely many solutions are found whose symmetry corresponds to the symmetry of A. Constant magnetic fields seem to be excluded, however. The constrained minimization problem (2.1), (2.2) with non-vanishing magnetic field does not seem to have been studied yet. Nevertheless, as our methods are not new, we would not be surprised if some of our results on the existence of a minimizer for (2.1),(2.2) with $A \neq 0$ could be inferred from existing results in the literature.

Section 2 is devoted to the problem of existence of minimizers for (2.1), (2.2); in Section 3 the binding of polarons is established. There is an appendix where technical auxiliaries are collected.

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2.2 The Magnetic Pekar Functional

This section contains all our results on the existence of a minimizer for the Pekar functional, as well as the main parts of the proofs. Some technical auxiliaries have been deferred to the appendix.

The *minimal assumptions* that we shall make throughout the paper, are that A, V are real-valued with $A_k, V \in L^2_{loc}(\mathbb{R}^3)$ and that V is infinitesimally small with respect to $-\Delta$, $V \ll -\Delta$. This means that for every $\varepsilon > 0$ there exists $C_\varepsilon \in \mathbb{R}$ such that

$$\|V\varphi\| \leq \varepsilon\|\Delta\varphi\| + C_\varepsilon\|\varphi\|$$

for all $\varphi \in C_0^\infty(\mathbb{R}^3)$. Here and henceforth $\|\cdot\|$ denotes an L^2-norm. Every potential V that admits a decomposition $V = V_1 + V_2$ with $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$ is infinitesimally small w.r.t. $-\Delta$.

We define $D_A := -i\nabla + A$ and

$$H^1_A(\mathbb{R}^3) = \big\{\varphi \in L^2(\mathbb{R}^3) \mid D_A\varphi \in L^2(\mathbb{R}^3;\mathbb{C}^3)\big\}.$$

Equipped with the norm $\|\varphi\|_A^2 := \|D_A\varphi\|^2 + \|\varphi\|^2$ this space is complete and $C_0^\infty(\mathbb{R}^3)$ is dense. This means that the quadratic form $\langle D_A\varphi, D_A\varphi\rangle$ is closed on $H^1_A(\mathbb{R}^3)$ and that $C_0^\infty(\mathbb{R}^3)$ is a core. The unique self-adjoint operator associated with this form is denoted D_A^2.

We define the Pekar functional $\mathcal{E}^{A,V}(\varphi)$ by the expression (2.1). For the domain of this functional we take $\big\{\varphi \in H^1_A(\mathbb{R}^3) | \int |\varphi|^2 dx = 1\big\}$ unless explicitly stated otherwise. In particular, by a *minimizer* of $\mathcal{E}^{A,V}$ we mean a vector φ from this domain. It is not hard to see, using the Hardy and the diamagnetic inequalities, that $\mathcal{E}^{A,V}$ is bounded below and that every minimizing sequence is bounded in $H^1_A(\mathbb{R}^3)$, see Lemma 2.4.2. We set

$$C^{A,V}(\lambda) := \inf\big\{\mathcal{E}^{A,V}(\varphi)\big|\varphi \in H^1_A(\mathbb{R}^3),\ \|\varphi\|^2 = \lambda\big\} \tag{2.3}$$

where $\lambda > 0$. As a preparation for the proofs of the theorems of this section we first establish a few general properties of the Pekar functional (2.1) and its lower bounds (2.3). To this end, and for use throughout the paper, we introduce the following notation:

$$V_\varphi(x) := \int \frac{|\varphi(y)|^2}{|x-y|}\,dy, \qquad D(\rho) := \int \frac{\rho(x)\rho(y)}{|x-y|}\,dxdy,$$

where usually $\rho = \rho_\varphi := |\varphi|^2$.

Lemma 2.2.1. *Under the above minimal assumptions on V, A, the following is true:*

(i) If $\mathcal{E}^{A,V}(\varphi_n) \to C^{A,V}(1)$ and $\varphi_n \to \varphi$ as $n \to \infty$, where $\|\varphi_n\| = 1$, then $\mathcal{E}^{A,V}(\varphi) = C^{A,V}(1)$ and $\varphi_n \to \varphi$ in $H^1_A(\mathbb{R}^3)$.

(ii) If $\mathcal{E}^{A,V}(\varphi) = C^{A,V}(1)$, then φ is an eigenvector of $D_A^2 + V - 2V_\varphi$ associated with the lowest eigenvalue of this operator, which is $C^{A,V}(1) - D(\rho_\varphi)$.

(iii) The map $\lambda \mapsto C^{A,V}(\lambda)$ is continuous.

(iv) If $\liminf_{n\to\infty} D(\rho_{\varphi_n}) > 0$ for every (normalized) minimizing sequence of $\mathcal{E}^{A,V}$, then for all $\lambda \in (0,1)$,

$$C^{A,V}(1) < C^{A,V}(\lambda) + C^{A,V}(1-\lambda).$$

Proof. (i) Since (φ_n) is bounded in $H^1_A(\mathbb{R}^3)$ and $\varphi_n \to \varphi$ we see that $\varphi_n \rightharpoonup \varphi$ in $H^1_A(\mathbb{R}^3)$, and hence that $\mathcal{E}^{A,V}(\varphi) \leq \liminf_{n\to\infty} \mathcal{E}^{A,V}(\varphi_n)$, by Lemma 2.4.2, (ii). It follows that $\mathcal{E}^{A,V}(\varphi) =$

$C^{A,V}(1) = \lim_{n\to\infty} \mathcal{E}^{A,V}(\varphi_n)$ and, using Lemma 2.4.2 again, that $\|D_A\varphi_n\|^2 \to \|D_A\varphi\|^2$. This proves (i).

(ii) We claim that

$$\mathcal{E}^{A,V}(\psi) \le \langle\psi, (D_A^2 + V - 2V_\varphi)\psi\rangle + D(\rho_\varphi) \tag{2.4}$$

for any given $\psi \in H_A^1(\mathbb{R}^3)$. This follows from $0 \le D(\rho_\varphi - \rho_\psi) = D(\rho_\varphi) + D(\rho_\psi) - 2\langle\psi, V_\varphi\psi\rangle$. If φ is a minimizer of $\mathcal{E}^{A,V}$, then it follows from (2.4) that for every normalized $\psi \in H_A^1(\mathbb{R}^3)$,

$$C^{A,V}(1) \le \langle\psi, (D_A^2 + V - 2V_\varphi)\psi\rangle + D(\rho_\varphi)$$

with equality if $\psi = \varphi$. This proves part (ii).

(iii) Clearly for all $\lambda > 0$,

$$C^{A,V}(\lambda) = \lambda \cdot \inf\left\{\|D_A\varphi\|^2 + \langle\varphi, V\varphi\rangle - \lambda D(\rho_\varphi)\big|\|\varphi\| = 1\right\}. \tag{2.5}$$

We see that $g(\lambda) = C^{A,V}(\lambda)/\lambda$ is the infimum of linear functions of λ. It follows that g is concave and hence continuous.

(iv) It suffices to show that

$$C^{A,V}(\lambda) > \lambda C^{A,V}(1) \quad \text{for all} \quad \lambda \in (0,1). \tag{2.6}$$

Then $C^{A,V}(1-\lambda) > (1-\lambda)C^{A,V}(1)$ and the asserted inequality follows. Since, by (2.5), $C^{A,V}(\lambda) \ge \lambda C^{A,V}(1)$, it remains to exclude equality. Again by (2.5), the equality $C^{A,V}(\lambda) = \lambda C^{A,V}(1)$ would imply the existence of a normalized sequence (φ_n) with $\|D_A\varphi_n\|^2 + \langle\varphi_n, V\varphi_n\rangle - \lambda D(\rho_{\varphi_n}) \to C^{A,V}(1)$. A fortiori, this sequence would be minimizing for $\mathcal{E}^{A,V}$ and $D(\rho_{\varphi_n}) \to 0$, in contradiction with the assumption. □

Lemma 2.2.2. *If A is* linear *with $B = \operatorname{curl} A$, then*

(i) $C^{0,0}(1) \le C^{A,0}(1) \le C^{0,0}(1) + |B|$, and $C^{0,0}(1) < 0$.

(ii) If (φ_n) is a minimizing sequence for $\mathcal{E}^{A,0}$ then $\liminf_{n\to\infty} D(\rho_{\varphi_n}) > 0$.

Proof. The inequality $C^{0,0}(1) \le C^{A,0}(1)$ follows from the diamagnetic inequality, and $C^{0,0}(1) < 0$ follows from a simple variational argument. By combining (2.4) with the enhanced binding inequality of Lieb [4, Theorem A.1], we conclude that, for $\varphi \in H^1(\mathbb{R}^3)$ with $\|\varphi\| = 1$,

$$\begin{aligned} C^{A,0}(1) &\leq \inf \sigma(D_A^2 - 2V_\varphi) + D(\rho_\varphi) \\ &\leq \inf \sigma(-\Delta - 2V_\varphi) + D(\rho_\varphi) + |B| \\ &\leq \langle \varphi, (-\Delta - 2V_\varphi)\varphi \rangle + D(\rho_\varphi) + |B| \\ &= \mathcal{E}^{0,0}(\varphi) + |B|. \end{aligned}$$

To prove (ii), suppose that $D(\rho_{\varphi_n}) \to 0$ as $n \to \infty$ for some minimizing sequence (φ_n) of $\mathcal{E}^{A,0}$. Then

$$C^{A,0}(1) = \lim_{n\to\infty} \mathcal{E}^{A,0}(\varphi_n) = \lim_{n\to\infty} \|D_A \varphi_n\|^2 \geq |B|, \tag{2.7}$$

which is in contradiction with the fact that $C^{A,0}(1) \leq C^{0,0}(1) + |B| < |B|$, by (i). □

Theorem 2.2.3. *Suppose that A is linear. Then there exists a $\varphi \in H^1_A(\mathbb{R}^3)$ with $\int |\varphi|^2 \, dx = 1$ such that*

$$\mathcal{E}^{A,0}(\varphi) = C^{A,0}(1),$$

and every minimizing sequence for $\mathcal{E}^{A,0}$ has a subsequence that converges to a minimizer after suitable translations and phase shifts.

Remark. The Pekar functional $\mathcal{E}^{A,0}$ with a linear vector potential A is invariant under magnetic translations $\psi \mapsto \psi_v$, $v \in \mathbb{R}^3$, where

$$\psi_v(x) := e^{-i\chi(x)}\psi(x - v), \qquad \chi(x) := A(v) \cdot x, \quad v \in \mathbb{R}^3. \tag{2.8}$$

This means that minimizing sequences will in general not be relatively compact. By the concentration compactness principle every minimizing sequence has a subsequence that becomes relatively compact upon suitable translations of the type (2.8).

Proof. Let (φ_n) be a minimizing sequence for $\mathcal{E}^{A,0}$ and let (φ_{n_k}) be the subsequence given by Lemma 2.4.1. We shall exclude vanishing and dichotomy in order to conclude compactness of the sequence of suitably shifted functions. In the following we use ρ_n as a short hand for ρ_{φ_n}.

Vanishing does not occur. We show that vanishing implies $D(\rho_{n_k}) \to 0$ as $k \to \infty$, which contradicts Lemma 2.2.2 (ii). To this end we use that $D(\rho_\varphi) = \int V_\varphi \rho_\varphi \, dx \leq \|V_\varphi\|_\infty$ where $\varphi \in L^2(\mathbb{R}^3)$ is normalized. For every $R > 0$, by the Hölder and the magnetic Hardy inequalities,

$$
\begin{aligned}
|V_{\varphi_{n_k}}(x)| &\leq \int_{B_R(x)} \frac{|\varphi_{n_k}(y)|^2}{|x-y|} dy + \frac{1}{R} \\
&\leq 2\|D_A\varphi_{n_k}\| \left(\int_{B_R(x)} |\varphi_{n_k}(y)|^2 \, dy \right)^{1/2} + \frac{1}{R}.
\end{aligned}
$$

Since $\sup_k \|D_A\varphi_{n_k}\| < \infty$, vanishing implies $\|V_{\varphi_{n_k}}\|_\infty \to 0$ and $D(\rho_{n_k}) \to 0$ as $k \to \infty$.

Dichotomy does not occur. Suppose dichotomy holds, that is, there exists some $\lambda \in (0,1)$, such that for every $\varepsilon > 0$ there exists $k_0 \in \mathbb{N}$ and bounded sequences $(\varphi_k^{(1)})$, $(\varphi_k^{(2)})$ in $H^1_A(\mathbb{R}^3)$ having the properties (a)–(d) from Lemma 2.4.1. Then, from (a), (c) and the continuity of $\varphi \mapsto D(\rho_\varphi)$, Lemma 2.4.2, we see that for $k \geq k_0$

$$
\begin{aligned}
&\left| D(\rho_{n_k}) - D(\rho_k^{(1)}) - D(\rho_k^{(2)}) \right| \\
&\leq \left| D(\rho_{n_k}) - D(|\varphi_k^{(1)} + \varphi_k^{(2)}|^2) \right| + \left| D(|\varphi_k^{(1)} + \varphi_k^{(2)}|^2) - D(\rho_k^{(1)}) - D(\rho_k^{(2)}) \right| \\
&= \delta(\varepsilon) + o(1), \qquad (k \to \infty),
\end{aligned}
$$

where $\delta(\varepsilon) = o(1)$ as $\varepsilon \to 0$. It follows that, using Lemma 2.2.1 (iii) and Lemma 2.4.1 (d),

$$
\begin{aligned}
& C^{A,0}(1) \\
= & \lim_{k\to\infty} \mathcal{E}^{A,0}(\varphi_{n_k}) \\
\geq & \liminf_{k\to\infty} \left[\mathcal{E}^{A,0}(\varphi_{n_k}) - \mathcal{E}^{A,0}(\varphi_k^{(1)}) - \mathcal{E}^{A,0}(\varphi_k^{(2)}) \right] + C^{A,0}(\lambda) + C^{A,0}(1-\lambda) + o(1) \\
\geq & \liminf_{k\to\infty} \int_{\mathbb{R}^3} |D_A\varphi_{n_k}|^2 - |D_A\varphi_k^{(1)}|^2 - |D_A\varphi_k^{(2)}|^2 \, dx + C^{A,0}(\lambda) + C^{A,0}(1-\lambda) + o(1) \\
\geq & C^{A,0}(\lambda) + C^{A,0}(1-\lambda) + o(1), \qquad (\varepsilon \to 0).
\end{aligned}
$$

This proves that $C^{A,0}(1) \geq C^{A,0}(\lambda) + C^{A,0}(1-\lambda)$ for some $\lambda \in (0,1)$, which contradicts Lemma 2.2.1 (iv).

Compactness. Since vanishing and dichotomy have been excluded, the subsequence (φ_{n_k}) must have the compactness property of Lemma 2.4.1. Let $\chi_k(x) := A(y_k) \cdot x$ with $y_k \in \mathbb{R}^3$ given by this lemma, and let $u_{n_k}(x) = e^{i\chi_k(x)}\varphi_{n_k}(x + y_k)$. Then, for every $\varepsilon > 0$ there exists $R > 0$ such that

$$
\int_{B_R(0)} |u_{n_k}|^2 dx \geq 1 - \varepsilon \qquad \text{for all } k. \tag{2.9}
$$

The phase χ_k has been chosen in such a way that $A(x) + \nabla\chi_k(x) = A(x + y_k)$, which implies that $\|D_A u_{n_k}\| = \|D_A\varphi_{n_k}\|$. It follows that $\mathcal{E}^{A,0}(u_{n_k}) = \mathcal{E}^{A,0}(\varphi_{n_k})$ and that (u_{n_k}) is bounded in $H^1_A(\mathbb{R}^3)$. Hence there exists a $u \in H^1_A(\mathbb{R}^3)$ and a subsequence of (u_{n_k}), denoted by (u_{n_k}) as well, such that

$$u_{n_k} \rightharpoonup u, \quad \text{in } H^1_A(\mathbb{R}^3), \tag{2.10}$$

and therefore $u_{n_k} \rightharpoonup u$ in $L^2(\mathbb{R}^3)$. We claim that $\|u\| = 1$ and hence that $u_{n_k} \to u$ in $L^2(\mathbb{R}^3)$. Indeed, since A is locally bounded, (2.10) implies that $u_{n_k} \to u$ locally in $L^2(\mathbb{R}^3)$, and by (2.9) we conclude that

$$1 \geq \|u\|^2 \geq \int_{B_R(0)} |u|^2\, dx = \lim_{k\to\infty} \int_{B_R(0)} |u_{n_k}|^2\, dx \geq 1 - \varepsilon$$

for every $\varepsilon > 0$. The theorem now follows from Lemma 2.2.1 (i). □

We say A is *asymptotically linear* if there exists a linear vector potential A_∞ such that

$$|A(x) - A_\infty(x)| \to 0, \qquad \text{as } |x| \to \infty.$$

In addition we shall assume that $A \in L^3_{loc}(\mathbb{R}^3)$ whenever A is asymptotically linear. This technical assumption ensures, e. g. that $H^1_A(\mathbb{R}^3) = H^1_{A_\infty}(\mathbb{R}^3)$ and that the norms of these spaces are equivalent (see Lemma 2.4.3).

To ensure relative compactness of minimizing sequences we shall impose one of the following *trapping assumptions*:

(T1) $V(-\Delta + 1)^{-1}$ is compact and

$$C^{A,V}(1) < C^{A,0}(1).$$

(T2) $V(-\Delta + 1)^{-1}$ is compact, A is asymptotically linear and

$$C^{A,V}(1) < C^{A_\infty,0}(1).$$

Further below we shall give examples of potentials that satisfy either (T1) or (T2).

Theorem 2.2.4. *Suppose that one of the trapping assumptions (T1) or (T2) is satisfied. Then every minimizing sequence of $\mathcal{E}^{A,V}$ has a convergent subsequence, the limit being a minimizer.*

Remark. If $V(-\Delta + 1)^{-1}$ is compact and A is asymptotically linear, then the inequality $C^{A,V}(1) < C^{A_\infty,0}(1)$ is not only sufficient, but also necessary for the conclusion of Theorem 2.2.4 to hold.

Proof. Let (φ_n) be a minimizing sequence for $\mathcal{E}^{A,V}$. After passing to a subsequence we may assume that $\varphi_n \rightharpoonup \psi$ in $H^1_A(\mathbb{R}^3)$. We claim that $\psi = 0$ is in contradiction with (T1) and (T2).

Indeed, if $\varphi_n \rightharpoonup 0$ then $\langle \varphi_n, V\varphi_n\rangle \to 0$, by Lemma 2.4.4, which implies that $C^{A,V}(1) \geq C^{A,0}(1)$ in contradiction with (T1). If A is asymptotically linear, then $D_A\varphi_n = D_{A_\infty}\varphi_n + (A - A_\infty)\varphi_n$ where $(A - A_\infty)\varphi_n \to 0$ by Lemma 2.4.3. It follows that

$$C^{A,V}(1) = \lim_{n\to\infty} \mathcal{E}^{A,V}(\varphi_n) = \lim_{n\to\infty} \mathcal{E}^{A_\infty,0}(\varphi_n) \geq C^{A_\infty,0}(1).$$

This is in contradiction with (T2).

Using that the weak limit of a minimizing sequence cannot vanish, we conclude, from Lemma 2.4.2 (iii), that

$$\liminf_{n\to\infty} D(\rho_{\varphi_n}) > 0$$

for every minimizing sequence (φ_n). It follows that $\lambda \mapsto C^{A,V}(\lambda)$ is subadditive in the sense of Lemma 2.2.1. We now use this to show that a weakly convergent minimizing sequence (φ_n) is in fact strongly convergent. To this end suppose that $\varphi_n \rightharpoonup \psi$ where $\lambda := \|\psi\|^2 \in (0,1)$ and consider the decomposition $\varphi_n = \psi + (\varphi_n - \psi) =: \psi + \beta_n$. Clearly, $\beta_n \rightharpoonup 0$ in $H^1_A(\mathbb{R}^3)$ and $\|\beta_n\|^2 \to 1-\lambda$. We claim that

$$\mathcal{E}^{A,V}(\varphi_n) = \mathcal{E}^{A,V}(\psi) + \mathcal{E}^{A,V}(\beta_n) + o(1), \qquad (n \to \infty). \tag{2.11}$$

The kinetic and potential energy $\|D_A\varphi_n\|^2 + \langle\varphi_n, V\varphi_n\rangle$ decompose as desired, which is a direct consequence of the weak convergence $\beta_n \rightharpoonup 0$ in $H^1_A(\mathbb{R}^3)$ and the compactness of $V(-\Delta+1)^{-1}$. It is not hard to see, using $\beta_n \to 0$ locally in $L^2(\mathbb{R}^3)$, that

$$D(\rho_{\psi+\beta_n}) = D(\rho_\psi) + D(\rho_{\beta_n}) + o(1), \qquad (n \to \infty).$$

From (2.11) we see that

$$\begin{aligned} \mathcal{E}^{A,V}(\varphi_n) &\geq C^{A,V}(\lambda) + C^{A,V}(\|\beta_n\|^2) + o(1) \\ &= C^{A,V}(\lambda) + C^{A,V}(1-\lambda) + o(1) \end{aligned}$$

for $n \to \infty$, by the continuity of $C^{A,V}$ (Lemma 2.2.1 (iii)). Thus $C^{A,V}(1) \geq C^{A,V}(\lambda) + C^{A,V}(1-\lambda)$ which contradicts the subadditivity of $C^{A,V}$, i.e. Lemma 2.2.1 (iv).

Since we have shown that $\|\psi\| < 1$ is impossible, we conclude that $\|\psi\| = 1$ and $\varphi_n \to \psi$ in $L^2(\mathbb{R}^3)$. The theorem now follows from Lemma 2.2.1 (i). □

Examples:

1) Suppose A is any C^1-vector potential for which $\mathcal{E}^{A,0}$ has a minimizer φ, see Theo-

rems 2.2.3 and 2.2.4. Then the Euler-Lagrange equation satisfied by φ is a Schrödinger equation and hence φ cannot vanish a.e. on a non-trivial open set, see [19]. It follows that $\int V|\varphi|^2\, dx < 0$ for every potential $V \leq 0$ with the property that $V < 0$ on some non-empty open set. If, moreover, $V(-\Delta+1)^{-1}$ is compact, then (T1) is satisfied.

2) We choose $V = 0$ and we define the vector potential A by $A = A_R$ where

$$A_R(x) = \chi_R(x) A_\infty(x)$$

and $A_\infty(x) = (-Bx_2, 0, 0)$, with $\chi \in C_0^\infty(\mathbb{R}^3; [0,1])$, $\chi(x) = 0$ for $|x| \leq 1/2$, $\chi(x) = 1$ for $|x| \geq 1$ and $\chi_R(x) := \chi(x/R)$. We claim that $C^{A,0}(1) < C^{A_\infty,0}(1)$ for $B \geq 4$ and R sufficiently large. Indeed, by Lemma 2.4.2, $\mathcal{E}^{A_\infty,0}(\varphi) = \|D_{A_\infty}\varphi\|^2 - D(\rho_\varphi) \geq B - 2\|\varphi\|^3 \|D_{A_\infty}\varphi\| \geq 0$, while $C^{A_R,0}(1) \to C^{0,0}(1) < 0$ as $R \to \infty$.

The following corollary summarizes the conclusions of Example 1) above and Theorem 2.2.4.

Corollary 2.2.5. *Suppose that $V(-\Delta+1)^{-1}$ is compact, $V \leq 0$, and $V < 0$ on some non-empty open set. Then $\mathcal{E}^{A,V}$ has a minimizer, provided $\mathcal{E}^{A,0}$ has a minimizer and A belongs to C^1. In particular $\mathcal{E}^{A,V}$ has a minimizer for every linear vector potential A.*

2.3 Binding of Polarons

Let V and A satisfy the minimal assumption introduced in the previous section. The magnetic Pekar-Tomasevich functional $\mathcal{E}_U^{A,V} : H^1_{(A,A)}(\mathbb{R}^6) \to \mathbb{R}$ is defined by

$$\begin{aligned}\mathcal{E}_U^{A,V}(\psi) := &\sum_{k=1}^{2} \int \left(|D_{A,x_k}\psi(x_1,x_2)|^2 + V(x_k)|\psi(x_1,x_2)|^2 \right) dx_1 dx_2 \\ &+ U \int \frac{|\psi(x_1,x_2)|^2}{|x_1 - x_2|} dx_1 dx_2 - \int \frac{\rho(x_1)\rho(x_2)}{|x_1 - x_2|} dx_1 dx_2,\end{aligned}$$

where

$$\rho(x) := \int (|\psi(x,y)|^2 + |\psi(y,x)|^2) dy$$

denotes the density. The minimal energy of $\mathcal{E}_U^{A,V}$ is defined by

$$C_U^{A,V} = \inf \left\{ \mathcal{E}_U^{A,V}(\psi) \,\middle|\, \psi \in H^1_{(A,A)}(\mathbb{R}^6), \|\psi\| = 1 \right\}.$$

Theorem 2.3.1. *Suppose that $\mathcal{E}^{A,V}$ possesses a minimizer φ_0; see Theorem 2.2.3, Theorem 2.2.4, and Corollary 2.2.5. Then there exists $U_A > 2$ such that for $2 < U < U_A$ we have*

$$C_U^{A,V} < 2C^{A,V}(1).$$

Proof. Since $C_U^{A,V}$ is continuous with respect to U it suffices to prove that $C_U^{A,V} < 2C^{A,V}(1)$ for $U = 2$. By a straightforward computation

$$\mathcal{E}_{U=2}^{A,V}(\varphi_0 \otimes \varphi_0) = 2\mathcal{E}^{A,V}(\varphi_0) = 2C^{A,V}(1),$$

and it remains to prove that $\varphi_0 \otimes \varphi_0$ is not a minimizer of $\mathcal{E}_{U=2}^{A,V}$. To this end, suppose $\varphi_0 \otimes \varphi_0$ were a minimizer of $\mathcal{E}_{U=2}^{A,V}$. Then it would have to solve the Euler equation of the functional, which implies that

$$\left\langle \eta \otimes \eta \,\middle|\, \textstyle\sum_{k=1}^2 (D_{A,x_k}^2 + V(x_k) - 4V_{\varphi_0}(x_k)) + 2|x_1 - x_2|^{-1} - E \,\middle|\, \varphi_0 \otimes \varphi_0 \right\rangle = 0 \tag{2.12}$$

for some E and all $\eta \in H_A^1(\mathbb{R}^3)$. We claim that (2.12) cannot be true for all η. Since φ_0 minimizes $\mathcal{E}^{A,V}$, we know from Lemma 2.2.1 (ii), that $(D_A^2 + V - 2V_{\varphi_0})\varphi_0 = \lambda\varphi_0$ for some $\lambda \in \mathbb{R}$. Hence equation (2.12) reduces to

$$\left\langle \eta \otimes \eta \,\middle|\, 2\lambda - E - 2\textstyle\sum_{k=1}^2 V_{\varphi_0}(x_k) + 2|x_1 - x_2|^{-1} \,\middle|\, \varphi_0 \otimes \varphi_0 \right\rangle = 0 \tag{2.13}$$

for all $\eta \in H_A^1(\mathbb{R}^3)$. Since V_{φ_0} is bounded while $|x_1 - x_2|^{-1}$ is positive and unbounded, we can choose $r > 0$ so that for all $z \in \mathbb{R}^3$ and all $x_1, x_2 \in B_r(z)$,

$$g(x_1, x_2) := 2\lambda - E - 2\sum_{k=1}^2 V_{\varphi_0}(x_k) + 2|x_1 - x_2|^{-1} \geq 1. \tag{2.14}$$

Let $\chi_{(r,z)} \in C_0^\infty(\mathbb{R}^3; [0,1])$ with $\chi_{(r,z)}(x) = 1$ for $x \in B_{r/2}(z)$ and $\chi_{(r,z)}(x) = 0$ for $x \notin B_r(z)$. In view of (2.14) the choice $\eta = \chi_{(r,z)}\varphi_0$ in (2.13) leads to

$$0 = \left\langle \chi_{(r,z)}\varphi_0 \otimes \chi_{(r,z)}\varphi_0 \,\middle|\, g \,\middle|\, \varphi_0 \otimes \varphi_0 \right\rangle \geq \left(\int_{B_{r/2}(z)} |\varphi_0(x)|^2 \, dx \right)^2,$$

for all $z \in \mathbb{R}^3$. It follows that $\varphi_0 = 0$ in contradiction with $\|\varphi_0\| = 1$. $\square$

2.4 Appendix

The following is a variant of the Lions' concentration compactness principle, Lemma III.1, in [25], the only difference being that $D = -i\nabla$ is replaced by D_A in our version. This does not affect the proof.

Lemma 2.4.1 (Concentration Compactness Lemma)**.** *Suppose that $A : \mathbb{R}^3 \to \mathbb{R}^3$ is real-valued and in $L^2_{loc}(\mathbb{R}^3)$. Let $(\varphi_n)_{n\in\mathbb{N}}$ be a bounded sequence in $H^1_A(\mathbb{R}^3)$, let $\rho_n = |\varphi_n|^2$ and suppose*

$$\int \rho_n(x)dx = 1 \qquad \text{for all } n \in \mathbb{N}.$$

Then there exists a subsequence (φ_{n_k}) which has one of the following three properties:

1. Compactness: *There exists a sequence $(y_k)_{k\geq 0} \subset \mathbb{R}^3$ such that for all $\varepsilon > 0$ there is $R > 0$ with*
$$\int_{B_R(y_k)} \rho_{n_k}(x)dx \geq 1 - \varepsilon \quad \text{for all } k \geq 0.$$
2. Vanishing: *For all $R > 0$:*
$$\lim_{k\to\infty} \left(\sup_{y\in\mathbb{R}^3} \int_{B_R(y)} \rho_{n_k}(x)dx \right) = 0.$$
3. Dichotomy: *There exists $\lambda \in (0,1)$ such that for every $\varepsilon > 0$ there exists $k_0 \in \mathbb{N}$ and bounded sequences $(\varphi_k^{(1)})$, $(\varphi_k^{(2)})$ in $H^1_A(\mathbb{R}^3)$ satisfying,*
   (a) $\|\varphi_{n_k} - (\varphi_k^{(1)} + \varphi_k^{(2)})\| = \delta(\varepsilon), \quad k \geq k_0,$
   (b) $|\|\varphi_k^{(1)}\|^2 - \lambda| \leq \varepsilon, \quad |\|\varphi_k^{(2)}\|^2 - (1-\lambda)| \leq \varepsilon, \quad k \geq k_0,$
   (c) $\mathrm{dist}(\mathrm{supp}(\varphi_k^{(1)}), \mathrm{supp}(\varphi_k^{(2)})) \to \infty \quad (k \to \infty),$
   (d) $\liminf_{k\to\infty} \int \left(|D_A\varphi_{n_k}(x)|^2 - |D_A\varphi_k^{(1)}(x)|^2 - |D_A\varphi_k^{(2)}(x)|^2\right)dx \geq 0,$

   where $\delta(\varepsilon) \to 0$ as $\varepsilon \to 0$ in property (a).

Lemma 2.4.2. *Under our minimal assumptions on A, V the following is true:*

(i) $D(\rho_\varphi) \leq 2\|\varphi\|^3\|D_A\varphi\|$ *for all* $\varphi \in H^1_A(\mathbb{R}^3)$.

(ii) On bounded subsets of $H^1_A(\mathbb{R}^3)$ the maps $\varphi \mapsto \langle\varphi, V\varphi\rangle$ and $\varphi \mapsto D(\rho_\varphi)$ are continuous w.r.t. the norm of $L^2(\mathbb{R}^3)$.

(iii) In $H_A^1(\mathbb{R}^3)$ the map $\varphi \mapsto D(\rho_\varphi)$ is weakly lower semi-continuous.

(iv) For every $\varepsilon \in (0,1)$ there exists C_ε such that for all $\varphi \in H_A^1(\mathbb{R}^3)$

$$\|D_A\varphi\|^2 \leq \frac{1}{1-\varepsilon}\mathcal{E}^{A,V}(\varphi) + C_\varepsilon\big(\|\varphi\|^2 + \|\varphi\|^6\big).$$

Proof. (i) We have $D(\rho_\varphi) = \int \rho_\varphi(x)V_\varphi(x)dx \leq \|\rho_\varphi\|_1\|V_\varphi\|_\infty$, where

$$\|V_\varphi\|_\infty \leq \|\varphi\| \left(\int \frac{|\varphi(y)|^2}{|x-y|^2}\,dy\right)^{1/2} \leq 2\|\varphi\|\|\nabla|\varphi|\|,$$

by the Hölder and the Hardy inequalities. (i) now follows from the diamagnetic inequality $|\nabla|\varphi|| \leq |D_A\varphi|$.

(ii) The continuity of $\varphi \mapsto D(\rho_\varphi)$ follows from

$$\begin{aligned}|D(\rho_\varphi) - D(\rho_\psi)| &= \left|\int \big(\rho_\varphi(x) - \rho_\psi(x)\big)\big(V_\varphi(x) + V_\psi(x)\big)\,dx\right| \\ &\leq \|\rho_\varphi - \rho_\psi\|_1\big(\|V_\varphi\|_\infty + \|V_\psi\|_\infty\big)\end{aligned}$$

where $\|\rho_\varphi - \rho_\psi\|_1 \leq \|\varphi - \psi\|(\|\varphi\| + \|\psi\|)$ and $\|V_\varphi\|_\infty \leq 2\|D_A\varphi\|\|\varphi\|$, by (i). We now turn to the map $\varphi \mapsto \langle\varphi, V\varphi\rangle$. The assumption $V \ll -\Delta$ is equivalent to $|V| \ll -\Delta$ which implies that $|V| \leq \varepsilon(-\Delta) + C_\varepsilon$ for all $\varepsilon > 0$. From here the continuity of $\varphi \mapsto \langle\varphi, V\varphi\rangle$ is easily established.

(iii) Let $\chi \in C_0^\infty(\mathbb{R}^3;[0,1])$ with $\chi(x) = 1$ for $|x| \leq 1$ and let $\chi_R(x) := \chi(x/R)$. The weak convergence $\varphi_n \rightharpoonup \varphi$ in $H_A^1(\mathbb{R}^3)$ implies the norm convergence $\chi_R\varphi_n \to \chi_R\varphi$ in $L^2(\mathbb{R}^3)$. This can be seen from Lemma 2.4.4 with the choice $V = \chi_R^2$. Since the sequence $(\chi_R\varphi_n)$ is bounded in $H_A^1(\mathbb{R}^3)$, it follows from (ii) that $\liminf_{n\to\infty} D(\rho_{\varphi_n}) \geq \liminf_{n\to\infty} D(\chi_R^2\rho_{\varphi_n}) = D(\chi_R^2\rho_\varphi)$ for all $R > 0$ and the desired inequality is obtained using monotone convergence.

(iv) The assumption $V \ll -\Delta$ and the diamagnetic inequality imply that $\varepsilon D_A^2 + V$ is bounded below for every $\varepsilon > 0$. With the help of (i) the inequality in (iv) now easily follows. □

Lemma 2.4.3. *(i) If A_1, A_2 belong to $L^3_{\mathrm{loc}}(\mathbb{R}^3;\mathbb{R}^3)$ and $A_1 - A_2$ is uniformly bounded in the complement of some compact set, then $H_{A_1}^1(\mathbb{R}^3) = H_{A_2}^1(\mathbb{R}^3)$ and the corresponding norms $\|\cdot\|_{A_1}$ and $\|\cdot\|_{A_2}$ are equivalent.*

(ii) If A is asymptotically linear, then the linear map $H_A^1(\mathbb{R}^3) \to L^2(\mathbb{R}^3;\mathbb{C}^3)$, $\varphi \mapsto (A - A_\infty)\varphi$ is compact.

Remark. Further embedding results similar to Lemma 2.4.3 can be found in [11].

Proof. (i) Suppose that $|A_1 - A_2| \leq C$ in the complement of the compact set $K \subset \mathbb{R}^3$. Then, for all $\varphi \in C_0^\infty(\mathbb{R}^3)$, $\|D_{A_2}\varphi\| \leq \|D_{A_1}\varphi\| + \|(A_1 - A_2)\varphi\|$ and

$$\begin{aligned} \|(A_1 - A_2)\varphi\|^2 &\leq \int_K |A_1 - A_2|^2 |\varphi|^2 dx + C^2\|\varphi\|^2 \\ &\leq \left(\int_K |A_1 - A_2|^3 dx\right)^{2/3} \|\varphi\|_6^2 + C^2\|\varphi\|^2. \end{aligned}$$

Since $\|\varphi\|_6 \leq \text{const}\|D_{A_1}\varphi\|$ by the Sobolev and the diamagnetic inequalities, it follows that $\|D_{A_2}\varphi\| \leq \text{const}\|\varphi\|_{A_1}$ for all $\varphi \in C_0^\infty(\mathbb{R}^3)$. This extends to all $\varphi \in H^1_{A_1}(\mathbb{R}^3)$ and then proves the lemma since the roles of A_1 and A_2 are interchangeable.

(ii) The boundedness of the map has been established in the proof of (i). To prove the compactness, let (φ_n) be a bounded sequence in $H^1_A(\mathbb{R}^3)$. After passing to a subsequence we may assume that $\varphi_n \rightharpoonup \varphi$ in $H^1_A(\mathbb{R}^3)$. By the Sobolev inequality, the sequence $(|\varphi_n - \varphi|^2)$ is bounded in $L^3(\mathbb{R}^3)$, which is a reflexive Banach space. Hence we may assume that $|\varphi_n - \varphi|^2 \rightharpoonup \psi$ in $L^3(\mathbb{R}^3)$ by passing to a subsequence once more. We claim that $\psi = 0$. Indeed, from $\varphi_n \rightharpoonup \varphi$ in $H^1_A(\mathbb{R}^3)$ it follows that $\int \chi|\varphi_n - \varphi|^2\, dx \to 0$ for $\chi \in C_0^\infty(\mathbb{R}^3)$, as explained in the proof of Lemma 2.4.2 (iii). On the other hand, $\int \chi|\varphi_n - \varphi|^2\, dx \to \int \chi\psi\, dx$ because $C_0^\infty(\mathbb{R}^3) \subset L^{3/2}(\mathbb{R}^3)$, which is the dual of $L^3(\mathbb{R}^3)$. Thus $\int \chi\psi\, dx = 0$ for all $\chi \in C_0^\infty(\mathbb{R}^3)$, which implies $\psi = 0$. Hence $|\varphi_n - \varphi|^2 \rightharpoonup 0$ in $L^3(\mathbb{R}^3)$ and it is easy to see that $(A - A_\infty)(\varphi_n - \varphi) \to 0$ in $L^2(\mathbb{R}^3; \mathbb{C}^3)$ using that $|A - A_\infty| \leq \varepsilon$ on the complement of some ball B_R and that $\chi_{B_R}|A - A_\infty|^2$ belongs to $L^{3/2}(\mathbb{R}^3)$, the dual of $L^3(\mathbb{R}^3)$. □

Lemma 2.4.4. *In addition to the minimal assumptions on A, V, suppose that $V(-\Delta + 1)^{-1}$ is compact. Then the map $\varphi \mapsto \langle\varphi, V\varphi\rangle$ is weakly continuous in $H^1_A(\mathbb{R}^3)$.*

Proof. The compactness of $V(-\Delta+1)^{-1}$ implies that $V(D_A^2+1)^{-1}$ is compact [4]. By interpolation it follows that $(D_A^2 + 1)^{-1/2}V(D_A^2 + 1)^{-1/2}$ is compact, which implies that $\varphi \mapsto \langle\varphi, V\varphi\rangle$ is weakly continuous. □

Chapter 3

The Strong-Coupling Polaron in Electromagnetic Fields

M. Griesemer and D. Wellig

Abstract

This paper is concerned with Fröhlich polarons subject to external electromagnetic fields in the limit of large electron-phonon coupling. To leading order in the coupling constant, $\sqrt{\alpha}$, the ground state energy is shown to be correctly given by the minimum of the Pekar functional including the electromagnetic fields, provided these fields in the Fröhlich model are scaled properly with α. As a corollary, the binding of two polarons in strong magnetic fields is obtained.

3.1 Introduction

The purpose of this paper is to determine the ground state energy $E(A, V, \alpha)$ of Fröhlich polarons subject to external electromagnetic fields $B = \operatorname{curl} A$ and $E = -\nabla V$ in the limit of large electron-phonon coupling, $\alpha \to \infty$. We show that $E(A, V, \alpha)$, to leading order in α, is given by the minimum of the Pekar functional including the electromagnetic fields, provided these fields in the Fröhlich model are scaled properly with α. Combining this result with our previous work on the binding of polarons in the Pekar-Tomasevich approximation, we prove here, for the first time, the existence of Fröhlich bipolarons in the presence of strong magnetic fields. These results were announced in [17].

The Fröhlich large polaron model without external fields has only one parameter, α, which describes the strength of the electron-phonon interaction. Hence the ground state energy $E(\alpha)$ is a function of α only, and since α is not small for many polar crystals, one is interested in the limit $\alpha \to \infty$. It had been conjectured long ago, and finally proved by Donsker and Varadhan [9], that

$$E(\alpha) = \alpha^2 E_P + o(\alpha^2), \qquad (\alpha \to \infty), \tag{3.1}$$

where E_P is the minimum of the Pekar functional

$$\int |\nabla\varphi(x)|^2 dx - \iint \frac{|\varphi(x)|^2 |\varphi(y)|^2}{|x-y|}\, dxdy, \tag{3.2}$$

constrained by

$$\int |\varphi(x)|^2\, dx = 1. \tag{3.3}$$

Statement (3.1) has later been reproved by Lieb and Thomas who also provided a bound on the error of the size $O(\alpha^{9/5})$ [24]. An interesting application of (3.1) is that it reduces the question of bipolaron formation, in the case $\alpha \gg 1$, to the analog question regarding the minimal energies of the Pekar and the Pekar-Tomasevich functionals. For these effective energy-functionals the binding of two polarons follows from a simple variational argument, provided the electron-electron repulsion constant belongs to the lower end of its physically admissible range. The minimizer of (3.2), (3.3), which is needed for the variational argument, is well-known to exist [23, 25]. This line of arguments, due to Miyao and Spohn [26], to our knowledge provides the only mathematically rigorous proof of the existence of bipolarons. While it assumes that $\alpha \gg 1$, numerical work suggest that $\alpha \geq 6.6$ may be sufficient for binding [32].

Whether or not polarons may form bound states if they are subject to external electromagnetic fields, e.g. constant magnetic fields, is an interesting open question. In view of [26, 17], this question calls for a generalization of (3.1) to systems including a magnetic field. In the present paper, for a large class of scalar and vector potentials V and A, respectively, we establish existence of a constant $C = C(A, V)$, such that

$$\alpha^2 E_P(A, V) \geq E(A_\alpha, V_\alpha, \alpha) \geq \alpha^2 E_P(A, V) - C\alpha^{9/5}, \tag{3.4}$$

where $A_\alpha(x) = \alpha A(\alpha x)$, $V_\alpha(x) = \alpha^2 V(\alpha x)$ and $E_P(A, V)$ is the infimum of the generalized

Pekar functional

$$\int |D_A\varphi(x)|^2 + V(x)|\varphi(x)|^2\, dx - \iint \frac{|\varphi(x)|^2|\varphi(y)|^2}{|x-y|}\, dxdy \tag{3.5}$$

constrained by (3.3). Here $D_A = -i\nabla + A$. Non-scaled electromagnetic potentials become negligible in the limit $\alpha \to \infty$. In fact, we show that $\alpha^{-2}E(A, V, \alpha) \to E_P$ as $\alpha \to \infty$.

As explained above, (3.4) allows us to explore the possibility of bipolaron formation in the external fields A, V. The corresponding question concerning the effective theories of Pekar and Tomasevich with electromagnetic fields was studied in [17]. It was found, under the usual condition on the electron-electron repulsion (see above), that two polarons will bind provided the functional (3.5) attains its minimum, which is the case, e.g., for constant magnetic fields and $V \equiv 0$. This leads to our second main result, the binding of two polarons in strong constant magnetic fields, which follows from the more general Theorem 3.4.1, below. Of course it would be interesting to know whether or not the binding of polarons is enhanced by the presence of a magnetic field, as conjectured in [5]. This question is not addressed in the present paper.

The strong coupling result (3.1) was generalized in the recent work [2] to many-polaron systems, and one of us, Wellig, is presently extending this work to include magnetic fields. In work independent and simultaneous to ours, Frank and Geisinger have analyzed the ground state energy of the polaron for *fixed* $\alpha > 0$ in the limit of large, constant magnetic field, i.e., $A = B \wedge x/2$ and $|B| \to \infty$ [12]. They show that the ground state energy, both in the Fröhlich and the Pekar models, is given by $|B| - \frac{\alpha^2}{48}(\ln|B|)^2$ up to corrections of smaller order. The question of binding is not addressed, however, and seems to require a similar analysis of the ground state energy of the Pekar-Tomasevich model. For the binding of $N > 2$ polarons in the Pekar-Tomasevich model with and without external magnetic fields we refer to [21] and [3], respectively. For the thermodynamic stability, the non-binding, and the binding-unbinding transition of multipolaron systems the reader may consult the short review [15] and the references therein.

3.2 The Lower Bound

In this section we study the strong coupling limit of the minimal energy of the polaron subject to given external electric and magnetic fields. To exhibit the general validity of the method we shall allow for fairly general electric and magnetic potentials $V : \mathbb{R}^3 \to \mathbb{R}$ and $A : \mathbb{R}^3 \to \mathbb{R}^3$.

We assume that $A_k \in L^2_{\mathrm{loc}}(\mathbb{R}^3)$, $V \in L^1_{\mathrm{loc}}(\mathbb{R}^3)$ and that for any $\varepsilon > 0$ and all $\varphi \in C_0^\infty(\mathbb{R}^3)$,

$$|\langle \varphi, V\varphi\rangle| \le \varepsilon \|\nabla\varphi\|^2 + C_\varepsilon \|\varphi\|^2. \tag{3.6}$$

This is satisfied, e.g., when $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, see [29] or the proof of (3.22). Of course, here $\langle \varphi, V\varphi\rangle$ denotes a quadratic form defined by $\langle \varphi, V\varphi\rangle = \int V|\varphi|^2 dx$. Since $\langle D_A\varphi, D_A\varphi\rangle$ on $H^1_A(\mathbb{R}^3) := \{\varphi \in L^2(\mathbb{R}^3) \mid D_A\varphi \in L^2(\mathbb{R}^3)\}$ is a closed quadratic form with form core $C_0^\infty(\mathbb{R}^3)$, it follows, by the KLMN-theorem, that $\langle D_A\varphi, D_A\varphi\rangle + \langle \varphi, V\varphi\rangle$ is the quadratic form of a unique self-adjoint operator $D_A^2 + V$ whose form domain is $H^1_A(\mathbb{R}^3)$. Our assumptions allow for constant magnetic fields, the case in which we are most interested.

We shall next define the Fröhlich model associated with V and A through a quadratic form, which we shall prove to be semi-bounded. In this way the introduction of an ultraviolet cutoff is avoided. However, such a cutoff is used in the proof of semi-boundedness. The Hilbert space of the model in this section is the tensor product $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathcal{F}$, where $\mathcal{F}$ denotes the symmetric Fock space over $L^2(\mathbb{R}^3)$, and the form domain is $\mathcal{Q} := H^1_A(\mathbb{R}^3) \otimes \mathcal{F}_0$ where

$$\mathcal{F}_0 := \big\{(\varphi^{(n)}) \in \mathcal{F} | \varphi^{(n)} \in C_0(\mathbb{R}^{3n}),\ \varphi^{(n)} = 0 \text{ for almost all } n\big\}.$$

We define a quadratic form H on $\mathcal{Q}$ by

$$\begin{aligned} H(\psi) &:= \langle \psi, (D_A^2 + V)\psi\rangle + N(\psi) + \sqrt{\alpha} W(\psi) \\ N(\psi) &:= \int \|a(k)\psi\|^2\, dk \qquad (3.7) \\ W(\psi) &:= \frac{1}{\sqrt{2}\pi} \int \frac{dk}{|k|} \left(\langle \psi, e^{ikx} a(k)\psi\rangle + \langle e^{ikx} a(k)\psi, \psi\rangle \right). \qquad (3.8) \end{aligned}$$

Note that $a(k)$ is a well-defined, linear operator on $\mathcal{F}_0$ but $a^*(k)$ is not and neither is $\int |k|^{-1} e^{-ikx} a^*(k)\, dk$, because $|k|^{-1}e^{-ikx}$ is not square integrable with respect to k. The Theorems 3.3.1 and 3.3.2 in the next section relate

$$E(A, V, \alpha) := \inf\{H(\psi) \mid \psi \in \mathcal{Q},\ \|\psi\| = 1\}$$

to the minimum, $E_P(A, V)$, of the Pekar functional (3.5) on the unit sphere $\|\varphi\| = 1$. For the proofs it is convenient to introduce a coupling constant α in the Pekar functional and to define $E_P(A, V, \alpha)$ as the minimum of

$$\mathcal{E}_\alpha(A, V, \varphi) = \int |D_A\varphi(x)|^2 + V(x)|\varphi(x)|^2\, dx - \alpha \iint \frac{|\varphi(x)|^2|\varphi(y)|^2}{|x-y|}\, dx dy$$

with the constraint $\|\varphi\| = 1$. We set $\mathcal{E}(\varphi) = \mathcal{E}_{\alpha=1}(0, 0, \varphi)$, which is the Pekar functional (3.2). It is easy to check that

$$E_P(A_\alpha, V_\alpha, \alpha) = \alpha^2 E_P(A, V) \tag{3.9}$$

where $A_\alpha(x) = \alpha A(\alpha x)$, $V_\alpha(x) = \alpha^2 V(\alpha x)$.

The number $E_P(A, V, \alpha)$ is finite because $E_P(A, V, \alpha) \geq E_P(0, V, \alpha)$, by the diamagnetic inequality [22], and $E_P(0, V, \alpha) > -\infty$ by assumption on V and a simple exercise using the Hölder and Hardy inequalities. Our key result is the following lower bound on $E(A, V, \alpha)$:

Proposition 3.2.1. *Suppose that A, V satisfy the assumptions described above and $\beta = 1 - \alpha^{-1/5}$. Then*

$$E(A, V, \alpha) \geq \beta E_P(A, \beta^{-1} V, \alpha\beta^{-2}) - O(\alpha^{9/5}), \quad (\alpha \to \infty), \tag{3.10}$$

the error bound being independent of A and V.

The proof of Proposition 3.2.1 is done in several steps following [24]. Some of them can be taken over verbatim upon the substitution $-i\nabla_x \to -i\nabla_x + A(x)$. Surprisingly, the translation invariance that seemed to play some role in [24] is not needed for the arguments to work. For the convenience of the reader we at least sketch the main ideas.

To begin with, we introduce a quadratic form $\langle \psi, H_\Lambda \psi \rangle$ on $\mathcal{Q}$ in terms of

$$H_\Lambda := \beta D_A^2 + V + N_{B_\Lambda} + \frac{\sqrt{\alpha}}{\sqrt{2}\pi} \int_{B_\Lambda} \frac{dk}{|k|} (e^{ikx} a(k) + e^{-ikx} a^*(k))$$

where $\beta := 1 - \frac{8\alpha}{\pi\Lambda}$, $B_\Lambda := \{k \in \mathbb{R}^3 : |k| \leq \Lambda\}$ and generally, for subsets $\Omega \subset \mathbb{R}^3$,

$$N_\Omega := \int_\Omega a^*(k) a(k) \, dk.$$

The quadratic form H_Λ is bounded below provided that $\Lambda > 8\alpha/\pi$.

Lemma 3.2.2. *In the sense of quadratic forms on $\mathcal{Q}$, for any $\Lambda > 0$,*

$$H(\psi) \geq \left\langle \psi, (H_\Lambda - \tfrac{1}{2})\psi \right\rangle.$$

This lemma, without electromagnetic fields, is due to Lieb and Thomas [24]. Its proof is based on the operator identity

$$e^{ikx} a(k) = \sum_{\ell=1}^{3} \left[D_{A,\ell}, \frac{k_\ell}{|k|^2} e^{ikx} a(k) \right] \tag{3.11}$$

where $D_{A,\ell} = -i\partial_{x_\ell} + A_\ell(x)$. Obviously, $A(x)$ plays no role in (3.11) as it drops out of the commutator, but we need it for the estimates to follow. For any given $\Lambda > 0$ and $x \in \mathbb{R}^3$ we define the Fock space operators

$$\phi_\Lambda(x) := \frac{1}{\sqrt{2}\pi}\int_{B_\Lambda} (e^{ikx}a(k) + e^{-ikx}a^*(k))\frac{dk}{|k|}$$
$$Z_\ell(x) := \frac{1}{\sqrt{2}\pi}\int_{\mathbb{R}^3\setminus B_\Lambda} \frac{k_\ell}{|k|^3}e^{ikx}a(k)\,dk$$

and we extend them to operators ϕ_Λ, Z_ℓ on $\mathcal{H}$ by setting $(\phi_\Lambda\psi)(x) := \phi_\Lambda(x)\psi(x)$, $(Z_\ell\psi)(x) := Z_\ell(x)\psi(x)$ for $\psi \in \mathcal{H} \simeq L^2(\mathbb{R}^3;\mathcal{F})$. Then, by (3.11), the electron-phonon interaction W can be written as

$$W(\psi) = \left\langle \psi, \left(\phi_\Lambda + \textstyle\sum_{\ell=1}^3 [D_{A,\ell}, Z_\ell - Z_\ell^*]\right)\psi \right\rangle. \tag{3.12}$$

Following [24] one now shows that

$$\sqrt{\alpha}\sum_{\ell=1}^{3}[D_{A,\ell}, Z_\ell - Z_\ell^*] \geq -\frac{8\alpha}{\pi\Lambda}D_A^2 - (N - N_{B_\Lambda}) - \frac{1}{2}. \tag{3.13}$$

The Lemma 3.2.2 follows from (3.12) and (3.13).

The next step is to *localize the electron* in a box of side length L. To this end we define the localization function

$$\varphi(x) = \begin{cases} \prod_{j=1}^3 \cos(\frac{\pi}{L}x_j) & \text{for } |x_j| \leq L/2, \\ 0 & \text{otherwise,} \end{cases}$$

and $\varphi_y(x) := \varphi(x-y)$.

Lemma 3.2.3. *For given $\Delta E > 0$ define $L > 0$ by $3\beta(\frac{\pi}{L})^2 = \Delta E$ and let φ be as above. Then for every non-vanishing $\psi \in \mathcal{Q}$ there exists a point $y \in \mathbb{R}^3$, such that $\varphi_y\psi \neq 0$ and*

$$\langle \varphi_y\psi, H_\Lambda\varphi_y\psi\rangle \leq (E + \Delta E)\|\varphi_y\psi\|^2,$$

where $E := \langle\psi, H_\Lambda\psi\rangle$.

Proof. Using $\varphi_y D_A^2\varphi_y = D_A\varphi_y^2 D_A + \varphi_y(-\Delta\varphi_y)$ and $\beta\varphi_y(-\Delta\varphi_y) = \varphi_y^2\Delta E$ one shows that

$$\int \langle\varphi_y\psi, (H_\Lambda - E - \Delta E)\varphi_y\psi\rangle\, dy = 0,$$

which proves the lemma. Note that $-\Delta\varphi_y$ is a distribution and not a function on the boundary of $\operatorname{supp}\varphi_y$. Nevertheless $\varphi_y(-\Delta\varphi_y)$ is a function, since φ_y is zero on the boundary of $\operatorname{supp}\varphi_y$. □

The Lemma 3.2.3 is to be read as a bound on $E = \langle\psi, H_\Lambda\psi\rangle$ from below: using that H_Λ is translation invariant, except for the terms involving A and V, it implies together with Lemma 3.2.2 that

$$E(A, V, \alpha) \geq \inf_{y\in\mathbb{R}^3} \left(\inf_{\psi\in\mathcal{Q}_L,\ \|\psi\|=1} \langle\psi, H_{\Lambda,y}\psi\rangle \right) - \Delta E - \frac{1}{2}, \tag{3.14}$$

where $H_{\Lambda,y}$ is defined in terms of the shifted potentials $A_y(x) = A(x+y)$ and $V_y(x) = V(x+y)$, $\mathcal{Q}_L := (L^2(C_L) \otimes \mathcal{F}) \cap \mathcal{Q}$, and $C_L = \operatorname{supp}(\varphi) \subset \mathbb{R}^3$ is the cube of side length L centered at the origin.

The next step is the passage to *block modes.* For given $P > 0$ and $n \in \mathbb{Z}^3$ we define

$$\begin{aligned} B(n) &:= \{k \in B_\Lambda \mid |k_i - n_i P| \leq P/2\}, \\ \Lambda_P &:= \{n \in \mathbb{Z}^3 \mid B(n) \neq \emptyset\}. \end{aligned}$$

In each set $B(n)$ we pick a point k_n, to be specified later, and we define block annihilation and creation operators a_n and a_n^* by

$$a_n := \frac{1}{M_n} \int_{B(n)} \frac{dk}{|k|} a(k), \qquad M_n = \left(\int_{B(n)} \frac{dk}{|k|^2} \right)^{1/2}.$$

For given $\delta > 0$ we define the block Hamiltonian

$$\begin{aligned} H_{\Lambda,y}^{block} &:= \beta D_{A_y}^2 + V_y + (1-\delta) \sum_{n\in\Lambda_P} a_n^* a_n \\ &\quad + \frac{\sqrt{\alpha}}{\sqrt{2}\pi} \sum_{n\in\Lambda_P} M_n \big(e^{ik_n x} a_n + e^{-ik_n x} a_n^*\big), \end{aligned}$$

and we set $H_\Lambda^{block} := H_{\Lambda,0}^{block}$. The reason for introducing block modes is well explained in [24] and related to (3.18).

Lemma 3.2.4. *In the sense of quadratic forms in $\mathcal{Q}_L$, for all (k_n),*

$$H_{\Lambda,y} \geq H_{\Lambda,y}^{block} - \frac{9\alpha P^2 L^2 \Lambda}{2\pi\delta}.$$

Proof. For each $n \in \Lambda_P$, by a completion of squares w.r.t. $a(k)$ and $a^*(k)$ we find, in the sense of quadratic forms in $\mathcal{Q}_L$,

$$\begin{aligned}
&\delta N_{B(n)} + \frac{\sqrt{\alpha}}{\sqrt{2}\pi}\int_{B(n)} \frac{dk}{|k|}\big(e^{ikx}a(k) + e^{-ikx}a^*(k)\big) \\
\geq\ & \frac{\sqrt{\alpha}}{\sqrt{2}\pi}\int_{B(n)} \frac{dk}{|k|}\big(e^{ik_nx}a(k) + e^{-ik_nx}a^*(k)\big) - \frac{\alpha}{2\pi^2\delta}\int_{B(n)} \frac{dk}{|k|^2}|e^{ikx} - e^{ik_nx}|^2 \\
\geq\ & \frac{\sqrt{\alpha}}{\sqrt{2}\pi} M_n\big(e^{ik_nx}a_n + e^{-ik_nx}a_n^*\big) - \frac{\alpha}{2\pi^2\delta}(\frac{3}{2}PL)^2\int_{B(n)} \frac{dk}{|k|^2},
\end{aligned} \tag{3.15}$$

where we used the definition of a_n and that

$$|e^{ikx} - e^{ik_nx}| \leq \frac{3}{2}PL, \quad \text{for } x \in C_L,\ k \in B(n).$$

After summing (3.15) with respect to $n \in \Lambda_P$, the lemma follows from $\int_{B_\Lambda} |k|^{-2}dk = 4\pi\Lambda$ and from $a_n^* a_n \leq N_{B(n)}$. □

We now use Lemma 3.2.4 to bound (3.14) from below and then we replace $\mathcal{Q}_L$ by $\mathcal{Q}$. This leads to

$$E(A, V, \alpha) \geq \inf_{\psi\in\mathcal{Q}, \|\psi\|=1} \sup_{k_n} \left\langle \psi, H^{block}_{\Lambda,y}\psi \right\rangle - \frac{9\alpha P^2L^2\Lambda}{2\pi\delta} - \Delta E - \frac{1}{2}. \tag{3.16}$$

Recall that L depends on ΔE. It remains to compare $\left\langle \psi, H^{block}_{\Lambda,y}\psi \right\rangle$ with the minimum of the Pekar functional. This will be done in the proof of the following lemma using coherent states.

Lemma 3.2.5. *Let $\mu = \alpha\beta^{-1}(1-\delta)^{-1}$. Then for every normalized $\psi \in \mathcal{Q}$ and every $y \in \mathbb{R}^3$,*

$$\sup_{k_n} \left\langle \psi, H^{block}_{\Lambda,y}\psi \right\rangle \geq \beta E_P(A, V, \mu) - |\Lambda_P|.$$

Proof. Since $E_P(A_y, V_y, \mu)$ is independent of y it suffices to prove the asserted inequality without the y-shift in the block Hamiltonian. Let $M = \text{span}\{|\cdot|^{-1}\chi_{B(n)} \mid n \in \Lambda_P\}$, which is a finite dimensional subspace of $L^2(\mathbb{R}^3)$. From $L^2(\mathbb{R}^3) = M \oplus M^\perp$ it follows that $\mathcal{F}$ is isomorphic to $\mathcal{F}(M) \otimes \mathcal{F}(M^\perp)$ with the isomorphism given by

$$\begin{aligned}
\Omega &\mapsto \Omega \otimes \Omega \\
a^*(h) &\mapsto a^*(h_1) \otimes 1 + 1 \otimes a^*(h_2)
\end{aligned}$$

where h_1 and h_2 are the orthogonal projections of h onto M and $M^\perp$ respectively. Here Ω

denotes the normalized vacuum in any Fock space. Note that

$$\mathcal{F}(M) = \overline{\text{span}}\Big\{ \prod_{n\in\Lambda_p} (a_n^*)^{m_n}\Omega \Big| m_n \in \mathbb{N}\Big\} \tag{3.17}$$

where $\overline{\text{span}}$ denotes the closure of the span. With respect to the factorization $\mathcal{H} = \mathcal{H}_M \otimes \mathcal{F}(M^\perp)$ where $\mathcal{H}_M = L^2(\mathbb{R}^3) \otimes \mathcal{F}(M)$, the block Hamiltonian is of the form $H_\Lambda^{block} \otimes 1$. To bound $H_\Lambda^{block} \otimes 1$ on $\mathcal{H}_M \otimes \mathcal{F}(M^\perp)$ from below we introduce coherent states $|z\rangle \in \mathcal{F}(M)$ for given $z = (z_n)_{n\in\Lambda_P}$, $z_n \in \mathbb{C}$, by

$$|z\rangle := \prod_{n\in\Lambda_P} e^{z_n a_n^* - \bar{z}_n a_n}\Omega.$$

Clearly, $\langle z, z\rangle = 1$ and it is easy to check that $a_n|z\rangle = z_n|z\rangle$. On $\mathcal{F}(M)$, in the sense of weak integrals,

$$\begin{aligned} \int dz|z\rangle\langle z| &= 1, \\ \int dz(|z_n|^2 - 1)|z\rangle\langle z| &= a_n^* a_n, \end{aligned} \tag{3.18}$$

where $\int dz := \prod_{n\in\Lambda_P} \frac{1}{\pi}\int dx_n dy_n$. The second equation follows from $a_n^* a_n = a_n a_n^* - 1$ and from the first one. Now suppose that $\psi \in \mathcal{Q}$ and let $\psi_z(x) = \langle z, \psi(x)\rangle$. Then $\psi_z \in L^2(\mathbb{R}^3)\otimes\mathcal{F}(M^\perp)$ and

$$\big\langle \psi, H_\Lambda^{block}\psi\big\rangle = \int dz\langle\psi_z, (h_z \otimes 1)\psi_z\rangle$$

where h_z denotes the Schrödinger operator in $L^2(\mathbb{R}^3)$ given by

$$h_z = \beta D_A^2 + V + (1-\delta)\sum_{n\in\Lambda_P}(|z_n|^2 - 1) + \frac{\sqrt{\alpha}}{\sqrt{2}\pi}\sum_{n\in\Lambda_P} M_n\big(z_n e^{ik_n x} + \overline{z_n}e^{-ik_n x}\big).$$

Let $\widehat{\rho_z}(k) := \big\langle \psi_z, e^{-ikx}\psi_z\big\rangle$ be the Fourier transform of $\rho_z(x) = |\psi_z(x)|^2$. By completion of the square w.r.to z_n and $\overline{z_n}$ it follows that

$$\begin{aligned} &\sup_{k_n}\int dz\langle\psi_z, (h_z\otimes 1)\psi_z\rangle \\ &\quad\geq \int dz\beta\|D_A\psi_z\|^2 + \langle\psi_z, V\psi_z\rangle - \frac{\alpha}{2\pi^2(1-\delta)}\int dz\int_{B_\Lambda}\frac{dk}{|k|^2}|\widehat{\rho_z}(k)|^2\frac{1}{\|\psi_z\|^2} - |\Lambda_P| \\ &\quad\geq \int dz\Big(\beta\|D_A\psi_z\|^2 + \langle\psi_z, V\psi_z\rangle - \frac{\alpha}{(1-\delta)\|\psi_z\|^2}\int\frac{\rho_z(x)\rho_z(y)}{|x-y|}\,dxdy\Big) - |\Lambda_P|. \end{aligned}$$

The integrand is readily recognized as

$$\beta\|\psi_z\|^2\mathcal{E}_\mu(A,\beta^{-1}V,\psi_z/\|\psi_z\|),$$

with coupling constant $\mu := \alpha\beta^{-1}(1-\delta)^{-1}$. Its minimum is

$$\beta\|\psi_z\|^2 E_P(A,\beta^{-1}V,\mu).$$

Since $\int \|\psi_z\|^2 dz = 1$, the proof of the lemma is complete. □

Proof of Proposition 3.2.1. By (3.16) and Lemma 3.2.5 it follows that

$$E(A,V,\alpha) \geq \beta E_P(A,\beta^{-1}V,\mu) - |\Lambda_P| - \frac{9\alpha P^2 L^2 \Lambda}{2\pi\delta} - \Delta E - \frac{1}{2}$$

where $\beta = 1-\frac{8\alpha}{\pi\Lambda}$, $\mu = \alpha\beta^{-1}(1-\delta)^{-1}$ and $L^2 = \pi^2 3\beta/\Delta E$. Λ, δ, P and ΔE are free parameters. We choose $\Lambda = \frac{8}{\pi}\alpha^{6/5}$, $\delta = \alpha^{-1/5}$, $P = \alpha^{3/5}$ and $\Delta E = \alpha^{9/5}$. Then $\beta = 1-\delta$ and hence the proposition follows. □

3.3 The Strong Coupling Limit

Equipped with Proposition 3.2.1 we can turn to the proofs of the results described in the introduction in the more precise forms of Theorems 3.3.1 and 3.3.2, below.

Theorem 3.3.1. *Suppose the potentials A and V satisfy the assumptions of Proposition 3.2.1, $A_\alpha(x) := \alpha A(\alpha x)$ and $V_\alpha(x) := \alpha^2 V(\alpha x)$. Then there exists a constant $C = C(A,V)$ such that for $\alpha > 0$ large enough,*

$$\alpha^2 E_P(A,V) \geq E(A_\alpha,V_\alpha,\alpha) \geq \alpha^2 E_P(A,V) - C\alpha^{9/5}.$$

Proof. The first inequality follows from the well-known $E_P \geq E$, see the proof of (3.30), and from the scaling property (3.9) of E_P. Using Proposition 3.2.1 and (3.9), we see that

$$E(A_\alpha,V_\alpha,\alpha) \geq \alpha^2\beta E_P(A,\beta^{-1}V,\beta^{-2}) - O(\alpha^{9/5}) \tag{3.19}$$

where $\beta = 1-\alpha^{-1/5}$ and where the function $\lambda \mapsto E_P(A,\lambda V,\lambda^2)$, as an infimum of concave functions, is concave. Therefore it has one-sided derivatives, which implies that

$$E_P(A,\beta^{-1}V,\beta^{-2}) \geq E_P(A,V) - O(\alpha^{-1/5}). \tag{3.20}$$

Combining (3.19) and (3.20) the second inequality from Theorem 3.3.1 follows. $\square$

Theorem 3.3.2.

(a) If $A \in L^3_{\mathrm{loc}}(\mathbb{R}^3)$ and $V \in L^{3/2}_{\mathrm{loc}}(\mathbb{R}^3)$ with (3.6), then $\alpha^{-2}E(A,V,\alpha) \to E_P$ as $\alpha \to \infty$.

(b) If $A = (B \wedge x)/2$ and $V \in L^{5/3}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, then

$$\frac{E(A,V,\alpha)}{\alpha^2} = E_P + O(\alpha^{-1/5}), \qquad (\alpha \to \infty).$$

The fact that non-scaled fields A, V should become negligible in the limit $\alpha \to \infty$ is seen as follows: by Proposition 3.2.1 and by (3.9), $\alpha^{-2}E(A,V,\alpha)$ is bounded from above and from below by

$$E_P(A_{\alpha^{-1}}, V_{\alpha^{-1}}) \geq \frac{E(A,V,\alpha)}{\alpha^2} \geq \beta E_P(A_{\alpha^{-1}}, \beta^{-1}V_{\alpha^{-1}}, \beta^{-2}) - O(\alpha^{-1/5}), \tag{3.21}$$

where $A_{\alpha^{-1}}(x) = \alpha^{-1}A(x/\alpha)$ and $V_{\alpha^{-1}}(x) = \alpha^{-2}V(x/\alpha)$. In the limit $\alpha \to \infty$ these fields are vanishing in the sense of the following lemma. The theorem will thus follow from parts (b) and (c) of Lemma 3.3.4 below. As a preparation we need:

Lemma 3.3.3. *(i) Suppose $A \in L^3_{\mathrm{loc}}(\mathbb{R}^3)$ and $V \in L^{3/2}_{\mathrm{loc}}(\mathbb{R}^3)$. Then*

$$\begin{aligned} A_{\alpha^{-1}} &\to 0 \quad (\alpha \to \infty) \quad \text{in } L^2_{\mathrm{loc}}(\mathbb{R}^3), \\ V_{\alpha^{-1}} &\to 0 \quad (\alpha \to \infty) \quad \text{in } L^1_{\mathrm{loc}}(\mathbb{R}^3). \end{aligned}$$

(ii) If $V = V_1 + V_2 \in L^{5/3}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, then for all $\varphi \in H^1(\mathbb{R}^3)$

$$|\langle \varphi, V\varphi \rangle| \leq C\|V_1\|_{5/3}\|\varphi\|^2_{H^1} + \|V_2\|_\infty \|\varphi\|^2. \tag{3.22}$$

In particular, V is infinitesimally form bounded w.r.to $-\Delta$.

Proof. (i) Let $\Omega \subset \mathbb{R}^3$ be compact. By Cauchy-Schwarz,

$$\begin{aligned} \int_\Omega |A_{\alpha^{-1}}(x)|^2 dx &= \alpha \int_{\alpha^{-1}\Omega} |A(x)|^2 dx \\ &\leq \left(\int |A(x)|^3 \chi_{\alpha^{-1}\Omega}(x) dx \right)^{2/3} |\Omega|^{1/3} \to 0 \quad (\alpha \to \infty). \end{aligned}$$

The second statement of (i) is proved similarly.

In statement (ii) the contribution due to V_2 is obvious. Let us assume that $V = V_1 \in L^{5/3}(\mathbb{R}^3)$. By Hölder's inequality $|\langle\varphi, V\varphi\rangle| \leq \|V\|_{5/3}\|\varphi\|_5^2$ and

$$\int |\varphi|^5 \, dx \leq \|\varphi\|^{1/2} \left(\int |\varphi|^6 \, dx\right)^{3/4}. \tag{3.23}$$

Using the general inequality $ab \leq p^{-1}a^p + q^{-1}b^q$ with $p = 10$ and $q = 10/9$ we obtain

$$\|\varphi\|_5^2 \leq \|\varphi\|^{1/5}\|\varphi\|_6^{9/5} \leq \frac{1}{10}\|\varphi\|^2 + \frac{9}{10}\|\varphi\|_6^2.$$

Statement (ii) now follows from the Sobolev inequality $\|\varphi\|_6^2 \leq C\|\nabla\varphi\|^2$. The infinitesimal form bound follows from the fact that the norm of the $L^{5/3}$-part of V can be chosen arbitrarily small. $\square$

Lemma 3.3.4. *Let A, V be real-valued potentials satisfying the hypothesis of Lemma 3.3.3 (i), and suppose that* (3.6) *holds. If* $\lim_{\alpha\to\infty} \lambda(\alpha) = 1$*, then*

(a) $\lim_{\alpha\to\infty} \mathcal{E}_{\lambda^2}(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \varphi) = \mathcal{E}(\varphi)$ *for all* $\varphi \in C_0^\infty(\mathbb{R}^3)$*,*

(b) $\lim_{\alpha\to\infty} E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) = E_P$*.*

If $A = (B \wedge x)/2$*,* $V \in L^{5/3}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ *and* $\lim_{\alpha\to\infty} \lambda(\alpha) = 1$*, then*

(c) $E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) = \lambda^4 E_P + O(\alpha^{-1/5}), \quad (\alpha \to \infty)$*.*

Proof. (a) For $\varphi \in C_0^\infty(\mathbb{R}^3)$, Lemma 3.3.3 implies that $\|A_{\alpha^{-1}}\varphi\| \to 0$ and $\langle\varphi, V_{\alpha^{-1}}\varphi\rangle \to 0$ as $\alpha \to \infty$. This proves (a).

(b) For any normalized $\varphi \in C_0^\infty(\mathbb{R}^3)$, by (a),

$$\limsup_{\alpha\to\infty} E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) \leq \limsup_{\alpha\to\infty} \mathcal{E}_{\lambda^2}(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \varphi) = \mathcal{E}(\varphi).$$

This implies that $\limsup_{\alpha\to\infty} E_P(A, \lambda V, \lambda^2\alpha)\alpha^{-2} \leq E_P$.

For (b) it remains to prove that $\liminf_{\alpha\to\infty} E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) \geq E_P$. By the hypothesis on V, for any $\varepsilon > 0$ and any normalized $\varphi \in C_0^\infty(\mathbb{R}^3)$,

$$|\langle\varphi, V_{\alpha^{-1}}\varphi\rangle| \leq \varepsilon\|\nabla|\varphi|\|^2 + \frac{C_\varepsilon}{\alpha^2}. \tag{3.24}$$

From (3.24), the diamagnetic inequality and the scaling property of E_P, it follows that

$$\mathcal{E}_{\lambda^2}(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \varphi) \geq (1-\lambda\varepsilon) E_P(0,0,\lambda^2/(1-\lambda\varepsilon)) - \lambda \frac{C_\varepsilon}{\alpha^2} \tag{3.25}$$

$$\geq \frac{\lambda^4}{(1-\lambda\varepsilon)} E_P - \lambda \frac{C_\varepsilon}{\alpha^2}, \tag{3.26}$$

and hence that

$$E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) \geq \frac{\lambda^4}{(1-\lambda\varepsilon)} E_P - \lambda \frac{C_\varepsilon}{\alpha^2}.$$

Now letting first $\alpha \to \infty$ and then $\varepsilon \to 0$, the desired lower bound is obtained.

The proof of the lower bound in (c) is similar to the proof of the lower bound in (b), the main difference being that we now have (3.22) from Lemma 3.3.3, which implies that

$$|\langle \varphi, V_{\alpha^{-1}} \varphi \rangle| \leq C\alpha^{-1/5} \big(\|\varphi\|^2 + \|\nabla|\varphi|\|^2 \big) \tag{3.27}$$

with some $C > 0$ that is independent of α and φ. By the diamagnetic inequality and by (3.27), for any normalized $\varphi \in C_0^\infty(\mathbb{R}^3)$,

$$\begin{aligned}
\mathcal{E}_{\lambda^2}(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \varphi) &\geq \mathcal{E}_{\lambda^2}(0,0,|\varphi|) - C\lambda\alpha^{-1/5} \big(1 + \|\nabla|\varphi|\|^2\big) \\
&\geq (1 - C\lambda\alpha^{-1/5}) E_P(0,0,\frac{\lambda^2}{1-C\lambda\alpha^{-1/5}}) - C\lambda\alpha^{-1/5} \\
&= \frac{\lambda^4}{1-C\lambda\alpha^{-1/5}} E_P - C\lambda\alpha^{-1/5}.
\end{aligned}$$

Hence $E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) \geq \lambda^4 E_P - O(\alpha^{-1/5})$.

It remains to prove the upper bound on $E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2)$ in (c). To this end let φ_0 be a (real-valued) minimizer of the Pekar functional [23], i.e. $\mathcal{E}(\varphi_0) = E_P$ and let φ_λ be scaled in such a way that $\mathcal{E}_{\lambda^2}(\varphi_\lambda) = \lambda^4 \mathcal{E}(\varphi_0)$. Then

$$\begin{aligned}
E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) &\leq \mathcal{E}_{\lambda^2}(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \varphi_\lambda) \\
&= \lambda^4 E_P + \|A_{\alpha^{-1}}\varphi_\lambda\|^2 + \lambda\langle \varphi_\lambda, V_{\alpha^{-1}}\varphi_\lambda \rangle \\
&= \lambda^4 E_P + O(\alpha^{-1/5}).
\end{aligned}$$

We have used that $\mathrm{Re}\,\langle -i\nabla\varphi_\lambda, A_{\alpha^{-1}}\varphi_\lambda \rangle = 0$, since φ_λ is real-valued, and (3.22) from Lemma 3.3.3

$\square$

3.4 Existence of Bipolarons

Let A, V be vector and scalar potentials, respectively, satisfying the assumptions of the Section 3.2. Let $\alpha, U > 0$. We define a two-body Hamiltonian $H_U^{A,V}$ on $L^2(\mathbb{R}^6)$ by

$$H_U^{A,V} := (D_A^2 + V) \otimes 1 + 1 \otimes (D_A^2 + V) + UV_C \tag{3.28}$$

where $V_C(x,y) := |x-y|^{-1}$. More precisely, we define $H_U^{A,V}$ in terms of the quadratic form given by the right hand side of (3.28) on $C_0^\infty(\mathbb{R}^6)$. Its form domain will be denoted by $H_A^1(\mathbb{R}^6)$.

In the two-polaron model of Fröhlich, the minimal energy, $E_2(A,V,U,\alpha)$ of two electrons in a polar crystal is the infimum of the quadratic form

$$\left\langle \psi, (H_U^{A,V} \otimes 1)\psi \right\rangle + N(\psi) + \sqrt{\alpha} W_2(\psi), \tag{3.29}$$

whose domain is the intersection of $H_A^1(\mathbb{R}^6) \otimes \mathcal{F}_0$ with the unit sphere of the Hilbert space $L^2(\mathbb{R}^6) \otimes \mathcal{F}$. Here $N(\psi)$ and $W_2(\psi)$ are defined by expressions similar to (3.7) and (3.8), the main difference being that e^{ikx} in (3.8) becomes $e^{ikx_1} + e^{ikx_2}$ in $W_2(\psi)$.

In the two-polaron model of Pekar and Tomasevich the minimal energy, $E_{PT}(A,V,U,\alpha)$ of two electrons in a polar crystal is the infimum of the functional

$$\left\langle \varphi, H_U^{A,V} \varphi \right\rangle - \alpha \iint \frac{\rho(x)\rho(y)}{|x-y|}\, dxdy$$

on the L^2-unit sphere of $H_A^1(\mathbb{R}^6)$, where $\rho(x) := \int \left(|\varphi(x,y)|^2 + |\varphi(y,x)|^2 \right) dy$. For any fixed $\varphi \in L^2(\mathbb{R}^6) \cap H_A^1(\mathbb{R}^6)$, $\|\varphi\| = 1$, and corresponding density ρ the identity

$$\inf_{\|\eta\|=1} \left(N(\varphi \otimes \eta) + \sqrt{\alpha} W_2(\varphi \otimes \eta) \right) = -\alpha \iint \frac{\rho(x)\rho(y)}{|x-y|}\, dxdy$$

holds. By choosing $\psi = \varphi \otimes \eta$ in (3.29) it follows that

$$E_{PT}(A,V,U,\alpha) \geq E_2(A,V,U,\alpha), \tag{3.30}$$

which, together with Theorem 3.3.1 and the results of [17] enables us to prove the following theorem on the *binding of polarons*:

Theorem 3.4.1. *Suppose $A, V \in L^2_{\mathrm{loc}}(\mathbb{R}^3)$ and that V is infinitesimally operator bounded w.r.to Δ. Let $A_\alpha(x) = \alpha A(\alpha x)$ and $V_\alpha(x) = \alpha^2 V(\alpha x)$. If the Pekar functional (3.5) attains* *its minimum, then there exists* $u_{A,V} > 2$ *such that for* $U < \alpha u_{A,V}$ *and* α *large enough*

$$2E(A_\alpha, V_\alpha, \alpha) > E_2(A_\alpha, V_\alpha, U, \alpha).$$

Proof. Let $U = \alpha u$. By a simple scaling argument

$$E_{PT}(A_\alpha, V_\alpha, \alpha u, \alpha) = \alpha^2 E_{PT}(A, V, u, 1), \tag{3.31}$$

which is analogous to (3.9). By Theorem 3.1 of [17] there exists $u_{A,V} > 2$ such that for $u < u_{A,V}$,

$$2E_P(A, V) > E_{PT}(A, V, u, 1). \tag{3.32}$$

From Theorem 3.3.1, (3.32), (3.31), and (3.30) it follows that, for α large enough,

$$\begin{aligned} 2\alpha^{-2}E(A_\alpha, V_\alpha, \alpha) &= 2E_P(A, V) - o(1) \\ &> E_{PT}(A, V, u, 1) \\ &= \alpha^{-2}E_{PT}(A_\alpha, V_\alpha, \alpha u, \alpha) \\ &\geq \alpha^{-2}E_2(A_\alpha, V_\alpha, U, \alpha), \end{aligned}$$

which proves the theorem. □

Chapter 4

On the Strong Coupling Limit of Many-Polaron Systems in Electromagnetic Fields

D. Wellig

Abstract

In this paper estimates on the ground state energy of Fröhlich N-polarons in electromagnetic fields in the strong coupling limit, $\alpha \to \infty$, are derived. It is shown that the ground state energy is given by α^2 multiplied by the minimal energy of the corresponding Pekar-Tomasevich functional for N particles, up to an error term of order $\alpha^{42/23}N^3$. The potentials A, V are suitably rescaled in α. As a corollary, binding of N-polarons for strong constant magnetic fields for large coupling constants is established.

4.1 Introduction and Main Results

An ionic crystal is deformed by the presence of an excess electron via the Coulomb attraction resp. repulsion. The distortion induces a potential which acts on the electron. The resulting composite particle is called a polaron. More generally a N-polaron is a system of N electrons with the corresponding distortions of the ionic lattice. In the physically admissible region the coupling constant α between electron and lattice, in our units, is bounded from above by the electron-electron repulsion strenght U. Energetically it is more favorable if the electrons deform the lattice in a small region, hence they tend to stay close together. Therefore an attractive force operates between the electrons which is counteracted by their Coulomb repulsion. Which force is stronger, depending on α and U, is discussed further below. For more information about the physical properties of polarons we refer to [8, 1] and references therein.

The goal of this work is to prove that in the leading order of the coupling constant the ground state energy of N-polarons subject to a certain class of electromagnetic fields is given by the minimal energy of the Pekar-Tomasevich functional. For large values of α the effect of the external fields is negligible. Hence they are rescaled such that they grow with increasing α. Combining this with the binding of Pekar-Tomasevich N-polarons subject to a constant magnetic field, which was recently established in [3], we prove binding for Fröhlich N-polarons in strong constant magnetic fields for large couplings. In the N-particle case without external fields, similar asymptotic exactness and binding results have recently been derived in [2]. The common strategy of the latter work and ours is to split up the N-polaron into disjoint groups of polarons, to estimate the interaction energy between the groups, and to derive the asymptotic coincidence with Pekar-Tomasevich for the individual groups by the techniques developed by Lieb and Thomas [24].

We consider the model, introduced by H. Fröhlich [16], that describes large polarons, i.e. polarons with large spatial extension compared to the lattice spacing. Additionally external potentials $V : \mathbb{R}^3 \to \mathbb{R}$ and $A : \mathbb{R}^3 \to \mathbb{R}^3$ are introduced, which generate the electric field $-\nabla V$ and the magnetic field $\operatorname{curl} A$. The Fröhlich hamilton operator for N-polarons on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^{3N}) \otimes \mathcal{F}$, with $\mathcal{F}$ as the bosonic Fock space over $L^2(\mathbb{R}^3)$, is given by

$$H^{(N)} = \sum_{j=1}^{N} \left(D^2_{A,x_j} + V(x_j) + \sqrt{\alpha}\phi(x_j) \right) + H_{ph} + UV_C(x_1, \dots, x_N), \tag{4.1}$$

where $D_{A,x_j} = -i\nabla_{x_j} + A(x_j)$. $V_C(x_1, \dots, x_N) = \sum_{i<j} \frac{1}{|x_i - x_j|}$ is the Coulomb potential and the interaction between the electron and the quantized lattice vibrations (i.e. phonons) is

$$\phi(x) = \frac{1}{\sqrt{2}\pi} \int \frac{dk}{|k|} \left(a(k)e^{ikx} + a^*(k)e^{-ikx} \right).$$

Where $a(k)$ represents the creation- and $a^*(k)$ the annihilation operator with momentum k and $H_{ph} = \int_{\mathbb{R}^3} dka^*(k)a(k)$ denotes the phonon energy. The ground state energy of $H^{(N)}$ is defined by

$$E^{(N)}(A, V, U, \alpha) = \inf_{\|\psi\|=1} \left\langle \psi \left| H^{(N)} \right| \psi \right\rangle.$$

For simplicity reasons $E^{(N)}(A,V,U,\alpha)$ sometimes is written as $E^{(N)}$. Because of Lemma 4.4.1 $E^{(N)}(A,V,U,\alpha)$ is bounded from below and hence it exists.

The Fröhlich model is closely related to the Pekar-Tomasevich functional $\mathcal{E}^{(N)}_{U,\alpha}(A,V,.)$, which for normalized $\varphi \in L^2(\mathbb{R}^{3N})$ may be defined by

$$\mathcal{E}^{(N)}_{U,\alpha}(A,V,\varphi) = \inf_{\|\eta\|=1} \left\langle \varphi\otimes\eta \,\middle|\, H^{(N)} \,\middle|\, \varphi\otimes\eta \right\rangle. \tag{4.2}$$

See Section 4.4 for a more explicit definition. The minimal energy of the Pekar-Tomasevich functional with external magnetic and electric fields is denoted by

$$C_N(A,V,U,\alpha) = \inf_{\|\varphi\|=1} \mathcal{E}^{(N)}_{U,\alpha}(A,V,\varphi).$$

Sometimes the short hand C_N instead of $C_N(A,V,U,\alpha)$ is used. By (4.2)

$$C_N \geq E^{(N)}. \tag{4.3}$$

The dimensionless constant $\nu := U/\alpha$ describes the physical region for $\nu > 2$. Does there exist a similar estimate converse to (4.3)? In the following theorem we give an affirmative answer.

Theorem 4.1.1. *For any values of $\nu > 0$ and N, the following is true:*

(a) Suppose A, V satisfy assumptions (AV1) and (4.10) *described in Section 4.2, then there exists $c(A,V)$*

$$E^{(N)}(A_\alpha, V_\alpha, \alpha\nu, \alpha) \geq \alpha^2 C_N(A,V,\nu,1) - c(A,V)\alpha^{42/23}N^3,$$

for α large and $A_\alpha(x) = \alpha A(\alpha x)$, $V_\alpha(x) = \alpha^2 V(\alpha x)$.

(b) Suppose A, V satisfy assumptions (AV2) and (4.10) *described in Section 4.2, then*

$$\lim_{\alpha\to\infty} \alpha^{-2} E^{(N)}(A,V,\alpha\nu,\alpha) = C_N(0,0,\nu,1), \quad (\alpha\to\infty), \quad \textit{for all } N. \tag{4.4}$$

Theorem 4.1.1 b) shows what one physically would expect, that the ground state energy of the Fröhlich model does not depend on the external fields in the leading order of the coupling constant for $\alpha \to \infty$. The external fields are rescaled such that they are appreciable for large α. Furthermore the scaling property from Theorem 4.1.1 a) ensures that the minimal energy of the electromagnetic Pekar functional is proportional to α^2, i.e.

$$C_N(A_\alpha, V_\alpha, \alpha\nu, \alpha) = \alpha^2 C_N(A, V, \nu, 1). \tag{4.5}$$

In the case $N = 1$ Theorem 4.1.1 was recently proved in [18]. The previous results without external fields are discussed further below.

Furthermore, we want to study the formation of multipolarons in constant magnetic fields. Binding for N-polarons is established if

$$\Delta E^{(N)} := \min_{1\leq k\leq N-1} \left(E^{(k)} + E^{(N-k)}\right) - E^{(N)} > 0, \tag{4.6}$$

and analogously for Pekar-Tomasevich N-polarons

$$\min_{1\leq k\leq N-1} (C_k + C_{N-k}) - C_N > 0. \tag{4.7}$$

We already know binding for Pekar-Tomasevich N-polarons in constant magnetic fields for ν in some neighborhood of $\nu = 2$ [3], hence as a corollary of Theorem 4.1.1, it follows the existence of bound states for Fröhlich N-polarons in strong constant magnetic fields for α large enough. Thus:

Theorem 4.1.2. *For any values of N, let A be linear, i.e. the corresponding magnetic field is constant, then there exists $\nu_{N,A} > 2$ such that for $\nu < \nu_{N,A}$ and α large enough*

$$\Delta E^{(N)}(A_\alpha, 0, \alpha\nu, \alpha) > 0,$$

where $A_\alpha(x) = \alpha A(\alpha x)$.

Remark. Suppose A, V satisfy (4.10) and assumption (AV2) described in Section 4.2, then there exists $\nu_N > 2$ such that for $\nu < \nu_N$ and α large enough

$$\Delta E^{(N)}(A, V, \alpha\nu, \alpha) > 0. \tag{4.8}$$

This follows from (4.4) and the binding of N-polarons in the Pekar-Tomasevich model without external fields (see [21] or [3] for $A = 0$). In other words, in the leading order for $\alpha \to \infty$ the binding energy does not depend on the (non-scaled) external fields.

For $N = 1$ without external fields a first proof of Theorem 4.1.1 was given by means of stochastic integration by Donsker and Varadhan [9], however they did not mention an explicit error bound. Later, Lieb and Thomas [24] gave another proof using operator theoretical methods, which was the basis for subsequent generalizations, i.e. to the case of polarons subject to electromagnetic fields [18] and to the case of N-polarons without external fields [2]. Since the idea of the proof in [24] only applies to multipolarons in a neighborhood of one another, Theorem 4.1.1 can not simply be adapted. Considering that, in Proposition 4.3.2 we estimate the interaction-energy between different clusters of multipolarons by a generalization of a lemma recently appeared in [14].

The basic idea of our proof of Theorem 4.1.2 goes back to Miyao and Spohn [26], where they proved formation of bipolarons. They argued that in the strong coupling regime, binding for bipolarons is implied by the binding for Pekar-Tomasevich bipolarons and the fact that in the leading order for $\alpha \to \infty$ the Fröhlich ground state energy is exactly described by the Pekar minimal energy. By a similar reasoning, the existence of bipolarons subject to electromagnetic fields was recently derived in [18] with the help of binding of the corresponding Pekar bipolarons [17]. For binding of N-polarons, but without external fields we refer to [2, 21]. There are further binding and non-binding results in the mathematical and physical literature. Namely non-binding for N-polarons without external fields have been proved for the Fröhlich model and the Pekar functional for sufficiently large values of $\nu > 0$ [14]. Numerical calculations suggest that binding for bipolarons does not occur for small couplings [31, 32], but there exists no rigorous proof yet.

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4.2 Preparations and Structure of the Proof

Let the aforementioned external potential $V : \mathbb{R}^3 \to \mathbb{R}$ be form-bounded with bound zero, i.e. for all $\varepsilon > 0$ there exists $C_\varepsilon > 0$

$$|\langle \varphi, V\varphi \rangle| \leq \varepsilon \|\nabla\varphi\|^2 + C_\varepsilon \|\varphi\|^2, \quad \varphi \in C_0^\infty(\mathbb{R}^3). \tag{4.9}$$

Two different assumptions on the magnetic and electric fields are given

(AV1) $A_k \in L^2_{loc}(\mathbb{R}^3)$, $V \in L^1_{loc}(\mathbb{R}^3)$ and (4.9),

(AV2) $A_k \in L^3_{loc}(\mathbb{R}^3)$, $V \in L^{3/2}_{loc}(\mathbb{R}^3)$ and (4.9).

Obviously (AV2) is contained in (AV1). If nothing is mentioned, always (AV1) is supposed. (AV1) ensures that the quadratic form $\sum_{j=1}^N \left\langle D_{A,x_j}\varphi, D_{A,x_j}\varphi \right\rangle$ on $C_0^\infty(\mathbb{R}^{3N})$ is well defined. It is closable and the domain of the closure is $H^1_A(\mathbb{R}^{3N}) := \{\varphi \in L^2(\mathbb{R}^{3N}) | (-i\partial_{x_j,\ell} + A_\ell(x_j))\varphi \in L^2(\mathbb{R}^{3N}), 1 \leq \ell \leq 3, 1 \leq j \leq N\}$ (see [4]).

We recall the important diamagnetic inequality that is frequently used in the present paper. It states, that if $\varphi \in H^1_A(\mathbb{R}^3)$, then $|\varphi| \in H^1(\mathbb{R}^3)$ and

$$|\nabla|\varphi|(x)| \leq |D_A\varphi(x)|, \quad \text{pointwise for almost every } x \in \mathbb{R}^3.$$

For a proof see [22].

(AV1) and the diamagnetic inequality imply that $\sum_{j=1}^N \langle D_{A,x_j}\varphi, D_{A,x_j}\varphi\rangle + \langle \varphi, V(x_j)\varphi\rangle$ is a closed quadratic form on $H^1_A(\mathbb{R}^{3N})$. Since $\int dk|k|^{-1}a^*(k)$ makes no sense on $\mathcal{F}_0 = \{(\varphi^{(n)}) \in \mathcal{F} | \varphi^{(n)} \in C_0(\mathbb{R}^{3N}), \varphi^{(n)} = 0$ for all but finitely many $n\}$, the Fröhlich hamiltonian is not well-defined on $Q = C_0^\infty(\mathbb{R}^{3N}) \otimes \mathcal{F}_0$. This drawback is avoided by interpreting $H^{(N)}$ as a quadratic form $\langle \psi \left| H^{(N)} \right| \psi \rangle$ on $\mathcal{Q}$. Because of Lemma 4.4.1 it is closable and semibounded on $\mathcal{Q}$, therefore the closure is a quadratic form of a self-adjoint operator.

Further, we assume the following energy inequality

$$C_n + C_m \geq C_{m+n}, \quad \text{for } m + n \leq N. \tag{4.10}$$

The following choices of potentials A, V satisfy (4.10).

1) There exists $w \in \mathbb{R}^3$ and $f \in H^2(\mathbb{R}^3)$, $f(x+w) = f(x)$: $A(x+w) = A(x) + \nabla f(x)$ and $V(x+w) = V(x)$ (periodic electric potential and periodic magnetic field).
   Proof. Let $\varphi_i \in L^2(\mathbb{R}^{3n_i})$, $1 \leq i \leq 2$ be approximative minimizers of $\mathcal{E}^{(n_i)}_{\nu,1}(A, V, .)$ up to an error of ε. We define the discrete magnetic translation by

$$\varphi_2^k(x) = \varphi_2(x + kw)e^{if(x)k}, \quad k \in \mathbb{Z}$$

   then $\|D_A\varphi_2^k\| = \|D_A\varphi_2\|$ for all $k \in \mathbb{Z}$. Hence

$$\mathcal{E}^{(n_1+n_2)}_{\nu,1}(A, V, \varphi_1 \otimes \varphi_2^k) < \sum_{i=1}^{2} C_{n_i}(A, V, \nu, 1) + 2\varepsilon + o(1)_{k\to\infty},$$

   where $o(1)_{k\to\infty}$ stems from the mixing terms of the self-interaction and the Coulomb interaction of the first n_1 and the last n_2 particles.

2) A linear, and $V \in L^\infty(\mathbb{R}^3)$, $V \geq 0$, $\lim_{|x|\to\infty} V(x) = 0$.

Structure of the Proof. Our proof of Theorem 4.1.1 is a generalization of the N-polaron case without external fields [2]. In [2] the polarons are divided into clusters in order to distinguish the ones that are in a neighborhood of each other to the ones that are not. With the help of a formula from Feynman and Kac (see Lemma 1 of [14]), derived by stochastic integration, the energy of the inter-cluster interactions is bounded from above. The formula from Feynman and Kac seems not to be easily generalizable to magnetic Schrödinger operators. Instead, in this paper the polarons are grouped into disjoint balls with sufficiently large distances to each other and bounded radii. The localization and the regrouping into suitable balls is done in Lemma 4.3.1. In Proposition 4.3.2 then the energy of the inter-ball interactions are estimated by a generalization of Lemma 3 of [14].

In the next step, the energies of N-polarons localized in balls are bounded from below by the ground state energy of the N-particle Pekar-Tomasevich functional. A proof is done in Proposition 4.4.2, which is based on [24]. From the proof it is also clear that the estimate does not depend on the concrete centers of the balls, although the fields A, V do not have to be translation invariant.

4.3 Estimate of the Multipolaron Interaction Energy

The N-polarons are first localized into N arbitrarily distributed equal sized balls. These balls then can be grouped in the following manner: There exist bigger disjoint balls that contain the smaller ones, additionally each radius is bounded in terms of the number of smaller balls in the corresponding bigger one. The following lemma addresses this issue.

Lemma 4.3.1. *Suppose $R > 0$, then for every normalized $\psi \in \mathcal{Q}$ there exists a normalized $\psi_0 \in \mathcal{Q}$ satisfying*

$$\left\langle \psi \left| H^{(N)} \right| \psi \right\rangle \geq \left\langle \psi_0 \left| H^{(N)} \right| \psi_0 \right\rangle - \frac{9N\pi^2}{4R^2} \tag{4.11}$$

and $\operatorname{supp} \psi_0 \subset \bigtimes_{i=1}^{m} B_i^{n_i}$, $B_i^{n_i} = \bigtimes_{j=1}^{n_i} B_i$. *Here B_i are balls with radius R_i, $n_i > 0$, $\sum_{i=1}^{m} n_i = N$ such that*

(i) $\operatorname{dist}(B_i, B_j) \geq R$ *for* $i \neq j$,

(ii) $R_i = \frac{1}{2}(3n_i - 1)R$.

Proof. In Step 1 $\psi \in \mathcal{Q}$ is localized. More explicitly: We show that for every $\psi \in \mathcal{Q}$ there exists $\tilde{\psi}_0 \in \mathcal{Q}$ satisfying (4.11) and $\operatorname{supp} \tilde{\psi}_0 \subset \bigtimes_{k=1}^{N} B_R(y_k)$, where $B_R(y_k)$ are balls with radius R and centers $y_k \in \mathbb{R}^3$. Then in Step 2 we regroup the N balls $B_R(y_k)$ found in Step 1 and inscribe them into disjoint bigger balls, i.e. we prove the existence of balls B_i, $1 \leq i \leq m$, where $m \leq N$, satisfying (i), (ii) and of a permutation $\sigma \in S_N$ such that $\times_{k=1}^N B_R(y_{\sigma(k)}) \subset \times_{i=1}^m B_i^{n_i}$. The lemma then follows by $\psi_0(x_1,\dots,x_N) := \tilde{\psi}_0(x_{\sigma^{-1}(1)},\dots,x_{\sigma^{-1}(N)})$ and the fact that $\langle . \left| H^{(N)} \right| . \rangle$ is invariant under permutations of the variables $x_1,\dots,x_N$.

Proof of Step 1. For arbitrary $L>0$, which later will be chosen as $L = 2R/\sqrt{3}$, a suitable localization function on $\mathbb{R}^{3N}$ is defined by

$$\phi(x) := \prod_{j=1}^{3N} \cos(x_j \pi/L) \chi_{[-L/2,L/2]}(x_j) \quad \text{and} \quad \phi_y(x) := \phi(x-y), \quad y \in \mathbb{R}^{3N}.$$

Thus ϕ_y is supported in a $3N$-dimensional cube of sidelength L and center y. By straightforward calculations

$$\begin{aligned} &\int_{\mathbb{R}^{3N}} dy \langle \phi_y\psi \left| H^{(N)} \right| \phi_y\psi \rangle \\ &= \int_{\mathbb{R}^{3N}} dy \left[\langle \psi \left| H^{(N)} \right| \psi \rangle \|\phi_y\psi\|^2 + 2\,\mathrm{Re}\,\langle (-i\nabla\phi_y)\psi, \phi_y D_A \psi \rangle + \|(-i\nabla\phi_y)\psi\|^2 \right] \\ &= \int_{\mathbb{R}^{3N}} dy \left[\langle \psi \left| H^{(N)} \right| \psi \rangle \|\phi_y\psi\|^2 + \frac{3N\pi^2}{L^2} \|\phi_y\psi\|^2 \right]. \end{aligned} \tag{4.12}$$

By (4.12)

$$\int_{\mathbb{R}^{3N}} dy \left[\langle \phi_y\psi \left| H^{(N)} \right| \phi_y\psi \rangle - \left(\frac{3N\pi^2}{L^2} + \langle \psi \left| H^{(N)} \right| \psi \rangle \right) \|\phi_y\psi\|^2 \right] = 0.$$

Hence there exists $y = (y_1,\dots,y_N)$, $y_k \in \mathbb{R}^3$, $1 \le k \le N$, such that

$$\langle \phi_y\psi \left| H^{(N)} \right| \phi_y\psi \rangle \le \left(\frac{3N\pi^2}{L^2} + \langle \psi \left| H^{(N)} \right| \psi \rangle \right) \|\phi_y\psi\|^2$$

and $\|\phi_y\psi\| \neq 0$. The support of $\tilde{\psi}_0 := \phi_y\psi\|\phi_y\psi\|^{-1}$ is contained in the cartesian product of N boxes of sidelength L and centers $y_k \in \mathbb{R}^3$, $1 \le k \le N$, and since $L = 2R/\sqrt{3}$ then the support is also located in $\times_{k=1}^N B_R(y_k)$.

Proof of Step 2. Proof by induction in N. For $N=1$ the statement is trivial. Now let us assume that for some N there exist $m \le N$, balls $B_1,\dots B_m$ and a permutation $\sigma \in S_N$ such that $\times_{k=1}^N B_R(y_{\sigma(k)}) \subset \times_{i=1}^m B_i^{n_i}$ and (i), (ii) hold. For $N+1$ balls $B_R(y_k)$ two cases can arise.

Case 1: There exists $1 \le i \le m$ such that $\mathrm{dist}(B_i, B_R(y_{N+1})) \ge R$. Then we define

$B_{m+1} := B_R(y_{N+1})$. Thus $\times_{k=1}^{N+1} B_R(y_{\tilde{\sigma}(k)}) \subset \times_{i=1}^{m+1} B_i^{n_i}$ for $n_{m+1} = 1$ and (i), (ii) is satisfied for all balls B_i and where $\tilde{\sigma} \in S_{N+1}$ such that $\tilde{\sigma}(k) = \sigma(k)$, $1 \leq k \leq N$ and $\tilde{\sigma}(N+1) = N+1$.

Case 2: There exists $i_1 \in \{1, \dots m\}$ such that $\operatorname{dist}(B_{i_1}, B_R(y_{N+1})) < R$. Then there is a ball $B^{(1)} \supset B_{i_1} \cup B_R(y_{N+1})$ with radius $\frac{1}{2}(3(n_{i_1}+1)-1)R$. If there is a $i_2 \in \{1, \dots m\} \setminus \{i_1\}$ with $\operatorname{dist}(B_{i_2}, B^{(1)}) < R$, then there exists a ball $B^{(2)} \supset B^{(1)} \cup B_{i_2}$ with radius $\frac{1}{2}(3(n_{i_1}+n_{i_2}+1)-1)R$. By repeating this procedure Step 2 is proved by choosing a convenient permutation. □

Let $n \geq 1$ and let $\Omega \subset \mathbb{R}^3$ be a measurable set, then we define

$$E_n(\Omega) = \inf_{\substack{\operatorname{supp}\varphi \subset \Omega^n \\ \|\varphi\|=1}} \langle \varphi \,|H^{(n)}|\, \varphi \rangle.$$

With the help of Lemma 4.3.1 any wave function $\psi \in \mathcal{Q}$ can be localized into a collection of disjoint balls. The proposition below specifies a concrete estimate for the inter-ball interactions.

Proposition 4.3.2. *Let N be any positive integer and let A, V satisfy (AV1). Suppose $\psi \in \mathcal{Q}$ is normalized with $\operatorname{supp}\psi \subset \times_{i=1}^m B_i^{n_i}$. Let B_i be balls with radius R_i and define $d_i := \min_{j\neq i} \operatorname{dist}(B_i, B_j) > 0$ for $1 \leq i \leq m$. Then*

$$\langle \psi \,|H^{(N)}|\, \psi \rangle \geq \sum_{i=1}^m E_{n_i}(B_i) + (U - 2\alpha) \sum_{i<j} \sum_{\substack{s_i \in C_i \\ \ell_j \in C_j}} \left\langle \psi, \tfrac{1}{|x_{s_i} - x_{\ell_j}|} \psi \right\rangle - \frac{8\alpha N}{\pi^2} \sum_{i=1}^m \left(\frac{n_i}{d_i} \right). \tag{4.13}$$

C_i denotes the index set of the electrons supported in B_i.

Our proof of Proposition 4.3.2 is a generalization of Lemma 3 of [14], where the two-particle case was studied. The proof in [14] shows, that it is useful to localize the phonon field about the respective particles. The phonon field is divided into two half-spaces each including one particle. In our case we have N polarons that are localized in m balls B_i containing n_i particles. It turns out that it is suitable to split up the phonon field in such a way, that every point of it is allocated to the nearest ball. We define

$$S_i := \{y \in \mathbb{R}^3 |\operatorname{dist}(B_i, y) < \operatorname{dist}(B_j, y), j \neq i\}.$$

Since $\operatorname{dist}(B_i, B_j) > 0$ for $i \neq j$, the definition especially ensures $B_i \subset S_i$ for $1 \leq i \leq m$ and

$$\overline{\bigcup_i S_i} = \mathbb{R}^3, \quad \text{where} \quad S_i \cap S_j = \emptyset \text{ for } i \neq j. \tag{4.14}$$

Magnetic and electric fields that satisfy (AV1) can easily be added in Lemma 3 of [14], since no special properties of the laplacian are needed.

Proof of Proposition 4.3.2. It is useful to rearrange the Fröhlich hamiltonian (4.1) such that it allows for the partition into balls

$$H^{(N)} = \sum_{i=1}^{m} \left(\sum_{\ell_i \in C_i} \left(T_{\ell_i} - \sqrt{\alpha}\phi(x_{\ell_i}) \right) + U \sum_{\substack{s_i, \ell_i \in C_i \\ s_i < \ell_i}} \frac{1}{|x_{s_i} - x_{\ell_i}|} \right) + H_{ph} + U \sum_{i<j} \sum_{\substack{s_i \in C_i \\ \ell_j \in C_j}} \frac{1}{|x_{s_i} - x_{\ell_j}|}, \tag{4.15}$$

with $T_{\ell_i} = D^2_{A,x_{\ell_i}} + V(x_{\ell_i})$. Define

$$\hat{a}(x) = \frac{1}{(2\pi)^{3/2}} \int dk e^{ikx} a(k), \quad \hat{a}^*(x) = \frac{1}{(2\pi)^{3/2}} \int dk e^{-ikx} a^*(k).$$

$\hat{a}(x)$ is a properly defined operator on the Fock space, but $\hat{a}^*(x)$ is not. Below, the operators are interpreted as quadratic forms, in which case they are well-defined. By Plancherel

$$\phi(x) = \frac{1}{\pi^{3/2}} \int dy \frac{\hat{a}(y) + \hat{a}^*(y)}{|x-y|^2}, \quad H_{ph} = \int \hat{a}^*(y)\hat{a}(y) dy. \tag{4.16}$$

Let $1 \leq i \leq m$, then for the surrounding S_i of B_i we associate the annihilation operator $\hat{a}_i(y)$. It is defined by

$$\hat{a}_i(y) = \hat{a}(y) - g_i(y), \quad y \in S_i, \tag{4.17}$$

where

$$g_i(y) = \frac{\sqrt{\alpha}}{\pi^{3/2}} \sum_{\substack{j=1 \\ j \neq i}}^{m} \sum_{\ell_j \in C_j} \frac{1}{|x_{\ell_j} - y|^2} \chi_{S_i}(y). \tag{4.18}$$

Using (4.14), (4.16) and (4.17) and the phonon energy H_{ph} becomes

$$H_{ph} = \sum_{i=1}^{m} \int_{S_i} dy \hat{a}_i^*(y)\hat{a}_i(y) + \sum_{i=1}^{m} \int_{S_i} dy (\hat{a}_i(y) + \hat{a}_i^*(y)) g_i(y) + F_1, \tag{4.19}$$

with multiplication operator

$$F_1 = \sum_{i=1}^{m} \|g_i\|^2. \tag{4.20}$$

Using (4.14) and (4.16) the interaction-term $\phi(x)$ splits up into two parts

$$\begin{aligned}\sqrt{\alpha}\sum_{i=1}^{m}\sum_{\ell_i\in C_i}\phi(x_{\ell_i}) =& \frac{\sqrt{\alpha}}{\pi^{3/2}}\sum_{i=1}^{m}\sum_{\ell_i\in C_i}\int_{S_i} dy\frac{\hat{a}(y)+\hat{a}^*(y)}{|x_{\ell_i}-y|^2} + \sum_{i=1}^{m}\int_{S_i} dy(\hat{a}(y)+\hat{a}^*(y))g_i(y)\\ =& \frac{\sqrt{\alpha}}{\pi^{3/2}}\sum_{i=1}^{m}\sum_{\ell_i\in C_i}\int_{S_i} dy\frac{\hat{a}_i(y)+\hat{a}_i^*(y)}{|x_{\ell_i}-y|^2} + \sum_{i=1}^{m}\int_{S_i} dy(\hat{a}_i(y)+\hat{a}_i^*(y))g_i(y)\\ &+ 2F_1 + F_2,\end{aligned} \tag{4.21}$$

where in the second step (4.17) was used and

$$F_2(x_1,\dots x_N) = \frac{2\sqrt{\alpha}}{\pi^{3/2}}\sum_{i=1}^{m}\sum_{s_i\in C_i}\int_{S_i} dy\frac{g_i(y)}{|x_{s_i}-y|^2}. \tag{4.22}$$

Inserting (4.19) and (4.21) in (4.15), we obtain that

$$H^{(N)} = \sum_{i=1}^{m} K_i + U\sum_{i<j}\sum_{\substack{s_i\in C_i\\ \ell_j\in C_j}}\frac{1}{|x_{s_i}-x_{\ell_j}|} - (F_1+F_2), \tag{4.23}$$

where

$$K_i = \sum_{\ell_i\in C_i}\left(T_{\ell_i} - \frac{\sqrt{\alpha}}{\pi^{3/2}}\int_{S_i} dy\frac{\hat{a}_i(y)+\hat{a}_i^*(y)}{|x_{\ell_i}-y|^2}\right) + \int_{S_i} dy\hat{a}_i^*(y)\hat{a}_i(y) + U\sum_{\substack{s_i,\ell_i\in C_i\\ s_i<\ell_i}}\frac{1}{|x_{s_i}-x_{\ell_i}|}.$$

Let $\psi\in\mathcal{Q}$ be normalized and $\operatorname{supp}\psi\subset \bigtimes_{i=1}^{m} B_i^{n_i}$, then by (4.23)

$$\left\langle\psi\left|H^{(N)}\right|\psi\right\rangle = \sum_{i=1}^{m}\langle\psi\,|K_i|\,\psi\rangle + U\sum_{i<j}\sum_{\substack{s_i\in C_i\\ \ell_j\in C_j}}\left\langle\psi, \tfrac{1}{|x_{s_i}-x_{\ell_j}|}\psi\right\rangle - \langle\psi,(F_1+F_2)\psi\rangle. \tag{4.24}$$

A bound for $\langle\psi,(F_1+F_2)\psi\rangle$ is derived in Lemma 4.3.4. It remains to bound $\langle\psi\,|K_i|\,\psi\rangle$. Because $L^2(\mathbb{R}^3) = \bigoplus_{i=1}^{m} L^2(S_i)$ the corresponding symmetric Fock space satisfies $\mathcal{F} = \bigotimes_{i=1}^{m}\mathcal{F}_{S_i}$, where $\mathcal{F}_{S_i} := \mathcal{F}(L^2(S_i))$. Since the precise form of K_i is $1\otimes\ldots\otimes K_i\otimes\ldots\otimes 1$ on $\bigotimes_{i=1}^{m} L^2(\mathbb{R}^{3n_i})\otimes\mathcal{F}_{S_i} = L^2(\mathbb{R}^{3N})\otimes\mathcal{F}$ and since $\bigotimes_{i=1}^{m}\mathcal{F}_{S_i,0}\otimes C_0^\infty(\mathbb{R}^{3n_i})$ is a form-core, the proof of the theorem is a consequence of Lemma 4.3.3. □

The key ingredients Lemma 4.3.1 and Proposition 4.3.2, together with the generalization of [24] from Section 4.4 enables us to proof Theorem 4.1.1.

Proof of Theorem 4.1.1. Let $\psi \in \mathcal{Q}$ be normalized. By Lemma 4.3.1 and Proposition 4.3.2 there exists a constant $C > 0$

$$\left\langle \psi \left| H^{(N)} \right| \psi \right\rangle \geq \sum_{i=1}^{m} E_{n_i}(B_i) - C\alpha \frac{N^2}{R} - \frac{9N\pi^2}{4R^2}. \tag{4.25}$$

We choose $R = N^{-1}\alpha^{-19/23}$ and since we use scaled fields A_α, V_α, by Corollary 4.4.3 there exists a constant $c(A, V)$

$$E_{n_i}(B_i) \geq \alpha^2 C_{n_i}(A, V, \nu, 1) - c(A, V)\alpha^{42/23} n_i^3 \left(1 + \frac{n_i^2}{N^2}\right). \tag{4.26}$$

Statement a) of the theorem is then a consequence of (4.25), (4.26), of the fact $\sum_{i=1}^m n_i^q \leq N^q$ for $q \geq 1$ and the energy inequality (4.10). If the fields A, V are not rescaled, an analogous calculation as above proves (4.4), where Corollary 4.4.3 and Lemma 4.5.3 are used. □

Lemma 4.3.3. *Suppose* $1 \leq i \leq m$. *Let* $\psi_i \in L^2(B_i^{n_i}) \otimes \mathcal{F}_{S_i}$ *be normalized. Then*

$$\langle \psi_i | K_i | \psi_i \rangle \geq E_{n_i}(B_i).$$

Proof. Let Ω_i be the normalized vacuum of $\mathcal{F}_{S_i^c}$. Let g_i be defined by (4.18) and $\hat{a}(g_i)$ by (4.17), then $W(g_i) = e^{\hat{a}^*(g_i) - \hat{a}(g_i)}$ is a unitary operator acting on $\mathcal{F}$. Further it satisfies $W(g_i)\hat{a}(y) = \hat{a}_i(y)W(g_i)$, and therefore in the sense of quadratic forms

$$W(g_i)H^{(n_i)}W(g_i)^{-1} = K_i + \int_{S_i^c} dy \left[\hat{a}^*(y)\hat{a}(y) - \frac{\sqrt{\alpha}}{\pi^{3/2}} \sum_{\ell_i \in C_i} \frac{\hat{a}(y) + \hat{a}^*(y)}{|x_{\ell_i} - y|^2}\right], \tag{4.27}$$

which follows by (4.15), (4.16). By (4.27)

$$E_{n_i}(B_i) \leq \left\langle \psi_i \otimes \Omega_i \left| W(g_i)H^{(n_i)}W(g_i)^{-1} \right| \psi_i \otimes \Omega_i \right\rangle = \langle \psi_i | K_i | \psi_i \rangle.$$

□

Lemma 4.3.4. *Suppose* ψ *satisfies the assumptions of Proposition 4.3.2. Then for* F_1 *and* F_2 *defined in* (4.20) *and* (4.22) *a)* $\langle \psi, F_1 \psi \rangle \leq N \frac{8\alpha}{\pi^2} \sum_{i=1}^{m} \frac{n_i}{d_i} \|\psi\|^2$.

b) $\langle \psi, F_2 \psi \rangle \leq 2\alpha \sum_{i<j} \sum_{\substack{s_i \in C_i \\ \ell_j \in C_j}} \left\langle \psi, \frac{1}{|x_{s_i} - x_{\ell_j}|} \psi \right\rangle$.

Proof. a) By Cauchy-Schwarz

$$\left(\sum_{\substack{j=1 \\ j \neq i}}^{m} \sum_{\ell_j \in C_j} \frac{1}{|x_{\ell_j} - y|^2} \right)^2 \leq N \sum_{\substack{j=1 \\ j \neq i}}^{m} \sum_{\ell_j \in C_j} \frac{1}{|x_{\ell_j} - y|^4}. \tag{4.28}$$

By the definition of F_1 and (4.28)

$$\begin{aligned} F_1(x_1, \dots x_N) &\leq \frac{\alpha}{\pi^3} N \sum_{i=1}^{m} \sum_{\substack{j=1 \\ j \neq i}}^{m} \sum_{\ell_j \in C_j} \int_{S_i} \frac{1}{|x_{\ell_j} - y|^4} dy \\ &= \frac{\alpha}{\pi^3} N \sum_{j=1}^{m} \sum_{\ell_j \in C_j} \int_{S_j^c} \frac{1}{|x_{\ell_j} - y|^4} dy. \end{aligned} \tag{4.29}$$

In the last step we exchanged the sums with respect to i and j and used that $\sum_{\substack{i=1 \\ i \neq j}}^{m} \chi_{S_i} = \chi_{S_j^c}$. Since $x_{\ell_j} \in B_j$

$$\int_{S_j^c} \frac{1}{|x_{\ell_j} - y|^4} dy \leq \int_{B_{d_j/2}^c(0)} \frac{1}{|y|^4} dy = \frac{8\pi}{d_j}. \tag{4.30}$$

(4.30) and (4.29) now conclude a).

b) By the definition of F_2 and g_i

$$\begin{aligned} F_2(x_1, \dots x_N) &= \frac{2\alpha}{\pi^3} \sum_{i<j} \int dy \left(\sum_{\ell_j \in C_j} \frac{1}{|x_{\ell_j} - y|^2} \right) \left(\sum_{s_i \in C_i} \frac{1}{|x_{s_i} - y|^2} \right) \big(\chi_{S_i}(y) + \chi_{S_j}(y) \big) \\ &\leq \frac{2\alpha}{\pi^3} \sum_{i<j} \sum_{\substack{s_i \in C_i \\ \ell_j \in C_j}} \int dy \frac{1}{|x_{\ell_j} - y|^2} \frac{1}{|x_{s_i} - y|^2} \\ &= 2\alpha \sum_{i<j} \sum_{\substack{s_i \in C_i \\ \ell_j \in C_j}} \frac{1}{|x_{s_i} - x_{\ell_j}|}. \end{aligned}$$

In the second step $\chi_{S_i}(y) + \chi_{S_j}(y) \leq 1$ for $i \neq j$ was used. The last equality follows by direct integration using cylindrical coordinates. $\square$

4.4 Compactly Supported Multipolarons

The objective of this section is to bound the energy of compactly supported N-polarons in electromagnetic fields by the respective N-particle Pekar-Tomasevich functional from below. The Pekar-Tomasevich functional with external electric and magnetic fields for N particles acting on $L^2(\mathbb{R}^{3N})$ is defined by

$$\mathcal{E}_{U,\alpha}^{(N)}(A,V,\varphi)=\int_{\mathbb{R}^{3N}}dx\sum_{j=1}^{N}\left(|D_{A,x_j}\varphi|^2+V(x_j)|\varphi|^2\right)+UV_C(x_1,\dots x_N)|\varphi|^2-\alpha D(\rho_\varphi),\quad(4.31)$$

with density

$$\rho_\varphi(x)=\sum_{j=1}^{N}\int_{\mathbb{R}^3}dx|\varphi(x_1,\dots,x_{j-1},x,x_{j+1},\dots x_N)|^2dx_1\dots\widehat{dx_j}\dots dx_N,$$

and self-interaction term

$$D(\rho)=\int_{\mathbb{R}^6}\frac{\rho(x)\rho(y)}{|x-y|}dxdy.\qquad(4.32)$$

(4.31) coincides with the definition (4.2). This fact can be seen by choosing η to be the coherent state that is determined by $a(k)\eta=-\overline{f(k)}\eta$ and $f(k)=2\sqrt{\alpha\pi}\hat{\rho}_\varphi(k)|k|^{-1}$, then η minimizes $\xi\mapsto\left\langle\varphi\otimes\xi\left|H^{(N)}\right|\varphi\otimes\xi\right\rangle$. The argument goes back to Pekar [28].

This section is in principle based on [24]. For completeness reasons the main ideas of the proofs are performed nevertheless. Since we allow for general A,V the translation invariance of the Fröhlich, and the Pekar and Tomasevich model is abolished. The translation invariance seems to play some role in [24], however after a little modification it is not necessary for our proof to work. In the case $N=1$ this issue was already noticed in [18].

Let $h\in L^2(\mathbb{R}^3)$, then $a(h):=\int dkh(k)a(k)$ is a well-defined Fock space operator. Suppose $\Omega\subset\mathbb{R}^3$ be a measurable set, then

$$N_\Omega=\int_\Omega dka^*(k)a(k).$$

Let $h\in L^2(\mathbb{R}^3)$ be normalized and $\operatorname{supp}h\subset\Omega$, then in the sense of quadratic forms

$$a^*(h)a(h)\leq N_\Omega.\qquad(4.33)$$

Let $B_\Lambda:=B_\Lambda(0)$ denote the ball centered in the origin with arbitrary radius $\Lambda>0$. Suppose

$\beta = 1 - \frac{8\alpha N}{\pi\Lambda}$. For any positive integer N we define

$$H_\Lambda^{(N)} := \sum_{j=1}^{N} \left(\beta D_{A,x_j}^2 + V(x_j) + \sqrt{\alpha}(a(f_{x_j}) + a^*(f_{x_j}))\right) + \beta U V_C(x_1, \dots x_N) + N_{B_\Lambda}, \quad (4.34)$$

where $f_x(k) = \chi_{B_\Lambda}(k)|k|^{-1}e^{-ikx}$.

Lemma 4.4.1. *For any values of N and $\Lambda > 0$ in the sense of quadratic forms on $\mathcal{Q}$*

$$H^{(N)} \geq H_\Lambda^{(N)} - \frac{1}{2}. \quad (4.35)$$

$H^{(N)}$ can be interpreted as a selfadjoint Operator.

Proof. Let $\psi \in \mathcal{Q}$. The interaction term of the Fröhlich hamilton operator is rewritten in terms of Fock space operators

$$\langle \psi \,|\phi(x)|\, \psi \rangle = \left\langle \psi, (a(f_x) + \textstyle\sum_{l=1}^3 [D_{A,l}, a(g_{l,x})])\psi \right\rangle + c.c., \quad (4.36)$$

where $D_{A,l}$ denotes the l-th component of D_A and

$$g_{l,x}(k) = \frac{1}{\sqrt{2}\pi}\chi_{B_\Lambda^c}(k)\frac{e^{ikx}k_l}{|k|^3}.$$

For every $\varepsilon_1, \varepsilon_2 > 0$

$$\sqrt{\alpha}|\langle \psi, a(f_x)\psi\rangle| \leq \frac{\varepsilon_1}{2}\langle \psi, N_{B_\Lambda}\psi\rangle + \frac{\Lambda\alpha}{\pi\varepsilon_1}\|\psi\|^2, \quad (4.37)$$

$$\sqrt{\alpha}\left|\left\langle \psi, \textstyle\sum_{l=1}^3 [D_{A,l}, a(g_{l,x})]\psi \right\rangle\right| \leq \frac{\varepsilon_2}{2}\langle \psi, D_A^2\psi\rangle + \frac{4\alpha}{\varepsilon_2\pi\Lambda}\langle \psi, N_{B_\Lambda^c}\psi\rangle + \frac{2\alpha}{\varepsilon_2\pi\Lambda}\|\psi\|^2. \quad (4.38)$$

(4.37) is a consequence of the Cauchy-Schwarz inequality and (4.33). For the proof of (4.38) see [24].

Suppose $\varepsilon_2 = 8\alpha N/(\Lambda\pi)$, then (4.36) and (4.38) imply (4.35).

Let $\varepsilon_1 = N^{-1}\varepsilon_2$ and $\Lambda = 8\alpha N/(\varepsilon_2^2\pi)$, then by (4.37) and (4.38) $\sqrt{\alpha}\sum_{j=1}^N \langle \psi \,|\phi(x_j)|\, \psi\rangle$ is relatively form-bounded by $\sum_{i=1}^N D_{A,x_i}^2 + N$ with bound ε_2. Hence there exists a corresponding self-adjoint operator with form core $\mathcal{Q}$ (see [29]), where in addition (4.9) is used. □

Proposition 4.4.2. *Suppose $N > 0$ is an integer. Let $\psi \in \mathcal{Q}$ be normalized and* $\operatorname{supp}\psi \subset$

$B_r(y)^N$ for any $r > 0$ and $y \in \mathbb{R}^3$. Then for arbitrary $P, \Lambda > 0$

$$\left\langle \psi \left| H^{(N)} \right| \psi \right\rangle \geq \beta C_N(A, \beta^{-1}V, U, \alpha\beta^{-2}) - \frac{6N^2\alpha P^2 r^2 \Lambda}{(1-\beta)\pi} - \frac{1}{2} - \left(2\frac{\Lambda}{P} + 1\right)^3. \tag{4.39}$$

Proof. Since C_N is constant with respect to translations of the potentials, i.e. $A(.-y)$ and $V(.-y)$, we may assume that $y = 0$. By Lemma 4.4.1 the left-hand side of (4.39) is estimated from below by $\left\langle \psi, H_\Lambda^{(N)}\psi \right\rangle$ with error $\frac{1}{2}$.

In the next step the modes are replaced by the so called block modes, of which only finitely many exist. For a given $P > 0$, we define

$$\begin{aligned} B(n) &:= \{k \in B_\Lambda | k_i - n_i P| \leq P/2\}, \quad n \in \mathbb{Z}^3, \\ \Lambda_P &:= \{n \in \mathbb{Z}^3 | B(n) \neq \emptyset\}. \end{aligned}$$

In every $B(n)$ an arbitrary k_n is chosen, they are specified later. The block modes are defined by

$$a_n := \frac{1}{M_n}\int_{B(n)} \frac{dk}{|k|} a(k), \quad M_n = \left(\int_{B(n)} \frac{dk}{|k|^2}\right)^{1/2}.$$

They are well-defined normalized annihilation operators acting on the Fock space $\mathcal{F}$. For random $\delta > 0$

$$\begin{aligned} H_{block}^{(N)} = &\sum_{j=1}^{N}\left(\beta D_{A,x_j}^2 + V(x_j) + \frac{\sqrt{\alpha}}{\sqrt{2\pi}}\sum_{n\in\Lambda_P} M_n\left(e^{ik_n x_j}a_n + e^{-ik_n x_j}a_n^*\right)\right) \\ &+\beta U V_C(x_1, \dots x_N) + (1-\delta)N_{block}, \end{aligned} \tag{4.40}$$

where $N_{block} = \sum_{n\in\Lambda_P} a_n^* a_n$.

Next we show

$$\left\langle \psi, H_\Lambda^{(N)}\psi \right\rangle \geq \inf_{\substack{\tilde{\psi}\in\mathcal{Q} \\ \|\tilde{\psi}\|=1}} \sup_{\{k_n\}} \left\langle \tilde{\psi}, H_{block}^{(N)}\tilde{\psi} \right\rangle - \frac{6N^2\alpha P^2 r^2\Lambda}{\delta\pi}. \tag{4.41}$$

Let $1 \leq j \leq N$, then in the sense of quadratic forms

$$\begin{aligned} &\frac{\delta}{N}N_{B(n)} + \frac{\sqrt{\alpha}}{\sqrt{2\pi}}\int_{B(n)}\frac{dk}{|k|}\left((e^{ikx_j} - e^{ik_n x_j})a(k) + (e^{-ikx_j} - e^{-ik_n x_j})a^*(k)\right) \\ \geq &-\frac{N\alpha}{2\pi^2\delta}\int_{B(n)} dk \frac{|e^{ikx_j} - e^{ik_n x_j}|^2}{|k|^2}, \end{aligned} \tag{4.42}$$

which follows by completion of squares. Let $k \in B(n)$ and $|x_j| < r$, $1 \le j \le N$

$$|e^{ikx_j} - e^{ik_n x_j}|^2 \le 3P^2 r^2, \quad 1 \le j \le N. \tag{4.43}$$

(4.41) is a consequence of (4.42) summed over all $n \in \Lambda_P$, $\sum_{n\in\Lambda_P} a_n^* a_n \le N_{B_\Lambda}$ and (4.43).

It remains to prove that for all normalized $\psi \in \mathcal{Q}$

$$\sup_{\{k_n\}} \left\langle \psi, H_{block}^{(N)} \psi \right\rangle \ge \beta C_N(A, \beta^{-1}V, U, \alpha\beta^{-2}) - |\Lambda_P|. \tag{4.44}$$

To do so, the block operators a_n are replaced by complex numbers z_n using coherent states. The closed subspace $M := \operatorname{span}\{\chi_{B(n)}|.|^{-1}|n \in \Lambda_P\} \subset L^2(\mathbb{R}^3)$ generates the symmetric Fock space $\mathcal{F}(M)$, i.e. the Fock space that is constructed by the block operators a_n^*, $n \in \Lambda_P$. Since M is a closed subspace

$$\mathcal{F} = \mathcal{F}(M \oplus M^\perp) \cong \mathcal{F}(M) \otimes \mathcal{F}(M^\perp).$$

Suppose $z = (z_n)_{n\in\Lambda_P}$, $z_n \in \mathbb{C}$, then we define normalized coherent states $\eta_z \in \mathcal{F}(M)$ by

$$\eta_z := \prod_{n\in\Lambda_P} e^{z_n a_n^* - \overline{z_n} a_n} \Omega, \tag{4.45}$$

where $\Omega \in \mathcal{F}(M)$ denotes the normalized vacuum. From (4.45) $a_n \eta_z = z_n \eta_z$. If $\psi \in \mathcal{Q}$ normalized and $\psi_z = \langle \eta_z, \psi \rangle$, note that the inner product acts on $\mathcal{F}(M)$, then $\psi_z \in L^2(\mathbb{R}^{3N}) \otimes \mathcal{F}(M^\perp)$. For notational simplicity hereinafter the inner products are not labeled explicitly. By a short calculation in the sense of weak integrals on the Fock space $\mathcal{F}(M)$ for $dz = \prod_{n\in\Lambda_P} \frac{1}{\pi} \int dx_n dy_n$

$$\begin{aligned} &\int dz \langle ., \eta_z \rangle \eta_z = 1, && \int dz z_n \langle ., \eta_z \rangle \eta_z = a_n, \\ &\int dz (|z_n|^2 - 1) \langle ., \eta_z \rangle \eta_z = a_n^* a_n, && \int dz \overline{z_n} \langle ., \eta_z \rangle \eta_z = a_n^*, \end{aligned} \tag{4.46}$$

where the last equality follows from the first one and the fact $[a_n, a_n^*] = 1$ for all $n \in \Lambda_P$. Let the block modes be replaced by the identities (4.46), then

$$\left\langle \psi, H_{block}^{(N)} \psi \right\rangle = \int dz \langle \psi_z, h_z \otimes 1 \psi_z \rangle, \tag{4.47}$$

whereas h_z is a Schrödinger operator on $L^2(\mathbb{R}^{3N})$

$$
\begin{aligned}
h_z = & \sum_{j=1}^{N}(\beta D^2_{A,x_j} + V(x_j)) + \beta U V_C(x_1, \dots x_N) + (1-\delta) \sum_{n\in\Lambda_P}(|z_n|^2 - 1) \\
& + \frac{\sqrt{\alpha}}{\sqrt{2}\pi}\sum_{j=1}^{N}\sum_{n\in\Lambda_P} M_n \left(z_n e^{ik_n x_j} + \overline{z_n} e^{-ik_n x_j}\right).
\end{aligned}
$$

Since $\rho_z(x) := \sum_{j=1}^{N}\int_{\mathbb{R}^{3(N-1)}} |\psi_z(x_1,\dots,x_{j-1},x,x_{j+1},\dots,x_N)|^2 dx_1\dots\widehat{dx_j}\dots dx_N$, then

$$
\sum_{j=1}^{N}\left\langle \psi_z, e^{-ikx_j}\psi_z\right\rangle = (2\pi)^{3/2}\hat{\rho}_z(k).
$$

Obviously

$$
\inf_{\{k_n\}} \int dz |\hat{\rho}_z(k_n)|^2 \|\psi_z\|^2 \le \int dz |\hat{\rho}_z(k)|^2\|\psi_z\|^2, \quad \forall k \in B(n). \tag{4.48}
$$

By completion of squares of (4.47) with respect to z_n and (4.48)

$$
\begin{aligned}
& \sup_{\{k_n\}} \int dz \langle \psi_z, h_z\psi_z\rangle \\
\ge & \int dz \Big\langle \psi_z, \Big[\textstyle\sum_{j=1}^{N}(\beta D^2_{A,x_j} + V(x_j)) + \beta U V_C(x_1,\dots x_N)\Big]\psi_z\Big\rangle \\
& - \frac{4\pi\alpha}{(1-\delta)}\int dz \int_{B_\Lambda} dk \frac{|\hat{\rho}_z(k)|^2}{\|\psi_z\|^2|k|^2} - |\Lambda_P| \\
\ge & \int dz \Big\langle \psi_z, \Big[\textstyle\sum_{j=1}^{N}(\beta D^2_{A,x_j} + V(x_j)) + \beta U V_C(x_1,\dots x_N)\Big]\psi_z\Big\rangle \\
& - \frac{\alpha}{(1-\delta)}\int dz \int \frac{\rho_z(x)\rho_z(y)}{\|\psi_z\|^2|x-y|} dx dy - |\Lambda_P|.
\end{aligned}
$$

The integrand is estimated from below by

$$
\beta\|\psi_z\|^2 C_N(A, \beta^{-1}V, U, \alpha\beta^{-2}),
$$

where $\delta = 1-\beta$ has been chosen. The assumption follows by $\int \|\psi_z\|^2 dz = 1$ and $|\Lambda_P| \le \left(2\frac{\Lambda}{P} + 1\right)^3$. $\square$

Next we evaluate (4.39) on a single localized n-polaron found in Lemma 4.3.1. The constants Λ and P can be chosen freely, but the radius r of the corresponding ball is determined by Lemma 4.3.1 (ii), i.e. $r = \frac{1}{2}(3n-1)R$ for any $R > 0$ fixed.

Corollary 4.4.3. *Let $\nu > 0$ be arbitrary and let $n > 0$ be any integer. Let $R > 0$ and let B be a ball of radius $\frac{1}{2}(3n-1)R$. Suppose A, V satisfy (AV1) and (4.10), and let them be scaled by $A_\alpha(x) = \alpha A(\alpha x)$, $V_\alpha(x) = \alpha^2 V(\alpha x)$. Then there exists $c(A, V)$*

$$E_n(B) \geq \alpha^2 C_n(A, V, \nu, 1) - 3R^2\alpha^{80/23}n^5 - c(A, V)\alpha^{42/23}n^3. \tag{4.49}$$

Moreover, if A, V satisfy (AV2), then $c(A_{\alpha^{-1}}, V_{\alpha^{-1}})$ is uniformly bounded for α large.

Proof. Since $\lambda \mapsto C_n(A, \lambda V, \nu, \lambda^2)$ is concave, the one-sided derivatives exist and

$$C_n(A, \beta^{-1}V, \nu, \beta^{-2}) \geq C_n(A, V, \nu, 1) + (\beta^{-1} - 1)\frac{d}{d\lambda}C_n(A, \lambda V, \nu, \lambda^2)\Big|_{\lambda=2-}. \tag{4.50}$$

The derivation term of (4.50) is estimated by Lemma 4.5.1. The statement is then a consequence of Proposition 4.4.2, the scaling property (4.5), (4.50) and Lemma 4.5.1, where we determine the free parameters $\Lambda = n\alpha^{27/23}$, $P = \alpha^{13/23}$ and hence $\left(2\frac{\Lambda}{P} + 1\right)^3 \leq 9n^3\alpha^{42/23}$ and $1 - \beta = \frac{8}{\pi}\alpha^{-4/23}$.

If the fields A, V are not rescaled, then in (4.50) A, V are replaced by $A_{\alpha^{-1}}, V_{\alpha^{-1}}$. Hence the second statement follows by Lemma 4.5.1. □

4.5 Appendix

Lemma 4.5.1. *For any values of N and $\nu > 0$. Suppose (AV1) and (4.10) are satisfied, then there exists $c(A, V)$*

$$c(A, V)N \geq C_N(A, V, \nu, 1) \geq -c(A, V)N^3, \quad N \in \mathbb{N}. \tag{4.51}$$

Moreover, if (AV2) is satisfied, then there exists a constant $c > 0$ such that $c(A_{\alpha^{-1}}, V_{\alpha^{-1}}) \leq c$ for α large enough.

Remark. In the physical regime $\nu > 2$ without external fields, in [14] it was proven that $C_N(0, 0, \nu, 1) \geq -c(\nu)N$ for $c(\nu) > 0$.

Proof of Lemma 4.5.1. Let $\nu > 0$, then by (4.10)

$$C_N(A, V, \nu, 1) \leq NC_1(A, V, 1), \tag{4.52}$$

which proves the upper bound in (4.51). Let $\varphi \in C_0^\infty(\mathbb{R}^{3N})$ be normalized, then by the Hardy and the diamagnetic inequality

$$D(\rho_\varphi) \leq 2N^{3/2}\left(\sum_{j=1}^N \|D_{A,x_j}\varphi\|^2\right)^{1/2}. \tag{4.53}$$

Thus from (4.53), (4.9) and by completion of squares with respect to $\left(\sum_{j=1}^N \|D_{A,x_j}\varphi\|^2\right)^{1/2}$, we conclude

$$\mathcal{E}_{\nu,1}^{(N)}(A,V,\varphi) \geq -\frac{N^3}{(1-\varepsilon)} - C_\varepsilon N,$$

where $C_\varepsilon > 0$. This proves the lower bound of (4.51).

By a similar calculation

$$\mathcal{E}_{\nu,1}^{(N)}(A_{\alpha^{-1}},V_{\alpha^{-1}},\varphi) \geq -\frac{N^3}{(1-\varepsilon)} - C_\varepsilon \alpha^{-2} N. \tag{4.54}$$

For α large, there exists a constant $c > 0$ such that (4.54) is bounded from below by $-cN^3$. Lemma 4.5.3 and (4.52) finish the proof. $\square$

Lemma 4.5.2. *Suppose $A \in L^3_{\text{loc}}(\mathbb{R}^3)$ and $V \in L^{3/2}_{\text{loc}}(\mathbb{R}^3)$. Then*

$$\begin{aligned} A_{\alpha^{-1}} &\to 0 \quad (\alpha \to \infty) \quad \textit{in } L^2_{\text{loc}}(\mathbb{R}^3), \\ V_{\alpha^{-1}} &\to 0 \quad (\alpha \to \infty) \quad \textit{in } L^1_{\text{loc}}(\mathbb{R}^3). \end{aligned}$$

For the proof of this Lemma we refer to the proof of Lemma 3.3.3.

Lemma 4.5.3. *For any values of N and $\nu > 0$. If the assumptions (AV2) are satisfied, then*

$$\lim_{\alpha\to\infty} C_N(A_{\alpha^{-1}},V_{\alpha^{-1}},\nu,1) = C_N(0,0,\nu,1).$$

Proof of Lemma 4.5.3. For any normalized $\varphi \in C_0^\infty(\mathbb{R}^{3N})$

$$\limsup_{\alpha\to\infty} C_N(A_{\alpha^{-1}},V_{\alpha^{-1}},\nu,1) \leq \limsup_{\alpha\to\infty} \mathcal{E}_{\nu,1}^{(N)}(A_{\alpha^{-1}},V_{\alpha^{-1}},\varphi) = \mathcal{E}_{\nu,1}^{(N)}(0,0,\varphi),$$

where the last equality is a consequence of Lemma 4.5.2. This implies

$$\limsup_{\alpha\to\infty} C_N(A_{\alpha^{-1}},V_{\alpha^{-1}},\nu,1) \leq C_N(0,0,\nu,1).$$

It remains to prove the other direction. For all normalized $\varphi \in C_0^\infty(\mathbb{R}^{3N})$ and by (4.9) for all $1 > \varepsilon > 0$ there exists $C_\varepsilon > 0$ such that

$$\mathcal{E}_{\nu,1}^{(N)}(A_{\alpha^{-1}}, V_{\alpha^{-1}}, \varphi) \geq (1-\varepsilon) C_N(0, 0, \nu, (1-\varepsilon)^{-1}) - C_\varepsilon N \alpha^{-2} \tag{4.55}$$

where the diamagnetic inequality has been used. The Lemma follows immediately from (4.55). $\square$

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