Multipolarons in a Constant Magnetic Field

I. Anapolitanos* and M. Griesemer
Universität Stuttgart, Fachbereich Mathematik
70550 Stuttgart, Germany

Dedicated to the memory of Walter Hunziker

Abstract

The binding of a system of $N$ polarons subject to a constant magnetic field of strength $B$ is investigated within the Pekar-Tomasevich approximation. In this approximation the energy of $N$ polarons is described in terms of a non-quadratic functional with a quartic term that accounts for the electron-electron self-interaction mediated by phonons. The size of a coupling constant, denoted by $\alpha$, in front of the quartic is determined by the electronic properties of the crystal under consideration, but in any case it is constrained by $0 < \alpha < 1$. For all values of $N$ and $B$ we find an interval $\alpha_{N,B} < \alpha < 1$ where the $N$ polarons bind in a single cluster described by a minimizer of the Pekar-Tomasevich functional. This minimizer is exponentially localized in the $N$-particle configuration space $\mathbb{R}^{3N}$.

1 Introduction

The electron-phonon interaction in a polar crystal mediates an interaction between pairs of electrons which becomes an electrostatic Coulomb attraction in the Pekar-Tomasevich approximation. This attraction competes with the Coulomb repulsion between the equally charged electrons, and the question arises whether $N$ electrons may form a bound cluster. Due to the constraint on the parameters of the model, the $1/|x|-part of the electron-electron interaction is repulsive. There remains, however an attractive short range interaction, which seems to be of van der Waals type and which may lead to $N-$particle bound states [11]. This phenomenon of bound multipolarons had previously been observed in Fröhlich’s large polaron model on which the Pekar-Tomasevich approximation is based [17, 4]. Similarly, the binding of polarons subject to a constant magnetic field had been investigated within the Fröhlich model [3]. Yet, in that case, the analysis in the literature is based on poorly justified variational estimates, and the conclusions remain doubtful. The present paper establishes, within the Pekar-Tomasevich approximation, the existence of bound $N$-polaron clusters in a constant magnetic field of any strength. It is a continuation of a previous work of one of us, concerning the case $N = 2$ [8].

The Pekar-Tomasevich approximation to the large polaron model of Fröhlich describes the energy of $N$ polarons through an effective functional that depends on the wave function $\Psi \in \mathcal{H}_N := \Lambda^N L^2(\mathbb{R}^3 \times \{1, \ldots, q\})$ of the particles only. We are mainly interested in the case of spin-1/2 fermions but we can allow for arbitrary $q \in \mathbb{N}$ without more effort. The functional is then given by

$$E^{N,\alpha}(\Psi) = \left\langle \Psi, \left( \sum_{j=1}^{N} D_{A,x_j}^2 + \sum_{i < j} \frac{U}{|x_i - x_j|} \right) \Psi \right\rangle - \frac{\alpha}{2} \int \int \rho_\Psi(x)\rho_\Psi(y) \frac{|x - y|}{|x - y|} dx dy, \quad (1)$$

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where \( U, \alpha > 0 \) are constants, and

\[
\rho_\Psi(x) := \sum_{j=1}^{N} \sum_{\sigma_j=1}^{q} \int |\Psi(x_1, \ldots, x_{j-1}, (x, \sigma_j), x_{j+1}, \ldots, x_N)|^2 \, dx_1 \cdots dx_{j-1} \cdots dx_N, \tag{2}
\]

is the density associated to \( \Psi \). We have introduced the notations \( x_j = (x_j, \sigma_j) \) for elements of \( \mathbb{R}^3 \times \{1, \ldots, q\} \) and we set \( \int dx_j = \sum_{\sigma_j=1}^{q} \int dx_j \). Of course in (2) the sum with respect to \( j \) may be replaced by a factor of \( N \), due to the symmetry of \( \Psi \); but we shall allow for Boltzons later on, and hence we prefer (2) as the definition of \( \rho_\Psi \). Furthermore, \( D_{A,x} := -i \nabla + A(x) \) where the vector potential \( A : \mathbb{R}^3 \to \mathbb{R}^3 \) generates a magnetic field \( B = \text{curl} A \). We are primarily interested in the case where \( B \) is constant and hence \( A \) will be assumed linear. The positive parameters \( U, \alpha \) are constrained by \( \alpha < U \) due to their role in the Fröhlich large polaron model. Mathematically, any real values are conceivable for \( U \) and \( \alpha \), but \( 0 < U < \alpha \) leads to thermodynamic instability \([10]\). The energy of the fields \( U^{3N/2} \Psi(Ux_1, \sigma_1, \ldots, Ux_N, \sigma_N) \) and \( UA(Ux) \) upon the substitutions \( Ux \to x \) and \( \alpha/U \to \alpha \) becomes proportional to \( U^2 \). We therefore set \( U = 1 \) and we require that \( 0 < \alpha < 1 \).

It is easy to see, using the diamagnetic and the Hardy inequalities, that \( E_{N,\alpha} \) is bounded below if restricted to the unit sphere \( \|\Psi\| = 1 \). The minimal energy,

\[
E_{N,\alpha} := \inf_{\|\Psi\| = 1} E_{N,\alpha}(\Psi), \tag{3}
\]

is therefore finite. By moving particles apart, one can see that \( E_{N,\alpha}^{k,\alpha} \leq E_{N,\alpha}^{k,\alpha} + E_{N,\alpha}^{N-k,\alpha} \) for \( k = 1, \ldots, N-1 \). The question is, whether it takes energy to do this, that is, whether for some \( \alpha < 1 \),

\[
\Delta E_{N,\alpha} := \min_{1 \leq k \leq N-1} \left\{ E_{N,\alpha}^{k,\alpha} + E_{N,\alpha}^{N-k,\alpha} \right\} - E_{N,\alpha} > 0. \tag{4}
\]

Our main result is the following theorem:

**Theorem 1.1.** Assume that the vector potential \( A \) is linear (constant magnetic field \( B \)). Then, for all \( N \in \mathbb{N} \) there exists \( \alpha_{N,B} < 1 \) such that for \( \alpha_{N,B} < \alpha < 1 \) and \( U = 1 \):

(a) the binding inequality \([1]\) holds,

(b) the functional \([1]\) has a minimizer.

Analog results hold in the case of bosons and boltzons, that is, for \( \mathcal{H}_N = \otimes^N L^2(\mathbb{R}^3 \times \{1, \ldots, q\}) \), the symmetric product of \( N \) copies of \( L^2(\mathbb{R}^3 \times \{1, \ldots, q\}) \), or \( \mathcal{H}_N = \otimes^N L^2(\mathbb{R}^3) \) without symmetry requirements. The proofs in these cases are similar and in the case of Boltzons the proof of (a) becomes much easier. Yet the property (a) even for boltzons is a subtle correlation effect since the restriction \( \alpha < 1 \) means that the Coulomb repulsion dominates the attraction for states of the form \( \varphi_1 \otimes \cdots \otimes \varphi_N \). We remark that Theorem \([1]\) has consequences for the binding of boltzonic polarons in the large polaron model of Fröhlich \([2, 9]\).

For \( \alpha = 0 \) there is no minimizer and, in the absence of magnetic fields, there is no binding for \( \alpha \) small enough \([6]\). The existence of a minimizer is a phenomenon due to the non-linearity and it occurs whenever the binding inequality \([1]\) is satisfied (and \( \alpha > 0 \)). For other non-quadratic energy-functionals associated with many-body quantum systems this has previously been pointed out and described as a non-linear HVZ-Theorem \([11, 7]\). In this paper we show that (a) \( \Rightarrow \) (b) is a consequence of a linear HVZ-Theorem for an \( N \)-body Hamiltonian that is intimately related with the physics of the polaron problem: there is a Hamiltonian \( H_\sigma \) depending on a charge density \( \sigma \in L^1(\mathbb{R}^3) \) such that

\[
\mathcal{E}_{N,\alpha}(\Psi) \leq \langle \Psi, H_\sigma \Psi \rangle
\]
with equality for $\sigma = \rho_\Psi$. We may think of $\alpha \sigma$ as the charge density due to a hypothetical, possibly non-optimal, lattice deformation caused by the electrons. For $E_{N,\alpha}^{N,\alpha}(\Psi_n)$ near $E_{PT}^{N,\alpha}$, ($\Psi_n$) being a minimizing sequence with densities ($\rho_n$), the binding inequality implies that $H_{\rho_n}$ has an isolated ground state energy separated from the essential spectrum of $H_{\rho_n}$ by a gap that is uniform in $n$ along a subsequence. This uniformity implies uniform localization of $\Psi_n$ (or concentration of minimizing sequences) up to magnetic translations.

Our proof of part (a) in Theorem 1.1 is based on a variational argument that is inspired by [8] but is considerably more involved in the present case of particles with statistics.

The following theorem gives further information about the minimizers found in Theorem 1.1. In Theorem 1.2 and throughout the paper we use the notation $V_\rho := \rho \ast | \cdot |^{-1}$.

**Theorem 1.2.** If $\Psi \in \mathcal{H}_N$ is a minimizer of $E_{N,\alpha}$, then it solves the non-linear Schrödinger equation

$$
\left( \sum_{k=1}^{N} (D^2_{A,x_k} - \alpha V_\rho(x_k)) + \sum_{i<j} \frac{1}{|x_i - x_j|} \right) \Psi = \lambda \Psi,
$$

(5)

where $\lambda \in \mathbb{R}$ is the lowest point in the spectrum of the Schrödinger operator on the left hand side and $\rho$ is the density of $\Psi$. Moreover, if (4) holds then the spectrum of the Schrödinger operator on the left hand side is discrete below $\lambda + \Delta E_{PT}^{N,\alpha}$ and hence if $\beta \in \mathbb{R}$ with $\beta^2 < \Delta E_{PT}^{N,\alpha}$, then

$$
e^{\beta |\cdot|} \Psi \in \mathcal{H}_N.
$$

(6)

In the case $N = 1$, $A = 0$ the Pekar-Tomasevich functional reduces to the Pekar or Choquard functional which is well known to be minimized by a spherically symmetric, positive function that is unique up to translations $[12, 16]$.

Existence of a magnetic polaron and the binding of two polarons subject to an external magnetic field, not necessarily constant, was previously established in [8]. In the present paper, the methods developed in [8] are extended and generalized to the case of $N > 2$ particles of fermionic, bosonic or bolzonic nature. Results similar to ours in the case $A = 0$ where previously obtained by Lewin in [11]. Lewin establishes a bound on the binding energy of the form of a van der Waals potential with exponentially small corrections. To this end he uses the variational state introduced by Lieb and Thirring in connection with the van der Waals binding of neutral atoms and molecules [15]. This approach makes crucial use of spherical averaging and the Newton’s theorem. It breaks down in the presence of a magnetic field where the rotational invariance of $E_{N,\alpha}$ is broken. Moreover, in the absence of a magnetic field our Theorem 1.2 gives more information than the corresponding result of Lewin, as it relates the binding energy $\Delta E_{PT}^{N,\alpha}$ to the gap between $\lambda$ and the essential spectrum of the Hamiltonian in (5). Lewin, in the case of binding, merely finds that such a gap exists provided that $\alpha > 1 - 1/N$.

The Theorem 1.2 opens the following new view upon the phenomenon of $N$-polaron binding: if a Hamiltonian of the type in (5) with total positive charge $\alpha N$ is shown not to bind $N$ electrons, then binding of $N$ polarons is excluded. Here binding means positivity of the binding energy. – In the case where the density is spherically symmetric and $A = 0$ we deduce from [13] that the Hamiltonian has no ground state if $\alpha \leq (1 - N^{-1})/2$. This leads to the following corollary: if $\alpha \leq (1 - N^{-1})/2$ then a hypothetical minimizer of $E_{N,\alpha}$ cannot have a spherically symmetric density.

This paper is organized as follows: In Section 2 we outline the proof of our main Theorem and we introduce the most important tools. In Section 3 we prove an operator inequality which is of crucial importance for the proof of existence of a minimizer of the Pekar-Tomasevich functional, as well as the proof of the second part of Theorem 1.2. In
Section 4 we use the operator inequality to prove existence of a minimizer and exponential decay of any minimizer of the Pekar-Tomasevich functional. In Section 5 we establish the binding inequality (4).

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2 Preparations and elements of the proofs

The minimal energy \( E_{PT}^{k,\alpha} \) is continuous in \( \alpha \) because it is concave in \( \alpha \) as the infimum of the affine functions \( \alpha \mapsto E_{PT}^{k,\alpha}(\Psi) \). Hence, it suffices to establish the binding in the case \( \alpha = 1 \).

Our proof that binding implies existence of a minimizer, i.e (a) \implies (b) in Theorem 1.1, as well as the proof of Theorem 1.2 readily generalize from the case \( \alpha = 1 \) to any \( \alpha > 0 \).

We therefore put \( \alpha = 1 \) for notational simplicity, that is,

\[
E_N(\Psi) := \left\langle \Psi, \left( \sum_{k=1}^{N} D_{A,x_k}^2 + \sum_{j<k} \frac{1}{|x_j - x_k|} \right) \Psi \right\rangle - D(\rho_{\Psi}),
\]

where \( D(\rho) := D(\rho,\rho) \),

\[
D(\rho,\sigma) := \frac{1}{2} \int \frac{\rho(x)\sigma(y)}{|x-y|} dxdy,
\]

and

\[
E_{PT}^N := \inf_{\|\Psi\|=1} E_N(\Psi).
\]

The domain of \( E_N \) is the form domain, \( Q_{N,A} \), of \( \sum_{k=1}^{N} D_{A,x_k}^2 \), that is, \( Q_{N,A} = \{ \Psi \in \mathcal{H}_N : D_{A,x_k} \Psi \in L^2, \forall k \in \{1, \ldots, N\} \} \), and we use \( \| \cdot \|_{Q_{N,A}} \) for the corresponding form norm. By a minimizer of \( E_N \) we shall always mean a normalized vector \( \Psi \in \mathcal{H}_N \) with \( \Psi \in Q_{N,A} \) and \( E_N(\Psi) = E_{PT}^N \). Throughout the paper we use \((\cdot,\cdot)\) and \(\| \cdot \|\) for the usual inner products and norms of \( \otimes^N L^2(\mathbb{R}^3 \times \{1, \ldots, q\}) \) and \( \mathcal{H}_N \).

By the above explanations it remains to prove the following theorem in order to establish Theorem 1.1:

Theorem 2.1. Assume that the vector potential \( A \) is linear. Then,

(a) there exists a minimizer of \( E^1 \),

(b) if \( E^1, \ldots, E^{N-1} \) have minimizers then

\[
E_{PT}^N < E_{PT}^k + E_{PT}^{N-k}, \quad \forall k = 1, \ldots, N - 1,
\]

(c) if (10) holds then \( E^N \) has a minimizer.

Part (a) of Theorem 2.1 is known from [8] but we shall reprove it as a part of the proof of part (c). Part (b) is proved in Section 5 by variational arguments. Sections 3 and 4 are devoted to the proof of (c). The remainder of the present section describes the difficulties met in the proof of (c) and collects our tools for dealing with them.

Any proof of (c) must deal with the following translation invariance of \( E^N \): Let \( A : \mathbb{R}^3 \to \mathbb{R}^3 \) be linear, \( h \in \mathbb{R}^3 \), and \( \Psi \in \mathcal{H}_N \). If \( T_h \Psi \) is defined by

\[
(T_h \Psi)(x_1,\sigma_1,\ldots,x_N,\sigma_N) = \prod_{j=1}^{N} e^{iA(h) \cdot x_j} \Psi(x_1 + h,\sigma_1,\ldots,x_N + h,\sigma_N),
\]
then \( \rho_{T_h \Psi}(x) = \rho_{\Psi}(x + h) \) and
\[
\mathcal{E}^N(T_h \Psi) = \mathcal{E}^N(\Psi).
\]
Due to (11) and (12) a minimizing sequence of \( \mathcal{E}^N \) may converge to the zero function weakly. On the other hand in view of Lemma A.1, a weak limit \( \Psi \in H_N \) with \( \| \Psi \| = 1 \) is, indeed, a minimizer of \( \mathcal{E}^N \). Our task is thus to find a minimizing sequence of \( \mathcal{E}^N \) that does not suffer any loss of norm in the limit. One of our tools to this end is the following form of the Concentration Compactness Principle \[16\]:

**Proposition 2.2.** Let \( (\rho_k)_{k \geq 1} \) be a sequence of nonnegative functions in \( L^1(\mathbb{R}^3) \) with \( \int \rho_k = N \). Then there exists a subsequence of \( (\rho_k) \), denoted by \( (\rho_k) \) as well, such that one of the following holds:

(i) (Vanishing) For all \( R > 0 \) we have that
\[
\lim_{k \to \infty} \sup_{y \in \mathbb{R}^3} \int_{B(y, R)} \rho_k = 0.
\]

(ii) (Dichotomy or compactness) There exists \( \lambda \in (0, N] \) such that for all \( \varepsilon > 0 \) there exist \( R_\varepsilon > 0 \), a sequence \( y_k = y_k(\varepsilon) \) in \( \mathbb{R}^3 \), and a sequence \( P_k = P_k(\varepsilon) \) in \( \mathbb{R} \) with \( P_k \to \infty \) as \( k \to \infty \), such that the sequences of functions
\[
\rho_{k, 1} := \rho_k \chi_{B(y_k(\varepsilon), R_\varepsilon)}
\]
\[
\rho_{k, 2} := \rho_k \chi_{B(y_k(\varepsilon), P_k(\varepsilon))}
\]
satisfy for \( k \geq k_0(\varepsilon) \) the bounds
\[
\| \rho_k - \rho_{k, 1} - \rho_{k, 2} \|_{L^1} \leq \varepsilon, \quad (13)
\]
\[
\| \rho_{k, 1} \|_{L^1} - \lambda \leq \varepsilon, \quad \| \rho_{k, 2} \|_{L^1} - (N - \lambda) \leq \varepsilon \quad (14)
\]
and
\[
dist(\text{supp } \rho_{k, 1}, \text{supp } \rho_{k, 2}) \to \infty, \quad (k \to \infty). \quad (15)
\]
If \( m \) is a positive integer such that \( m\lambda > N \), then after passing to a subsequence once more, there exists \( \varepsilon_1, \ldots, \varepsilon_m > 0 \), and \( \delta > 0 \) such that
\[
\liminf_{k \to \infty} \int_{\bigcup_{i=1}^{m-1} B_{y_i, \varepsilon}} \rho_{k, 1} \geq \delta \quad (16)
\]
for all \( \varepsilon > 0 \) small enough. Here \( B_{y, R} = B(y, R) \).

**Proof.** We shall only prove the last part of (ii). The rest is a variation of the Concentration Compactness Principle. Let \( \varepsilon_1, \delta_1 > 0 \) be such that \( m(\lambda - \varepsilon_1) > N + m\delta_1 \). Assuming that the lemma is wrong we inductively construct \( \varepsilon_1 > \varepsilon_2 > \ldots > \varepsilon_m > 0 \) and a subsequence of \( \rho_k \) denoted by \( \rho_k \) as well, such that
\[
\int_{\bigcup_{i=1}^{m-1} B_{y_i, \varepsilon_i} \cap B_{y_{i+1}, \varepsilon_{i+1}}} \rho_k \leq \frac{\delta_i}{i-1}, \quad \forall i = 2, \ldots, m.
\]

Using this together with (14) and the inequality
\[
\chi_{\bigcup_{j=1}^m B_{y, \varepsilon}} \geq \sum_{j=1}^m \chi_{B_{y, \varepsilon_j}} - \sum_{i<j \leq m} \chi_{B_{y, \varepsilon_i} \cap B_{y, \varepsilon_j}},
\]
\( \chi_A \) denotes the characteristic function of the set \( A \) and \( B(y, R) \) is the ball of radius \( R \) centered at \( y \) in \( \mathbb{R}^3 \).
we obtain that
\[
\liminf \int_{\cup_{j=1}^{m} B_{k,\varepsilon_j}} \rho_k \geq \sum_{j=1}^{m} (\lambda - \varepsilon_j) - (m-1)\delta_1 \geq m(\lambda - \varepsilon_1) - (m-1)\delta_1 > N,
\]
where the last inequality follows by the choice of $\varepsilon_1$ and $\delta_1$. This is in contradiction with $\int \rho_k = N$, which concludes the proof of the lemma.

The following lemma is the reason for the new part (16) in the above version of the Concentration Compactness Principle.

**Lemma 2.3.** In the case (ii) of Proposition 2.2, if $(\rho_k)$ is chosen to satisfy (16), then
\[
\liminf_{k \to \infty} D(\rho_{k,1}) > 0 \quad (17)
\]
uniformly for small enough $\varepsilon$. (Recall that $\rho_{k,1}$ depends on $\varepsilon$.)

**Proof.** Let $\varepsilon$ be small enough for (16) and fixed. By (16) there exists $k_0(\varepsilon)$ such that for all $k \geq k_0(\varepsilon)$ we have
\[
\int_{\cup_{j=1}^{m-1} B_{k,\varepsilon_j}} \rho_{k,1} \geq \frac{(m-1)\delta}{m}. \quad (18)
\]
This means that $\int_{B_{k,\varepsilon_j}} \rho_{k,1} \geq \delta/m$ for some $j \in \{1, ..., m-1\}$ depending on $k \geq k_0(\varepsilon)$. Since $\text{diam}(B_{k,\varepsilon_j}) = 2R_{\varepsilon_j}$, we conclude that
\[
D(\rho_{k,1}) \geq \frac{1}{2R_{\varepsilon_j}} \left( \int_{B_{k,\varepsilon_j}} \rho_{k,1}(x)dx \right)^2 \geq \min_i \frac{\delta^2}{2R_{\varepsilon_i}m^2}, \quad (19)
\]
which proves the lemma. □

We want to construct a minimizing sequence $(\Psi_k)$ that is concentrated near the origin (after translations). Applying the Concentration Compactness Principle to $|\Psi_k|^2$ would not work, because the Pekar-Tomasevich functional is invariant under translations of the form (11), only, and not under general translations in $\mathbb{R}^{3N}$. Thus, we apply the Concentration Compactness Principle to the densities, where dichotomy may mean various things for the wave function. Rather than trying to exclude all of them we show directly that non-vanishing of the sequence $\rho_k$, leads to concentration of a subsequence of $\Psi_k$. This is possible thanks to an HVZ-type operator inequality for the Hamiltonians $H_{\rho_k}^N$ defined as follows:

for a given real-valued density $\sigma \in L^1(\mathbb{R}^3) \cap L^{6/5}(\mathbb{R}^3)$ we define
\[
V_\sigma := \sigma \ast \frac{1}{|\cdot|},
\]
and
\[
H_\sigma^N := \sum_{j=1}^{N} \left( D^2_{A,x_j} - V_\sigma(x_j) \right) + \sum_{i<j} \frac{1}{|x_i - x_j|} + D(\sigma), \quad (21)
\]
which is well defined by the choice of $\sigma$ ([14] Corollary 5.10). In all the following this operator is considered defined in $\mathcal{H}_N$ unless explicitly stated otherwise. The following lemma, taken from [6], relates the Pekar-Tomasevich functional to the linear Hamiltonian (21):

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Lemma 2.4 (Linearization of the Pekar-Tomasevich functional). For any density \( \sigma \in L^1(\mathbb{R}^3) \cap L^{6/5}(\mathbb{R}^3) \),
\[
\mathcal{E}^N(\Psi) \leq \langle \Psi, H^N_\sigma \Psi \rangle
\]  
with equality if and only if \( \sigma = \rho_\Psi \). In particular, for all \( N \in \mathbb{N} \),
\[
H^N_\sigma \geq E^N_{PT}.
\]  
In particular, if \((\Psi_k)\) is a minimizing sequence for \( \mathcal{E}^N \) and \((\rho_k)\) is the sequence of the corresponding densities, then
\[
\lim_{k \to \infty} \langle \Psi_k, H^N_{\rho_k} \Psi_k \rangle = E^N_{PT}. 
\]  
Proof. By the definitions of \( H^N_\sigma, \mathcal{E}^N, V_\sigma \) and \( D \) we have that
\[
\langle \Psi, H^N_\sigma \Psi \rangle - \mathcal{E}^N(\Psi) = D(\sigma) + D(\rho_\Psi) - 2D(\rho_\Psi, \sigma) = D(\sigma - \rho_\Psi) \geq 0,
\]  
where the last inequality follows from the positivity of the Fourier transform of \(|.|^{-1}\). This proves (22). Inequality (23) follows from (22) and from the definition, Equation (9), of \( E^N_{PT} \). Equation (24) follows from \( \langle \Psi_k, H^N_{\rho_k} \Psi_k \rangle = \mathcal{E}^N(\Psi_k) \) and from the choice of \((\Psi_k)\).

The main steps in our proof of part (c) of Theorem 2.1 are as follows:

**Step 1** is to exclude vanishing for the sequence of the densities \((\rho_k)\) associated with a minimizing sequence \((\Psi_k)\). To this end we prove that vanishing implies that \( D(\rho_k) \to 0 \) which is easily seen to be in contradiction with \( \mathcal{E}^N(\Psi_k) \to E^N_{PT} \).

As vanishing has now been excluded, the second alternative of Proposition 2.2 must apply to the densities \((\rho_k)\) of any minimizing sequence \((\Psi_k)\). Upon the translations \( \Psi_k \to T_{y_k} \Psi_k \), see (11), we may assume that some part of the densities \( \rho_k \) is concentrated near the origin.

**Step 2** is the proof of the operator inequality
\[
H^N_{\rho_k} \geq E^N_{PT} + d(1 - J_\varepsilon) + O(\sqrt{\varepsilon}),
\]  
where \( d > 0 \), \( J_\varepsilon \) is compactly supported and \( 0 \leq J_\varepsilon \leq 1 \). The proof of (26) is based on the properties of \( \rho_k \) as described by Proposition 2.2 (ii), on Lemma 2.3 and on a suitable partition of unity that is adjusted to the supports of \( \rho_{k,1} \) and \( \rho_{k,2} \).

**Step 3** is to show that (25) implies concentration of \((\Psi_k)\). This is easily done with the help of (24) and the fact that \( \varepsilon \) in (25) may be taken arbitrarily small.

## 3 Absence of vanishing and the operator inequality

Our goal in this Section is to establish absence of vanishing of the sequence of the densities \((\rho_k)\) associated with a minimizing sequence \((\Psi_k)\) and to prove the operator inequality of Proposition 3.2.

**Lemma 3.1 (Absence of vanishing).** The sequence of the densities \((\rho_k)\) associated with a minimizing sequence \((\Psi_k)\) of \( \mathcal{E}^N \) cannot be vanishing.

**Proof.** We shall derive a contradiction from the assumptions that \((\Psi_k)\) is minimizing and that \((\rho_k)\) is vanishing at the same time. The vanishing of \((\rho_k)\) implies that
\[
\lim_{k \to \infty} D(\rho_k) = 0,
\]  
(26)
as we will prove shortly. By \((7)\) and \((26)\) we have that
\[
\lim_{k \to \infty} E^N_{\Psi_k} \geq N \inf \sigma(D^2_{\lambda}) \geq N |B|.
\] (27)
On the other hand \(E^N_{\Psi_T} \leq NE^1_{\Psi_T}\) by general principles and \(E^1_{\Psi_T} < |B|\), by [8]. It follows that
\[
E^N_{\Psi_T} < N |B|,
\] (28)
which we combine with \((27)\) to conclude that the sequence \((\Psi_k)\) is not minimizing in contradiction to our assumption.

We now turn to the proof of \((26)\). From \(\|\rho_k\|_{L^1} = N\) it follows that, for any \(r > 0\),
\[
D(\rho_k) \leq \int_{|x-y| \leq r} \frac{\rho_k(x)\rho_k(y)}{|x-y|} dx dy + \frac{N^2}{r}
\] (29)
and
\[
\int_{|x-y| \leq r} \frac{\rho_k(x)\rho_k(y)}{|x-y|} dx dy \leq N \sup_{x \in \mathbb{R}^3} \int_{|x-y| \leq r} \frac{\rho_k(y)}{|x-y|} dy.
\] (30)
For each \(x \in \mathbb{R}^3\), by Cauchy-Schwarz,
\[
\int_{|x-y| \leq r} \frac{\rho_k(y)}{|x-y|} dy \leq \left( \int_{|x-y| \leq r} \rho_k(y) dy \right)^{1/2} \left( \int_{|x-y| \leq r} \frac{\rho_k(y)}{|x-y|} dy \right)^{1/2}.
\] (31)
On the right hand side of \((31)\), the first factor vanishes uniformly in \(x\) in the limit \(k \to \infty\), by the assumption that \((\rho_k)\) is vanishing. The second factor is bounded uniformly in \(x\) because of Lemma \(A.1\) and the estimate
\[
\int \frac{\rho_k(y)}{|x-y|^2} dy = \frac{N}{r} \sum_{j=1}^{N} \int \frac{\Psi_k(x_1, \ldots, x_N)}{|x-x_j|^2} dx_1 \ldots dx_N \leq 4 \|\Psi_k\|^2_{Q,N,A}.
\] (32)
Here we used the Hardy and diamagnetic inequalities. As we have now shown that \((31)\) vanishes uniformly in \(x\) in the limit \(k \to \infty\), we conclude, combining \((29)\) - \((31)\), that \(D(\rho_k) \to 0\) as \(k \to \infty\) because \(r > 0\) may be chosen arbitrarily large in \((29)\). \(\square\)

**Proposition 3.2.** Suppose that \((11)\) holds and let \((\Psi_k)\) be a minimizing sequence whose densities \(\rho_k = \rho_{\Psi_k}\) have the properties of Proposition \(2.2\) (ii). Then there exists a subsequence of \(\rho_k\), denoted by \(\rho_k\) as well, and a positive number \(d > 0\) such that for all \(\varepsilon > 0\) small enough there exists a function \(J_\varepsilon \in C^\infty_0(\mathbb{R}^3 \times [0,1])\) symmetric with respect to exchange of particle coordinates, such that for all \(k \geq k_0(\varepsilon)\)
\[
H^N_{\rho_k} \geq E^N_{\rho_k} + d(1 - \tau_{y_k}J_\varepsilon - N(2\sqrt{\varepsilon}C + \varepsilon N) - 2^N(\varepsilon N)^2,
\] (33)
where \(y_k = y_k(\varepsilon)\) is given by Proposition \(2.2\) (ii), \(\tau_{y_k}J_\varepsilon(x_1, \ldots, x_N) := J_\varepsilon(x_1 - y_k, \ldots, x_N - y_k)\) and \(C := 2 \sup \|\Psi_k\|_{Q,N,A} \infty\) (see Lemma \(A.1\)). If the sequence \((\rho_k)\) is concentrated, i.e. if \(\lambda = N\) in Proposition \(2.2\) (ii), then we may choose \(d = \Delta E^N := \min \{E^k_{\Psi_T} + E^{N-k}_{\Psi_T} | k = 1, \ldots, N - 1 \} - E^N_{\Psi_T}\).

We fix \(\varepsilon > 0\) and \((\Psi_k)\) as described in Proposition \(3.2\). Let \((y_k)\) be the corresponding sequence provided by Proposition \(2.2\) (ii). After the translations \(\Psi_k \mapsto T_{y_k} \Psi_k\) defined by Equation \((11)\) we may assume that the densities of \((\Psi_k)\) have the properties of Proposition \(2.2\) (ii) with \(y_k = 0\). It thus remains to prove Proposition \(3.2\) in the case \(y_k = 0\). As a preparation we will first establish the following two lemmas.

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Lemma 3.3 (Partition of unity). Let $\varepsilon$ and $\Psi_k$ be as explained above. Let also $\rho_k = \rho_{\Psi_k}$ and $\rho_{k,1}$ be as in Proposition 2.2 (ii). Then there exist $k_0 \geq 1$ and non-negative functions $j_1, j_2 : \mathbb{R}^3 \to \mathbb{R}$ with

$$0 \leq j_1, j_2 \leq 1, \quad j_1^2 + j_2^2 = 1, \quad \|\nabla j_i\|_{L^\infty} \leq \varepsilon, \quad \text{supp } j_1 \subset B(0, R_\varepsilon + \frac{3}{\varepsilon}),$$

such that for all $k \geq k_0$,

$$\text{dist}(\text{supp } \rho_{k,i}, \text{supp } j_{3-i}) \geq \frac{1}{\varepsilon}, \quad i = 1, 2.$$  

(35)

If $a = (a_1, \ldots, a_N) \in \{1, 2\}^N$, then the functions

$$J_a(x_1, \ldots, x_N) := \prod_{j=1}^N j_{a_j}(x_j)$$

have the following properties:

$$0 \leq J_a \leq 1, \quad \sum_{a \in \{1,2\}^N} J_a^2 = 1, \quad \|\nabla J_a\|_{L^\infty} \leq \varepsilon N.$$  

(37)

Proof. It is an elementary exercise to construct non-negative functions $f_1, f_2 \in C^\infty(\mathbb{R})$ with $\sup_x |f_i'(x)| \leq 1$, $f_1^2 + f_2^2 = 1$, $f_1 = 1$ on $(-\infty, 1]$ and $f_2 = 1$ on $[3, \infty)$. Let

$$j_i(x) = f_i(||x| - R_\varepsilon\varepsilon).$$

Using the properties of $f_1, f_2$ and the fact that $P_k(\varepsilon) \geq R_\varepsilon + 4\varepsilon^{-1}$ for $k$ large enough, see Proposition 2.2 (ii), one easily verifies that $j_1, j_2$ have the desired properties. \(\square\)

Lemma 3.4. Let $\varepsilon$ and $(\Psi_k)$ be as in Lemma 3.3 and $C := 2\sup \|\Psi_k\|_{Q_{N,A}}$ as in Proposition 2.2. If $\rho_k, \rho_{k,1}$ are given by Proposition 2.2 (ii), then for $k$ large enough,

$$V_{\rho_k} - V_{\rho_{k,1}} - V_{\rho_{k,2}} \leq \sqrt{\varepsilon} C,$$

$$\text{(38)}$$

$$\text{(V}_{\rho_k} - V_{\rho_{k,1}})j_i^2 \leq (\sqrt{\varepsilon} C + \varepsilon N)j_i^2, \quad i = 1, 2.$$  

(39)

Proof. By the definitions of $V_{\rho_k}, V_{\rho_{k,1}},$ and $V_{\rho_{k,2}}$, we have

$$V_{\rho_k} - V_{\rho_{k,1}} - V_{\rho_{k,2}} = (\rho_k - \rho_{k,1} - \rho_{k,2}) * \frac{1}{|\cdot|},$$

where $0 \leq \rho_k - \rho_{k,1} - \rho_{k,2} \leq \rho_k$. Hence, by Cauchy-Schwarz, (32), and (33),

$$\|V_{\rho_k} - V_{\rho_{k,1}} - V_{\rho_{k,2}}(x)\| \leq \left(\int \frac{\rho_k(y)}{|x-y|^2} \, dy\right)^{1/2} \left(\int (\rho_k - \rho_{k,1} - \rho_{k,2}) \, dy\right)^{1/2} \leq C\sqrt{\varepsilon}.$$  

To prove (38), by (32) it suffices to show that $V_{\rho_{k,3-i}}j_i^2 \leq \varepsilon N j_i^2$. This easily follows from (33) and $\|\rho_{k,3-i}\|_{L^1} \leq \|\rho_k\|_{L^1} = N$. \(\square\)

Proof of Proposition 3.2. In this proof we shall tacitly assume that $k$ is large enough so that the statements of the previous lemmas apply. By the IMS localization formula [5],

$$H_{\rho_k}^N = \sum_{a \in \{1,2\}^N} J_a H_{\rho_k}^N J_a - \sum_{a \in \{1,2\}^N} |\nabla J_a|^2.$$  

(40)
We will now estimate the terms $J_a H_{\rho_k}^N J_a$ from below.

1st Case: $a$ has $n$ ones and $N-n$ twos, $0 < n < N$. We may assume without loss of generality that $a = (1, \ldots, 1, 2, \ldots, 2)$. From $\rho_k \geq \rho_{k,1} + \rho_{k,2}$ it follows that
\begin{equation}
D(\rho_k) \geq D(\rho_{k,1}) + D(\rho_{k,2}).
\end{equation}
This, together with (39) and (28) implies that
\begin{equation}
J_a H_{\rho_k}^N J_a \geq J_a(H_{\rho_{k,1}}^n + H_{\rho_{k,2}}^{N-n})J_a - N(\sqrt{\varepsilon}C + \varepsilon N)J_a^2,
\end{equation}
\begin{equation}
\geq (E_{PT}^n + E_{PT}^{N-n})J_a^2 - N(\sqrt{\varepsilon}C + \varepsilon N)J_a^2.
\end{equation}
Note that $H_{\rho_{k,1}}^n$ acts on the coordinates labeled by $1, \ldots, n$, while $H_{\rho_{k,2}}^{N-n}$ acts on the ones labeled by $n + 1, \ldots, N$. Moreover, $J_a \mathcal{H}_N \subset \mathcal{H}_n \otimes \mathcal{H}_{N-n}$ by construction of $J_a$.

2nd case: $a = (2, \ldots, 2)$, i.e., only twos. By (39) and (11),
\begin{equation}
J_a H_{\rho_k}^N J_a \geq J_a(D(\rho_{k,1}) + H_{\rho_{k,2}}^N)J_a - N(\sqrt{\varepsilon}C + \varepsilon N)J_a^2.
\end{equation}
By (28) we have $H_{\rho_{k,2}}^N \geq E_{PT}^N$ and by Lemma 4.1 there exists a constant $\gamma > 0$ such that
\begin{equation}
D(\rho_{k,1}) \geq \gamma, \quad \text{for } \varepsilon \text{ small enough}.
\end{equation}
It follows that, for $\varepsilon$ small enough,
\begin{equation}
J_a H_{\rho_k}^N J_a \geq (E_{PT}^n + \gamma)J_a^2 - N(\sqrt{\varepsilon}C + \varepsilon N)J_a^2.
\end{equation}

3rd case: $a = a_0 := (1, \ldots, 1)$. Since $H_{\rho_k}^N \geq E_{PT}^n$, we have
\begin{equation}
J_{a_0} H_{\rho_k}^N J_{a_0} \geq E_{PT}^N J_{a_0}^2.
\end{equation}
Combining the results (12), (45) and (10) from the three cases above with (47) and (44) we obtain (43) with $J_\varepsilon = J_{a_0}^2$ and $d = \min\{\gamma, \Delta E^N\}$, which is positive due to the binding assumption (10).

In the case $\lambda = N$ we may improve our bound in the second case to get $d = \Delta E^N$. Indeed
\begin{equation}
H_{\rho_{k,2}}^N \geq \sum_{j=1}^N (D_{A,j}^2 - V_{\rho_{k,2}}(x_j)) \geq NE_{PT}^1 - NC\sqrt{\varepsilon},
\end{equation}
because $D_{A,j}^2 \geq E_{PT}^1$ and $V_{\rho_{k,2}}(x) \leq C||\rho_{k,2}||_{L^1}^{1/2} \leq C\sqrt{\varepsilon}$ by the Cauchy-Schwarz, Hardy and diamagnetic inequalities. Here we used $\lambda = N$ and (11). Since $NE_{PT}^1 \geq E_{PT}^1 + E_{PT}^{N-1}$ we conclude that
\begin{equation}
J_a H_{\rho_k}^N J_a \geq (E_{PT}^n + \Delta E^N)J_a^2 - N(\sqrt{\varepsilon}2C + \varepsilon N)J_a^2,
\end{equation}
which we use in place of (45).

\section{Existence of a minimizer and exponential decay}

In this Section we prove parts (a),(c) of Theorem 2.1 and then we prove Theorem 1.2. The part (b) of Theorem 2.1 will be proved in the next Section.

\textbf{Lemma 4.1.} Assume that (10) holds. Then, there exists a minimizing sequence $(\Phi_k)$ with the following property: for every $\delta > 0$ there exists $P > 0$ such that
\begin{equation}
\liminf_{k \to \infty} \int_{B(0,P)} |\Phi_k|^2 \geq 1 - \delta.
\end{equation}
Proof. Without loss of generality we may assume that \( \delta < 1/2 \). By Lemma 3.1 there exists a minimizing sequence \((\Psi_k)\) for which the sequence \((\rho_k)\) of the associated densities satisfies the properties of Proposition 2.2 (ii) and hence Proposition 3.2 applies to \((\Psi_k)\). The operator inequality (33) implies that

\[
\langle \Psi_k, H^N_{\rho_k} \Psi_k \rangle \geq E^N_{PT} + d - d(\Psi_k, \tau_{y_k} J_\varepsilon \Psi_k) - N(2\sqrt{\varepsilon}C + \varepsilon N) - 2^N(\varepsilon N)^2.
\]

Upon rearranging this inequality, it follows from (24) that

\[
\liminf_{k \to \infty} \langle \Psi_k, \tau_{y_k} J_\varepsilon \Psi_k \rangle \geq 1 - \frac{N}{d} \left( 2C\sqrt{\varepsilon} + \varepsilon N \right) - \frac{2^N}{d} (\varepsilon N)^2 \geq 1 - \delta,
\]

for \( \varepsilon \) small enough. Since \( J_\varepsilon \) is compactly supported and \( 0 \leq J_\varepsilon \leq 1 \) it follows that

\[
\liminf_{k \to \infty} \int_{B(y_k, R)} |\Psi_k|^2 \geq 1 - \delta,
\]

(49)

where \( R \) and \( y_k \) depend on \( \varepsilon \) and hence on \( \delta \). Using an argument of Lions (see [16]) we shall now replace \((y_k)\) by another sequence \((y'_k)\) that is independent of \( \delta \) such that (49) still holds after enlarging \( R \). Let \( R' \) and \( (y'_k) \) be determined in the same way as \( R \) and \( (y_k) \) in the case \( \delta = 1/2 \). That is,

\[
\liminf_{k \to \infty} \int_{B(y'_k, R')} |\Psi_k|^2 \geq \frac{1}{2},
\]

Since \( \|\Psi_k\| = 1 \) and since \( 1 - \delta > 1/2 \), by assumption, the balls \( B(y, R) \) and \( B(y_k, R') \) must overlap for \( k \) large enough. It follows that

\[
\liminf_{k \to \infty} \int_{B(y'_k, R' + 2R)} |\Psi_k|^2 \geq 1 - \delta.
\]

(50)

The sequence \( \Phi_k = T_{y'_k} \Psi_k \) is minimizing and it satisfies (18) with \( P = R' + 2R \). \( \square \)

Proof of Theorem 2.1 (a), (c) (existence of a minimizer). Let \((\Phi_k)\) be given by Lemma 4.1. By Lemma 4.1 part (b), \((\Phi_k)\) is bounded in \( Q_{N,A} \) and hence, after passing to a subsequence, we may assume that \( \Phi_k \to \Phi \in Q_{N,A} \) weakly in \( Q_{N,A} \). Since \( A \) is locally bounded it follows that \( \Phi_k \to \Phi \) locally in \( H_N \) and weakly in \( H_N \). Hence, by Lemma 4.1 for every \( \delta > 0 \) there exists \( P > 0 \) such that

\[
1 = \lim_{k \to \infty} \|\Phi_k\|^2 \geq \|\Phi\|^2 \geq \int_{B(0, P)} |\Phi|^2 dx = \liminf_{k \to \infty} \int_{B(0, P)} |\Phi_k|^2 dx \geq 1 - \delta.
\]

It follows that \( \|\Phi\| = 1 \) and hence that \( \Phi_k \to \Phi \) strongly in \( H_N \). Since \( \Phi_k \to \Phi \in Q_{N,A} \) weakly in \( Q_{N,A} \), the parts (a) and (c) of Theorem 2.1 follow from Lemma A.1 (c). \( \square \)

Proof of Theorem 1.2. This proof is based on Lemma 2.4 which clearly holds for any \( \alpha > 0 \). Let \( \Psi \) be a minimizer with density \( \rho \). By Lemma 2.4 \( H^N_\rho \geq E^N_{PT} \) and \( \langle \Psi, H^N_\rho \Psi \rangle = E^N_{PT} \). It follows that \( \Psi \) belongs to the domain of the Friedrichs’ extension of \( H^N_\rho \) and that \( H^N_\rho \Psi = E^N_{PT} \Psi \). This equation agrees with the Schrödinger equation (5) upon subtracting \( D(\rho) \Psi \) from both sides.

By [1] eigenvalues of \( H^N_\rho \) below

\[
\Sigma := \lim_{R \to \infty} \left( \inf_{\Phi \in D_R, \|\Phi\| = 1} \langle \Phi, H^N_\rho \Phi \rangle \right),
\]

\[
D_R := \{ \Phi \in Q_{N,A} \mid \Phi(x) = 0 \text{ for } |x| < R \},
\]

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are associated with exponentially decaying eigenfunctions. This means that $e^{\beta |\cdot|} \Psi \in L^2$ provided $\beta^2 < \Sigma - E_{PT}^N$. Applying Proposition 3.2 to the constant minimizing sequence $\Psi_k = \Psi$, for which the sequence of densities $\rho_k = \rho$ obviously is concentrated, we see that

$$H_\rho^N \geq E_{PT}^N + \Delta E^N (1 - J_\varepsilon) - O(\sqrt{\varepsilon}),$$

(51)

where $J_\varepsilon$ is compactly supported and $\varepsilon$ is small enough. Since $\varepsilon$ can be arbitrarily small we obtain that $\Sigma \geq E_{PT}^N + \Delta E^N$, which concludes the proof.

\[\square\]

5 Proof of Binding

In this Section we prove Theorem 2.1 part (b). To explain the main ideas in their pure form, without the difficulties due to the Pauli-principle, we first do the proof in the case of Bolzons, i.e., for Pekar-Tomasevich functional defined on $L^2(\mathbb{R}^{3N})$. Thereafter we shall describe the modifications necessary to accommodate fermions and bosons.

The case of Bolzons. The functionals $\mathcal{E}^1, \ldots, \mathcal{E}^{N-1}$ have minimizers $\Phi_1, \ldots, \Phi_{N-1}$ by assumption. Assuming that

$$E_{PT}^N = E_{PT}^k + E_{PT}^{N-k}$$

(52)

for some $k \in \{1, \ldots, N-1\}$ we shall prove in the Steps 1 and 2 below, that on the one hand $\Phi_k \otimes \Phi_{N-k}$ is a minimizer of $\mathcal{E}^N$, on the other hand it cannot satisfy the corresponding Euler-Lagrange equation. Hence the assumption (52) must be wrong.

Step 1: $\Phi_k \otimes \Phi_{N-k}$ is a minimizer of $\mathcal{E}^N$, that is

$$\mathcal{E}^N(\Phi_k \otimes \Phi_{N-k}) = E_{PT}^N.$$  

(53)

From the definitions of the density, $\rho_{\Phi}$, and interaction energy $D(\rho_{\Phi})$ associated with any $\Psi$ (see (5), (5)), we easily see that

$$\rho_{\Phi_k \otimes \Phi_{N-k}} = \rho_{\Phi_k} + \rho_{\Phi_{N-k}}$$

(54)

and

$$D(\rho_{\Phi_k \otimes \Phi_{N-k}}) = D(\rho_{\Phi_k}) + D(\rho_{\Phi_{N-k}}) + 2D(\rho_{\Phi_k}, \rho_{\Phi_{N-k}}),$$

(55)

where

$$2D(\rho_{\Phi_k}, \rho_{\Phi_{N-k}}) = \langle \Phi_k \otimes \Phi_{N-k}, \sum_{i=1}^{N} \sum_{j=k+1}^{N} \frac{1}{|x_i - x_j|} \Phi_k \otimes \Phi_{N-k} \rangle.$$  

(56)

From (55), (56), and the assumption (52) it follows that

$$\mathcal{E}^N(\Phi_k \otimes \Phi_{N-k}) = \mathcal{E}^k(\Phi_k) + \mathcal{E}^{N-k}(\Phi_{N-k}) = E_{PT}^k + E_{PT}^{N-k} = E_{PT}^N.$$  

(57)

Step 2: $\Phi_k \otimes \Phi_{N-k}$ does not solve the Euler Lagrange equation of $\mathcal{E}^N$. Suppose that $\Phi_k \otimes \Phi_{N-k}$ solves the Euler-Lagrange equation

$$\left( \sum_{j=1}^{N} D_{A,x_j}^2 + \sum_{i<j}^{N} \frac{1}{|x_i - x_j|} - \sum_{j=1}^{N} V_{\rho_{\Phi_k \otimes \Phi_{N-k}}}(x_j) - \lambda \right) \Phi_k \otimes \Phi_{N-k} = 0,$$

(57)

for some $\lambda \in \mathbb{R}$. Since $\Phi_k$ and $\Phi_{N-k}$ are minimizers of $\mathcal{E}^k$ and $\mathcal{E}^{N-k}$, respectively, they satisfy the Euler-Lagrange equations

$$\left( \sum_{j=1}^{k} D_{A,x_j}^2 + \sum_{i<j}^{k} \frac{1}{|x_i - x_j|} - \sum_{j=1}^{k} V_{\rho_{\Phi_k}}(x_j) - \lambda_1 \right) \Phi_k = 0,$$

(58)
and
\[
\left( \sum_{j=k+1}^{N} D_{A,j}^2 + \sum_{k+1 \leq i < j}^{N} \frac{1}{|x_i - x_j|} - \sum_{j=k+1}^{N} V_{\rho \Phi_{N-k}}(x_j) - \lambda_2 \right) \Phi_{N-k} = 0, \tag{59}
\]
with \(\lambda_1, \lambda_2 \in \mathbb{R}\). Note that, by (54),
\[
V_{\rho \Phi_k \otimes \Phi_{N-k}} = V_{\rho \Phi_k} + V_{\rho \Phi_{N-k}}. \tag{60}
\]

Taking tensor products of the Equations (58) and (59) with \(\Phi_N\) we shall apply smooth space cut-offs at distance \(\psi\) and let
\[
\text{time we may assume, after suitable magnetic translations of } \Phi_k \text{, respectively,}
\]
changing from one equation to another. Suppose that for some \(\lambda\) with
\[
\lambda \in \mathbb{R},
\]
origin and then move \(\Phi_k\) of the resulting
\[
\text{with (61), which completes the proof of Step 2.}
\]

The strict positivity of the lower bound (62), and the inequality (63) are in contradiction with (61), which completes the proof of Step 2.

The case of fermions. In the case of fermions, the tensor product \(\Phi_k \otimes \Phi_{N-k}\) of the minimizers \(\Phi_k\) and \(\Phi_{N-k}\) in Step 1 must be antisymmetrized and normalized. The density of the resulting \(N\)-particle state is not the sum of the densities of \(\Phi_k, \Phi_{N-k}\). In order to regain an analogue of (54) we shall apply smooth space cut-offs at distance \(R\) from the origin and then move \(\Phi_{N-k}\) by a distance of \(3R\). These cut-off minimizers, as well as their antisymmetrized tensor product, are approximate minimizers satisfying approximate Euler-Lagrange equations, the error being exponentially small. But such an exponentially small error is not compatible with the power laws decay of the Coulomb interaction between the first \(k\) and the last \(N-k\) particles.

We now proceed with the details. We use \(c, C\) to denote positive constants possibly changing from one equation to another. Suppose that for some \(k\)
\[
E_{PT}^N = E_{PT}^k + E_{PT}^{N-k}, \tag{64}
\]
and let \(\psi_m\) be a minimizer of \(\mathcal{E}_m\), \(m \in \{1, \ldots, N-1\}\). Let \(f \in C^\infty(\mathbb{R}; [0, 1])\) with \(f(s) = 1\) if \(s \leq -1\) and \(f(s) = 0\) if \(s \geq 0\), and let \(\chi_R(x) := f(|x| - R)\), a smoothed characteristic function of the ball \(B(0, R) \subset \mathbb{R}^3\). We define
\[
\phi_{m} = \frac{\psi_m \chi \overset{\otimes}{\chi}_R}{\|\psi_m \chi \overset{\otimes}{\chi}_R\|}.
\]

Let \(y \in \mathbb{R}^3\) with \(|y| = 3R\). Recall that \(T_y \phi_{N-k}\) denotes a magnetic translation of \(\phi_{N-k}\) as defined in (11). Due to the exponential decay of the minimizers \(\psi_k, \psi_{N-k}\) and their gradients and Laplacians we obtain that \(\phi_k, T_y \phi_{N-k}\) are approximate minimizers and satisfy
respectively the Euler-Lagrange equations of $\mathcal{E}^{k}, \mathcal{E}^{N-k}$ up to an exponentially small error. More precisely,

$$
(H^{N-k}_{\rho_{\phi_k}} - E^{N-k}_{P T})\phi_k = O_{Q_{N,A}}(e^{-cR}), \tag{65}
$$

$$
(H^{N-k}_{\rho_{T y\phi_{N-k}}} - E^{N-k}_{P T})T_y\phi_{N-k} = O_{Q_{N-k,A}}(e^{-cR}), \tag{66}
$$

where $O_{Q_{m,A}}$ refers to the $Q_{m,A}$ norm. Since $\mathcal{E}^m(\phi) = \langle \phi, H^m_{\rho_\phi} \phi \rangle$ it follows that

$$
\mathcal{E}^{k}(\phi_k) = E^{k}_{P T} + O(e^{-cR}),
$$

$$
\mathcal{E}^{N-k}(T_y\phi_{N-k}) = E^{N-k}_{P T} + O(e^{-cR}). \tag{67}
$$

Equations (65) and (66) correspond to (58) and (59) in the boltzonic case, note however the irrelevant constants $D_{\rho_{\phi_k}}$ and $D_{\rho_{T y\phi_{N-k}}}$ in the Hamiltonians defined by (21).

Let now $\Phi := P_k(\phi_k \otimes T_y\phi_{N-k})$. Here $P_k := \sqrt{\binom{N}{k}} P_A$ where $P_A$ denotes the projection onto the completely antisymmetric functions with respect to permutations of pairs of positions and spins. The factor in front of $P_A$ is chosen so that $\Phi$ is also normalized. Since the densities of $\phi_k, T_y\phi_{N-k}$ have disjoint supports we obtain that $\rho_\Phi = \rho_{\phi_k} + \rho_{T y\phi_{N-k}}$ which similarly to the case of Boltzons implies that

$$
\mathcal{E}^N(\Phi) = \mathcal{E}^{k}(\phi_k) + \mathcal{E}^{N-k}(T_y\phi_{N-k}) \tag{68}
$$

and that

$$
V_{\rho_\Phi} = V_{\rho_{\phi_k}} + V_{\rho_{T y\phi_{N-k}}} \tag{69}
$$

From (67) and (68) we obtain that

$$
\mathcal{E}^N(\Phi) = E^{k}_{P T} + E^{N-k}_{P T} + O(e^{-cR}). \tag{70}
$$

We show now that $\Phi$ satisfies an approximate Euler Lagrange equation. We take the tensor product of both sides of (65) with $T_y\phi_{N-k}$. Similarly, we take tensor product of both sides of (66) with $\phi_k$. By adding the resulting equations and then adding $J_k(\phi_k \otimes T_y\phi_{N-k})$ on both sides, where

$$
J_k(x_1, ..., x_N) := \sum_{i=1}^{k} \sum_{j=k+1}^{N} \frac{1}{|x_i - x_j|} - \sum_{i=1}^{k} V_{\rho_{T y\phi_{N-k}}}(x_i) - \sum_{j=k+1}^{N} V_{\rho_{\phi_k}}(x_j), \tag{71}
$$

we arrive at

$$
(H^{N}_{\rho_\phi} - c_R)\phi_k \otimes T_y\phi_{N-k} = J_k(\phi_k \otimes T_y\phi_{N-k}) + O_{Q_{N,A}}(e^{-cR}), \tag{72}
$$

where $c_R := E^{k}_{P T} + E^{N-k}_{P T} - 2D(\rho_{\phi_k}, \rho_{T y\phi_{N-k}})$ depends on $R$. We have used (21) and (59). The fact that the supports of $\phi_k, T_y\phi_{N-k}$ have distance $R$ in each particle coordinate implies that

$$
|J_k| = O(R^{-1}), \quad |\nabla J_k| = O(R^{-2}), \quad \text{uniformly in } (x_1, ..., x_N) \in \text{supp } \phi_k \otimes T_y\phi_{N-k}. \tag{73}
$$

Applying the antisymmetrization $P_k$ to both sides of (72) and using (73) as well as the symmetry of $H^{N}_{\rho_\phi}$ with respect to the $N$ particles, we arrive at

$$
\|H^{N}_{\rho_\phi} - c_R\|_{Q_{N,A}} = O(R^{-1}). \tag{74}
$$

We are now going to improve this error estimate by changing the Lagrange multiplier by $O(R^{-1})$. To this end we write

$$
H^{N}_{\rho_\phi} \Phi = \lambda R \Phi + f_R, \quad \text{with } \langle f_R, \Phi \rangle = 0. \tag{75}
$$
First observe that (74) and (75) imply that \( \lambda_R = c_R + O(R^{-1}) \) and therefore
\[
\|f_R\|_{Q_{N,A}} = O(R^{-1}). \tag{76}
\]
On the other hand using (75) twice we obtain that
\[
\langle f_R, f_R \rangle = \langle f_R, H^N_{\rho_p} \Phi \rangle = \langle f_R, (H^N_{\rho_p} - E^N_{PT})\Phi \rangle.
\]
Recall that \( (H^N_{\rho_p} - E^N_{PT})|_{\mathcal{H}_N} \geq 0 \) (see Lemma 2.4) and \( f_R, \Phi \in \mathcal{H}_N \). Hence, by Cauchy-Schwarz for positive (semi-)definite quadratic forms we find
\[
\|f_R\|^2 \leq \langle f_R, (H^N_{\rho_p} - E^N_{PT})f_R \rangle^{1/2} \langle \Phi, (H^N_{\rho_p} - E^N_{PT})\Phi \rangle^{1/2}.
\]
This estimate together with \( E^{(N)}(\Phi) = \langle \Phi, H^N_{\rho_p} \Phi \rangle \) (see Lemma 2.4, (64), (70) and (76) implies that
\[
\|(H^N_{\rho_p} - \lambda_R)\Phi\| = \|f_R\| = O(e^{-cR}). \tag{77}
\]
By definition of \( \Phi \), the equations (75) and (76) imply that
\[
\|(H^N_{\rho_p} - \lambda_R)\phi_k \otimes T_y\phi_{N-k}\| = O(e^{-cR}), \tag{78}
\]
because \( P_k \) acts isometrically on the left hand side of (78) and commutes with \( H^N_{\rho_p} \). From (72) and (78) it follows that
\[
\|(J_k + c_R - \lambda_R)\phi_k \otimes T_y\phi_{N-k}\| = O(e^{-cR}). \tag{79}
\]
This is in contradiction with Lemma 5.1 below. Hence, our assumption (64) must be wrong and (10) is proved.

**Lemma 5.1.** If the minimizers \( \psi_m, m \in \{k, N-k\} \) are chosen so that \( \int u\rho_{\psi_m}(u)du = 0 \), then there exists a constant \( C > 0 \) such that
\[
\inf_{M \in \mathbb{R}} \|(J_k + M)\phi_k \otimes T_y\phi_{N-k}\| \geq \frac{C}{R^3}
\]
(recall that \( |y| = 3R \)). In particular, (79) does not hold.

**Proof.** Let \( M \in \mathbb{R} \) be arbitrary. Recall that \( T_y\phi_{N-k} \) by definition is a magnetic translation by \( y \) with \( |y| = 3R \) of \( \phi_{N-k} \). By a change of variables for the particles with labels in \( \{k+1, \ldots, N\} \) we find that
\[
\|(J_k + M)\phi_k \otimes T_y\phi_{N-k}\| = \|I_R\|,
\]
where
\[
I_R := (J_k + M)\phi_k \otimes \phi_{N-k}
\]
and
\[
\tilde{J}_k(z_1, \ldots, z_N) := \sum_{i=1}^{k} \sum_{j=k+1}^{N} \frac{1}{|z_i - z_j + y|} \sum_{i=1}^{k} V_{\rho_{N-k}}(z_i + y) - \sum_{j=k+1}^{N} V_{\rho_{N-k}}(z_j - y). \tag{82}
\]
By (80) it remains to prove that there exists \( C > 0 \) independent of \( M \) so that
\[
\|I_R\| \geq \frac{C}{R^3}. \tag{83}
\]
From the assumption of the lemma and the exponential decay of \( \psi_m \) we obtain for \( \phi_m \) that

\[
\int u\rho_{\phi_m}(u)du = O(e^{-cR}), \quad \text{for } m \in \{k, N - k\}.
\]  

(84)

By normalization of \( \psi_m \) and the definition of \( \phi_m \) we may choose \( d > 0 \) such that

\[
\int_{B_d} dz_1 \ldots dz_N |\phi_k(z_1, \ldots, z_k)|^2 |\phi_{N-k}(z_{k+1}, \ldots, z_N)|^2 \geq \frac{1}{2},
\]  

(85)

for all \( R \geq d + 1 \) where \( B_d := B(0, d)^N \subset \mathbb{R}^{3N} \). To prove (83), and thus the lemma, it clearly suffices to show that

\[
\|I_{R\chi_{B_d}}\| \geq \frac{C}{R^3}, \quad C > 0,
\]  

(86)

where \( C \) is independent of \( M \).

We are going to expand (82) in powers of \( \frac{1}{|y|} \). To this end we first remark that

\[
\frac{1}{|w - y|} = \frac{1}{|y|} + \frac{\hat{g} \cdot w}{|y|^2} + \frac{3(\hat{g} \cdot w)^2 - |w|^2}{2|y|^3} + O\left(\frac{|w|^3}{|y|^4}\right), \quad \text{uniformly in } |w| \leq 2R,
\]  

(87)

where \( \hat{g} = y/|y| \). Using this, (84), \( \text{supp}\, \rho_{\phi_m} \subset B(0, R) \) and the definition of \( V_\rho \) (see (20)) we obtain for \( |z_i|, |z_j| \leq d \)

\[
V_{\rho_{\phi_k}}(z_j - y) = k \left( \frac{1}{|y|} + \frac{\hat{g} \cdot z_j}{|y|^2} + \frac{3(\hat{g} \cdot z_j)^2 - |z_j|^2}{2|y|^3} \right) + O(R^{-4}),
\]  

(88)

\[
V_{\rho_{\phi_{N-k}}}(z_i + y) = (N - k) \left( \frac{1}{|y|} - \frac{\hat{g} \cdot z_i}{|y|^2} + \frac{3(\hat{g} \cdot z_i)^2 - |z_j|^2}{2|y|^3} \right) + O(R^{-4}),
\]  

(89)

where

\[
f_m(\hat{x}) := \int \rho_{\phi_m}(u) \frac{3(\hat{x} \cdot u)^2 - |u|^2}{2} du.
\]  

(90)

Recall that \( \phi_m \) depends on \( R \) and hence the exponential decay of \( \psi_m \) is needed for establishing the bound \( O(R^{-4}) \). Using (87) again we obtain

\[
\frac{1}{|z_i - z_j + y|} = \left( \frac{1}{|y|} + \frac{\hat{g} \cdot (z_j - z_i)}{|y|^2} + \frac{3(\hat{g} \cdot (z_j - z_i))^2 - |z_j - z_i|^2}{2|y|^3} \right)
\]  

\[+ O\left(\frac{1}{|y|^4}\right), \quad \forall z_i, z_j \in B(0, d).
\]  

(91)

Inserting (88), (89) and (90) into (81) (see also (82)) an elementary but somewhat lengthy calculation gives that

\[
I_{R\chi_{B_d}}(z_1, \ldots, z_N) = \frac{1}{|y|^3} \left( \sum_{i=1}^{k} \sum_{j=k+1}^{N} (z_i \cdot z_j - 3(z_i \cdot \hat{g})(z_j \cdot \hat{g})) + C_{y,M} \right)
\times (\phi_k \otimes \phi_{N-k}) \chi_{B_d}(z_1, \ldots, z_N) + O(R^{-4}),
\]  

(92)

where \( C_{y,M} = -(N - k)f_k(\hat{g}) - kf_{N-k}(\hat{g}) - k(N - k)|y|^2 + M|y|^3 \) depends on \( y \) and \( M \) only.

We recognize in (92) the interaction energy \( (z_i \cdot z_j - 3(z_i \cdot \hat{g})(z_j \cdot \hat{g})) / |y|^3 \) of two dipoles \( z_i \) and \( z_j \) separated by \( y \). Let

\[
L(\hat{g}, D) = \int_{B_d} dz_1 \ldots dz_N \left| \sum_{i=1}^{k} \sum_{j=k+1}^{N} (z_i \cdot z_j - 3(z_i \cdot \hat{g})(z_j \cdot \hat{g})) + D \right|
\times \phi_k(z_1, \ldots, z_k) \phi_{N-k}(z_{k+1}, \ldots, z_N)^2.
\]  

(93)
Then, by (92),
\[ \|I_{R\mathbb{R}^d}\| = \frac{1}{|y|^3} L(\hat{y}, C_{y,M})^{1/2} + O(R^{-4}), \]  
and it remains to show that there exists a constant \( C > 0 \) such that
\[ L(\hat{y}, D) \geq C, \quad \forall \hat{y}, D. \]  
This estimate together with (94) concludes the proof of (86) and therefore of Lemma 5.1.

To prove (95) we first establish that \( L(\hat{y}, D) \) is everywhere positive. To this end we fix \( y, D \) and we consider the function
\[ f(z_1, z_2, ..., z_N) = \left( \sum_{i=1}^{k} z_i \right) \cdot \left( \sum_{j=k+1}^{N} z_j \right) - 3 \left( \sum_{i=1}^{k} z_i \cdot \hat{y} \right) \left( \sum_{j=k+1}^{N} z_j \cdot \hat{y} \right) + D, \]
which is part of the integrand in (93). One can show that \( f(z_1, z_2, ..., z_N) \neq 0 \) almost everywhere, which together with (85) implies that
\[ L(\hat{y}, D) > 0. \]  
Now we will use a continuity argument to show (95). Since \( f \) is continuous and thus bounded on \( B_d \) it follows, by the dominated convergence theorem, that \( L \) is a continuous function of \( \hat{y}, D \). Moreover, \( \lim_{|D| \to \infty} L(\hat{y}, D) = \infty \). These observations together with (96) and the fact that a continuous function on a compact set attains its minimum give (95).

A Properties of \( E^N \)

Lemma A.1.

(a) The functional \( E^N \) is bounded from below on the set \( S_N := \{ \Psi \in \mathcal{Q}_{N,A} : \| \Psi \| = 1 \} \).

(b) Every minimizing sequence \( (\Psi_k) \) of \( E^N \) on \( S_N \) is bounded in \( \mathcal{Q}_{N,A} \).

(c) If for a minimizing sequence \( (\Psi_k) \) of \( E^N \) we have that \( \Psi_k \to \Psi \) weakly in \( \mathcal{Q}_{N,A} \) and strongly in \( H_N \) then \( \Psi \) is a minimizer of \( E^N \).

Proof. (a),(b) They follow from the Hardy and diamagnetic inequalities. We recall from [13] that the diamagnetic inequality states that if \( \phi \in H^1_A \) then we have that \( |\nabla|\phi(x)| \leq |(D_{A,x} \phi(x), ..., D_{A,x_N} \phi(x))| \), for almost all \( x \in \mathbb{R}^{3N} \). In the case \( N = 1 \) and without spin a detailed proof of parts (a) and (b) of the Lemma is given in [8] and in the general case the argument is similar.

(c) We will now show that if \( \Psi_k \to \Psi \) weakly in \( \mathcal{Q}_{N,A} \) and strongly in \( H_N \) then
\[ E^N(\Psi) \leq \liminf_{k \to \infty} E^N(\Psi_k), \]  
from which we conclude that \( \Psi \) is a minimizer of the Pekar-Tomasevich functional \( E^N \). Indeed, recall that
\[ E^N(\Psi) = \langle \Psi, \left( \sum_{j=1}^{N} D_{A,x_j}^2 + \sum_{i<j} \frac{1}{|x_i - x_j|} \right) \Psi \rangle - D(\rho_\Psi). \]  
Since \( \Psi_k \to \Psi \) weakly in \( \mathcal{Q}_{N,A} \) and \( \| \Psi_k \| = \| \Psi \| = 1 \) we see that
\[ \langle \Psi, \sum_{j=1}^{N} D_{A,x_j}^2 \Psi \rangle \leq \liminf_{k \to \infty} \langle \Psi_k, \sum_{j=1}^{N} D_{A,x_j}^2 \Psi_k \rangle. \]
On the other hand, since $\Psi_k \to \Psi$ weakly in $Q_{N,A}$ and since $|x_i - x_j|^{-1}$ is a bounded operator from $Q_{N,A}$ to $H_N$ we obtain that

$$|x_i - x_j|^{-1}\Psi_k \to |x_i - x_j|^{-1}\Psi,$$ weakly in $H_N$.

Since, moreover, $\Psi_k \to \Psi$ strongly in $H_N$ we conclude that

$$\langle \Psi, |x_i - x_j|^{-1}\Psi \rangle = \lim_{k \to \infty} \langle \Psi_k, |x_i - x_j|^{-1}\Psi_k \rangle.$$ \hspace{1cm} (100)

In addition,

$$D(\rho_\Psi) - D(\rho_k) = D(\rho_\Psi - \rho_k, \rho_\Psi) + D(\rho_k, \rho_\Psi - \rho_k).$$ \hspace{1cm} (101)

We will show that

$$D(\rho_k, \rho_\Psi - \rho_k) \to 0.$$ \hspace{1cm} (102)

Indeed, using (8) and (20) we obtain that

$$D(\rho_k, \rho_\Psi - \rho_k) = \int V_{\rho_k}(\rho_\Psi - \rho_k) \, dx.$$ \hspace{1cm} (103)

But using Lemma A.1 (b) together with (20), (31) with $r = \infty$, and (32) we can prove that

$$\sup_k \|V_{\rho_k}\|_{L^\infty} < \infty.$$ \hspace{1cm} (104)

Since $\Psi_k \to \Psi$ in $H_N$ we obtain that $\|\rho_\Psi - \rho_k\|_{L^1} \to 0$ which together with (103) and (104) implies (102). Similarly,

$$D(\rho_\Psi - \rho_k, \rho_\Psi) \to 0.$$ \hspace{1cm} (105)

Combining (102), (105) and (101) we obtain that

$$D(\rho_\Psi) = \lim_{k \to \infty} D(\rho_k).$$ \hspace{1cm} (106)

The relations (98), (99), (100) and (106) give (97) as desired.

\[\square\]

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