PEKAR'S ANSATZ AND THE GROUND-STATE SYMMETRY OF A BOUND POLARON

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ABSTRACT. We consider a Fröhlich polaron bound in a symmetric Mexican hat-type potential. The ground state is unique and therefore invariant under rotations. However, we show that the minimizers of the corresponding Pekar problem are nonradial. Assuming these nonradial minimizers are unique up to rotation, we prove in the strong-coupling limit that the ground-state electron density converges in a weak sense to a rotational average of the densities of the minimizers.

1. Introduction

In order to develop a theory of dielectric breakdown in semiconductors, H. Fröhlich proposed a model in 1937 of an electron interacting with the quantized optical modes (phonons) of an ionic crystal. Known today as the (Fröhlich) polaron, it is one of the simplest examples of a particle interacting with a quantized field, and perhaps most notably, it has served as a testing ground for Feynman’s path integral formulation of quantum field theory. It is described by the Hamiltonian

\begin{equation}
H_\alpha^V = p^2 - \alpha^2 V(\alpha x) + \int_{\mathbb{R}^3} a_k^\dagger a_k dk - \frac{\sqrt{\alpha}}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \left[ a_k e^{i k \cdot x} + a_k^\dagger e^{-i k \cdot x} \right] \frac{dk}{|k|},
\end{equation}

acting on the Hilbert space \( \mathcal{H} := L^2(\mathbb{R}^3) \otimes \mathcal{F} \) where \( \mathcal{F} := \bigoplus_{n \geq 0} \otimes_n L^2(\mathbb{R}^3) \) is the (symmetric) phonon Fock space. An outstanding idiosyncrasy of the Fröhlich’s polaron is that for all its popularity over the years as a convenient “toy model” for a singularity-free field theory, the electron-phonon interaction term in the Hamiltonian makes it intractable for calculating even the most basic quantities such as the effective mass and the ground-state energy. This computational difficulty has led S.I. Pekar (in a series of collaborations with L.D. Landau, O.F. Tomasevich and others between 1944 and 1950) to derive from Fröhlich’s model a much simpler—albeit nonlinear—effective theory, built entirely on an (unjustified!) Ansatz for the ground-state wave function. Remarkably, Pekar’s effective minimization problem nevertheless yields the exact ground-state energy of the polaron in the strong-coupling limit, \( \alpha \to \infty \). It is therefore natural to conjecture that the ground-state electron density also converges (in a weak sense) to a minimizer of Pekar’s effective problem: after all, this is known to be the case for particular one-dimensional models. In this paper, however, using an intuitive example of a polaron localized in a radial potential, we shall showcase a discrepancy in spherical symmetry between a rotation-invariant Hamiltonian and its unique ground state on the one hand and the corresponding Pekar Ansatz for the wave function on the other. This in turn illustrates that such expected (weak) convergence of the ground state to Pekar’s minimizer is not in general true.

We denote by \( x \in \mathbb{R}^3 \) the electron coordinate and by \( k \in \mathbb{R}^3 \) the phonon mode; \( p = -i \nabla_x \) is the electron momentum, and the electric potential \( V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \) is nonnegative.
and vanishes at infinity and usually arises from an impurity in the crystal; $a_k^\dagger$ and $a_k$ are scalar creation and annihilation operators on $\mathcal{F}$ which satisfy the canonical commutation relation $[a_k, a_{k'}^\dagger] = \delta(k - k')$; and $\alpha > 0$ is the electron-phonon coupling parameter. The ground-state energy of the model is defined to be

$$E^V(\alpha) := \inf \left\{ (\Psi, H^V_\alpha \Psi)_{\mathcal{H}} \mid \|\Psi\|_\mathcal{H} = 1 \right\}.$$  

Any normalized vector $\Omega \in \mathcal{H}$ that achieves the infimum in (1.2) is called a ground-state wave function, and it satisfies the Schrödinger equation $H^V_\alpha \Omega = E^V(\alpha) \Omega$; integrating out its phonon coordinates, one has the electron density $\|\Omega\|^2_F(x)$. Most of the literature is concerned with the translation-invariant (TI-) polaron—i.e., the case where $V \equiv 0$ in (1.1). It was shown in the 1980s that for all values of the coupling parameter $\alpha > 0$, the TI-polaron does not have a ground state (finally settling a decades-long debate on the existence of a delocalization-localization transition). We are instead interested in the case of nonzero $V$, the bound polaron, which has attracted sizable attention (see [Dv1996] and the references therein; in particular, we refer to the rigorous work on pinning transitions by H. Spohn [Sp1986] and H. Löwen [Lw1988a], [Lw1988b]). In contrast to the TI-polaron, under physically natural conditions on the external potential $V$, the Fröhlich Hamiltonian $H^V_\alpha$ has a unique ground state for all $\alpha > 0$. This follows from now-standard techniques developed by F. Hiroshima [Ha2000] and by M. Griesemer, E.H. Lieb and M. Loss [GLL2001] to study the analogous Pauli-Fierz model in quantum electrodynamics (see Appendix). Note that we have added the potential in the scaled form $\alpha^2 V(\alpha x)$ to the Hamiltonian in order for its effect to survive in the limit $\alpha \to \infty$ (see Theorem 3.2 in [GW2013]). We work with the potential

$$V_R \in C^\infty_c(\mathbb{R}^3), \quad 0 \leq V_R \leq 1 \quad \text{and} \quad V_R(x) = \begin{cases} 0 & \text{when} \quad |x| \leq 1 \\ 1 & \text{when} \quad 2 \leq |x| \leq R \\ 0 & \text{when} \quad |x| \geq R + 1 \end{cases}.$$  

First we motivate our results with a general potential. When the coupling parameter $\alpha$ is large, Pekar guessed that the ground state has the product form

$$\Psi_\alpha = \psi_\alpha(x) \otimes \Phi_\alpha,$$

where $\psi_\alpha \in L^2(\mathbb{R}^3)$ is an electronic wave function, and $\Phi_\alpha \in \mathcal{F}$ is a coherent state depending only on the phonon coordinates:

$$\Phi_\alpha = \prod_k \exp \left( z_\alpha(k) a_k^\dagger - z_\alpha(k) a_k \right) |0\rangle$$

with the vacuum $|0\rangle \in \mathcal{F}$ and the phonon displacements $z_\alpha(k) \in L^2(\mathbb{R}^3)$, which are to be determined variationally. In particular, $a_k \Phi_\alpha = z(k) \Phi_\alpha$.

The optimization problem in (1.2) for the ground-state energy becomes considerably more tractable if we assume that the ground state has the product form in Pekar’s Ansatz. Minimizing the quantity $\langle \Psi, H^V_\alpha \Psi \rangle$ over the more restrictive set of product wave functions in (1.4) and completing the square, Pekar deduced that

$$z_\alpha(k) = \frac{1}{\pi |k|} \sqrt{\frac{\alpha}{2}} \int_{\mathbb{R}^3} e^{-ikx} |\psi_\alpha|^2 dx,$$
which in turn couples the coherent state to the electronic wave function in (1.4), and arrived at an upper bound for the ground-state energy:

\[ E^V_\alpha \leq \inf \{ \langle \Psi, H^V_\alpha \Psi \rangle \mid \|\Psi\| = 1 \text{ and } \Psi = \psi \otimes \Phi \} \]

(1.7)

\[ = \alpha^2 e(V). \]

The quantity \( e(V) \) in (1.7) can be calculated by minimizing the nonlinear Pekar functional:

\[ e(V) = \inf_{\|\psi\|_2 = 1} \mathcal{E}_V(\psi), \]

(1.8)

where

\[ \mathcal{E}_V(\psi) = \int_{\mathbb{R}^3} |\nabla \psi|^2 dx - \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\psi(x)|^2 |\psi(y)|^2}{|x - y|} dx \, dy - \int_{\mathbb{R}^3} V(x)|\psi(x)|^2 dx. \]

Furthermore, if the minimization problem problem in (1.8) admits a minimizer \( \phi(x) \), then \( \alpha^{3/2} \phi(\alpha x) \) is the electronic wave function in Pekar’s product ground state from (1.4):

\[ \Psi_\alpha = \alpha^{3/2} \phi(\alpha x) \prod_k \exp \left( z_\alpha(k) a^\dagger_k - z_\alpha(k) a_k \right) |0\rangle, \]

(1.10)

where

\[ z_\alpha(k) = \frac{1}{\pi |k|} \sqrt{\frac{\alpha}{2}} \int_{\mathbb{R}^3} e^{-ik \cdot x} |\alpha^{3/2} \phi(\alpha x)|^2 dx; \]

note that the electronic function becomes more localized as the coupling parameter \( \alpha > 0 \) increases.

Though Pekar’s result in (1.7) is only an upper bound, his Ansatz provides the convenience of eliminating all of the phonon coordinates from the calculation: the functional in (1.9) needs to be minimized just over a single electronic coordinate, a sharp contrast to the more demanding situation in (1.2).

Not being amenable to the direct method in the calculus of variations, Pekar’s minimization problem for approximating the ground-state energy in turn motivated mathematicians to develop novel and far-reaching techniques in nonlinear analysis such as the symmetrization arguments of E.H. Lieb, the Concentration-Compactness Lemma of P.L. Lions and the stability theory of T. Cazenave and P.L. Lions. Indeed, the first detailed analysis of the nonlinear problem in (1.9) was given in 1977 by Lieb, who used rearrangement inequalities to show that a minimizer exists when \( V = 0 \). He also established that this minimizer is unique up to a translation by proving uniqueness of a radial solution for the corresponding Euler-Lagrange equation

\[ \left\{ -\Delta - 2 \int_{\mathbb{R}^3} |\phi(y)|^2 |x - y|^{-1} dy \right\} \phi(x) = \phi(x), \]

known in the literature as the Choquard-Pekar or Schrödinger-Newton equation. For showing the existence of a minimizer when \( V \neq 0 \) in (1.9), Lieb’s symmetrization argument applies for a symmetric decreasing potential. This motivated Lions to develop his famous Concentration Compactness Principle from 1984: for a general \( V \geq 0 \) that vanishes at infinity, he showed that the problem in (1.9) admits a minimizer. Uniqueness of a minimizer when \( V \neq 0 \), however, remains an elusive open problem.

Despite giving rise to a rich variational theory that continues to be a source of interesting mathematical problems, Pekar’s Produkt-Ansatz of the ground state in (1.4) lacks a rigorous
justification: It is based entirely on his feeling that (we quote the amusing yet accurate, anthropomorphic description from \[LT1997\]) “...at large coupling the phonons cannot follow the rapidly moving electron (as they do at weak coupling) and so resign themselves to interacting with the “mean” electron density \(\psi^2(x)\).” This “mean-field” interaction is reflected in the phonon displacements, given in equation (1.6), for Pekar’s coherent state.) It is therefore remarkable that Pekar’s crude upper bound for the ground-state energy in (1.7)– derived after all from his unjustified Ansatz– becomes exact (to the leading order) in the strong-coupling limit:

\[
\lim_{\alpha \to \infty} E^V_{\alpha} = e(V).
\]

The convergence in (1.11) was first argued by M.D. Donsker and S.R.S. Varadhan in \[DV1983\] using large deviation theory. In 1997, Lieb and L.E. Thomas gave an alternate, pedestrian proof of the convergence in (1.11) using simple modifications of the Hamiltonian (\[LT1997\]), a philosophy that can be traced back to the inspiring work of Lieb and K. Yamaazaki (\[LY1958\]).

In light of the convergence in (1.11) for the ground state energy, it is now only natural to investigate how well Pekar’s theory describes the ground-state wave function (in the strong-coupling limit). Using the now-standard techniques developed by F. Hiroshima \[Ha2000\] and by M. Griesemer, E.H. Lieb and M. Loss \[GLL2001\] to study the analogous Pauli-Fierz model in quantum electrodynamics, it can be argued that, under physically natural conditions on the external potential, the Fröhlich Hamiltonian \(H^V_{\alpha}\) has a unique ground state for all values of the coupling paramater \(\alpha > 0\). Because it is straightforward to adapt the arguments in \[Ha2000\] and \[GLL2001\] to the Fröhlich Hamiltonian and because the arguments are rather long, we do not provide a proof of the existence and uniqueness of a ground state here; a sketch of the main ideas is given in the Appendix.

Let \(\|\Psi^V_{\alpha}\|^2(x)\) denote the electron density of the ground state, and recall that a minimizer of the Pekar functional from (1.9) is the electronic wave function in his Produkt-Ansatz. Since the ground state energy in the strong-coupling limit can be obtained (to a leading order in the electron-phonon coupling) by minimizing the Pekar functional, shouldn’t the electron density \(\|\Psi^V_{\alpha}\|^2_{\alpha}\) also converge to a minimizer of the Pekar functional? Indeed, if the minimization problem in (1.9) for the Pekar energy admits a unique minimizer \(u_V\), then for all \(W \in C^\infty_c(\mathbb{R}^3)\)

\[
\lim_{\alpha \to \infty} \frac{1}{\alpha^3} \int_{\mathbb{R}^3} \|\Psi^V_{\alpha}\|^2_{\alpha} \left(\frac{x}{\alpha}\right) W(x) \, dx = \int_{\mathbb{R}^3} |u_V(x)|^2 \, W(x) \, dx
\]

This follows from a technique developed by Lieb and Simon in 1977 (for studying the Thomas-Fermi problem), and consists of differentiating the (concave) map \(\delta \mapsto e(V + \delta W)\) at \(\delta = 0\), where

\[
e(V + \delta W) = \inf_{\|\psi\|_{L^2} = 1} \left\{ \mathcal{E}_V(\psi) - \delta \int_{\mathbb{R}^3} |\psi(x)|^2 \, W(x) \, dx \right\}.
\]

However, it is not necessarily the case that the Pekar minimization problem admits a unique minimizer (See Theorem 1 below). The contribution of this paper is to address the discrepancy between a unique ground state and the non-unique Pekar minimizers.

Let the potential \(V_R\) be as above. For each \(\alpha > 0\) the Hamiltonian \(H^V_{\alpha_R}\), \(R > 2\) has a unique ground-state wave function. Since the potential \(V_R(x) \geq 0\) is short-range, i.e.
decays exponentially at infinity, it is known that for each \( \alpha > 0 \) the Schrödinger operator \( \mathbf{p}^2 - \alpha^2 V_R(\alpha x) \) has a negative energy bound state in \( L^2(\mathbb{R}^3) \) (see e.g. the introduction in [BV2004]). (To be precise: For the short-range potential \( V_R(x) \) it can be seen that there exists for all \( \alpha > 0 \) some \( \lambda_0 > 0 \) such that for \( \lambda > \lambda_0 \) the operator \( \mathbf{p}^2 - \lambda \alpha^2 V(\alpha x) \) has a negative energy bound state in \( L^2(\mathbb{R}^3) \). But our proofs still hold true if for some \( \lambda > \lambda_0 \) the function \( V_R(x) \) in (1.3) is replaced by \( \lambda V_R(x) \), so we do not inconvenience ourselves any further with this innocuous technicality.) So, \( V_R(x) \) satisfies the hypothesis of Proposition 7 in the Appendix. Furthermore, since \( V_R(x) \geq 0 \) and \( V_R \in L^\infty(\mathbb{R}^3) \), the form bound in (A.3) follows trivially from Hölder’s inequality; the potential \( V_R(x) \) also satisfies the hypothesis of Proposition 8 in the Appendix and the semigroup generated by the Hamiltonian is positivity improving in the Schroedinger representation. Hence, for \( R > 2 \) there exists a unique ground-state wave function \( \Psi_{V_R}^\alpha \), which is therefore invariant after a rotation in both the electron and phonon coordinates. We state this precisely: Denoting \( \mathbf{n} \) to be a vector in \( \mathbb{R}^3 \), the field (phonon) angular momentum relative to the origin is given by the operator (see [Sp2004])

\[
J_f = \int_{\mathbb{R}^3} dk \left( k \times i \nabla_k \right) a_k^\dagger a_k.
\]

Let \( \mathcal{R}_\theta \in SO(3) \) be a rotation by an angle \( \theta \) about \( \mathbf{n} \). Since for any vector \( \mathbf{n} \in \mathbb{R}^3 \) and all \( \theta \),

\[
(1.13) \quad \Psi_{V_R}^\alpha (x; k) = e^{- i \mathbf{n} \cdot J_f} \Psi_{V_R}^\alpha (\mathcal{R}_\theta x; k),
\]

we deduce that the electron density \( \| \Psi_{V_R}^\alpha \|^2 \mathcal{J}_\alpha (x) \) is radial for all \( R \).

But we show that the minimizers of the corresponding Pekar functional are not radial, for \( R \) large. Since the Pekar functional is, however, invariant under rotations, this implies that the non-radial minimizer is also not unique.

**Theorem 1.** For \( R \) large, the Pekar problem \( e(V_R) \) admits only nonradial minimizers.

We shall show Theorem 1 using a proof by contradiction. Our arguments use in an essential way Lieb’s 1977 uniqueness result [Lb1977] for the translation-invariant problem. The discrepancy in ground-state symmetry shows that the expected convergence in (1.12) of the (radial) ground-state electron density to a minimizer of the Pekar functional is not possible. However, we have the following:

**Theorem 2.** Let \( R \) be large enough so that \( e(V_R) \) in (1.9) admits only nonradial minimizers. Let \( \Psi_{V_R}^\alpha \in \mathcal{H} \) be the unique ground-state wave function of the Fröhlich Hamiltonian \( H_{V_R}^\alpha \) in (1.7). If the minimization problem in (1.9) for the Pekar energy admits a minimizer \( u_{V_R} \) that is unique up to a rotation, then, denoting \( \gamma \) to be the Haar measure on \( SO(3) \),

\[
(1.14) \quad \lim_{\alpha \to \infty} \int_{\mathbb{R}^3} \| \Psi_{V_R}^\alpha \|^2 \mathcal{J}_\alpha (x) W(x) \, dx = \int_{\mathbb{R}^3} \left[ \int_{SO(3)} |u_{V_R}(\mathcal{R}x)|^2 \, d\gamma(\mathcal{R}) \right] W(x) \, dx
\]

for all \( W \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \).

We now describe the strategy for proving Theorem 2. To the Hamiltonian \( H_{V_R}^\alpha \) we add \( \delta \) times the rotational average \( \langle W \rangle (x) \) of a test potential \( W(x) \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \) that is scaled appropriately:

\[
(1.15) \quad H_{V_R}^\alpha - \delta \alpha^2 \langle W \rangle (\alpha x),
\]
where $\langle W \rangle = \int_{SO(3)} W(\mathcal{R} x) \, d\gamma(\mathcal{R})$. Denoting $E^{V_R+\delta(W)}_{\alpha}$ to be the ground-state energy of the Hamiltonian in (1.15), it follows from the variational principle that

$$E^{V_R+\delta(W)}_{\alpha} \leq \langle \Psi_{V_R}^{V_R}, H_{\alpha}^{V_R} \Psi_{V_R} \rangle - \delta \alpha^2 \int_{\mathbb{R}^3} \langle W \rangle (x) \|\Psi_{V_R}^{V_R} \|_{\mathcal{F}}^2 \left( \frac{x}{\alpha} \right) \, dx$$

$$= E^{V_R}_{\alpha} - \delta \alpha \int_{\mathbb{R}^3} \langle W \rangle (x) \|\Psi_{V_R}^{V_R} \|_{\mathcal{F}}^2 \left( \frac{x}{\alpha} \right) \, dx.$$

For $\delta > 0$, by subtraction and division, the following inequality holds:

$$\frac{E^{V_R+\delta(W)}_{\alpha} - E^{V_R}_{\alpha}}{\delta \alpha^2} \leq - \frac{1}{\alpha^3} \int_{\mathbb{R}^3} \langle W \rangle (x) \|\Psi_{V_R}^{V_R} \|_{\mathcal{F}}^2 \left( \frac{x}{\alpha} \right) \, dx.$$

By (1.11),

(1.16) \quad \frac{e (V_R + \delta \langle W \rangle) - e (V_R)}{\delta} \leq \lim_{\alpha \to \infty} \frac{1}{\alpha^3} \int_{\mathbb{R}^3} \langle W \rangle (x) \|\Psi_{V_R}^{V_R} \|_{\mathcal{F}}^2 \left( \frac{x}{\alpha} \right) \, dx \]

(1.17) \quad = \lim_{\alpha \to \infty} \frac{1}{\alpha^3} \int_{\mathbb{R}^3} W(x) \|\Psi_{V_R}^{V_R} \|_{\mathcal{F}}^2 \left( \frac{x}{\alpha} \right) \, dx;$$

Above, (1.17) follows from Fubini’s theorem and that $\|\Psi_{V_R}^{V_R} \|_{\mathcal{F}}^2(x)$ is a radial function.

When $\delta < 0$, the inequality in (1.16) is merely reversed with the “lim inf” replaced by “lim sup”. Hence, Theorem 2 will follow if the map $\delta \mapsto e (V_R + \delta \langle W \rangle)$ is differentiable at $\delta = 0$. Because the minimization problem for the energy $e (V_R)$ does not admit a unique minimizer, the map $\delta \mapsto e (V_R + \delta J)$ cannot be differentiable for every $J \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. However, since (by assumption) the minimizers $u_{V_R}$ for the energy $e (V_R)$ are unique up to rotation, we will show that for all radial $Z \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$,

(1.18) \quad \lim_{\delta \to 0} \frac{e (V_R + \delta Z) - e (V_R)}{\delta} = - \int_{\mathbb{R}^3} Z(x) |u_{V_R}(x)|^2 \, dx.$$

Choosing $Z(x) = \langle W \rangle (x)$ in (1.18), Theorem 2 then follows from Fubini’s theorem.

The paper is organized as follows. A proof of Theorem 1 will be given in Section 2 below. In Section 3, we establish the crucial differentiation result, (1.18), and then prove Theorem 2.

2. NONRADIALITY OF THE PEKAR MINIMIZERS

Let the Pekar functional $\mathcal{E}_V$ be as given in (1.9) above. We consider the potential $V_R \in C_c^\infty(\mathbb{R}^3)$, $0 \leq V_R \leq 1$ given in (1.3) above. The corresponding Pekar problem is

(2.1) \quad e (V_R) = \inf \{ \mathcal{E}_{V_R} (\varphi) : \|\varphi\|_2 = 1 \}.$$

Since $V_R$ vanishes at infinity, by Lions’ Concentration Compactness Principle, we have the following:

Lemma 3. The minimization problem in (2.1) for the energy $e (V_R)$ admits a minimizer.

Proof. Theorem III.1 in [Ls1984].

The goal of this section is to show that the minimizers in the above Lemma for the energy $e (V_R)$ are nonradial. But first, we consider the radial minimization problem:
Lemma 4. The minimization problem

\[ e^{\text{rad}} (V_R) = \inf \{ \mathcal{E}_{V_R} (\varphi) : \varphi \in H^1_{\text{rad}} (\mathbb{R}^3) \text{ and } \| \varphi \|_2 = 1 \} \]

admits a (radial) minimizer.

We do not provide a proof of the above Lemma, because it is standard (cf. Remark III.2 in [Ls1984] and also [Ls1981]) and proceeds along the lines of the argument from “Step 3” in the proof of Theorem 3 below; the main ingredient is the well-known observation of W.A. Strauss (“Radial Lemma 1” in [Ss1977]) that any \( u \in H^1_{\text{rad}} (\mathbb{R}^3) \) satisfies

\[ |u(x)| \leq \frac{\sqrt{2} |S^2|^{-\frac{1}{2}}}{|x|} \| u \|_{H^1} \text{ for a.e. } |x| \geq 2. \]

Indeed, with \( u \in C_{c}^{\infty} (\mathbb{R}^3) \cap H^1_{\text{rad}} (\mathbb{R}^3) \) (we abuse notation by writing \( u(x) = u(r) \) with \( r = |x| \)),

\[ (r^2 u^2)_r = 2 (ru)_r (ru) \leq (ru)_r^2 + (ru)^2 = r^2 (u_r^2 + u^2) + (ru)_r^2. \]

Then for all \( L \geq 2 \),

\[ \frac{u^2 (L)}{2} L^2 \leq u^2 (L) (L^2 - L) \leq \int_0^L (u_r^2 + u^2) r^2 dr \leq |S^2|^{-1} \| u \|_{H^1}^2, \]

and (2.3) follows from a density argument.

The minimizers for \( e^{\text{rad}} (V_R) \) from the above Lemma play an important role in our proof of nonradiality:

Lemma 5. Let the potential \( V_R \) be as given in (1.3), and let the energies \( e (V_R) \) and \( e^{\text{rad}} (V_R) \) be as defined by the minimization problems in (2.1) and (2.2) respectively. For \( R \) large,

\[ e (V_R) < e^{\text{rad}} (V_R). \]

Proof. Essential to the proof is the Free Pekar Problem (i.e. without an external potential):

\[ e(0) = \inf_{\| \psi \|_2 = 1} \mathcal{E}_0 (\psi) \]

where

\[ \mathcal{E}_0 (\psi) = \int_{\mathbb{R}^3} |\nabla \psi|^2 dx - \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\psi(x)|^2 |\psi(y)|^2}{|x-y|} dx dy. \]

We recall that the problem in (2.3) admits a symmetric decreasing minimizer \( Q \in H^1 (\mathbb{R}^3) \) with \( \| Q \|_2 = 1 \) (Theorem 7 in [Lb1977]). We consider the translate

\[ Q_R (x) := Q (x - \zeta_R) \text{ with } \zeta_R = \left( \frac{R + 2}{2}, 0, 0 \right). \]

Since the functional in (2.6) is invariant under translations,

\[ \mathcal{E}_0 (Q_R) = \mathcal{E}_0 (Q) = e(0) \text{ for all } R. \]

Most importantly, for \( R \) large the nonradial function \( Q_R \) is concentrated in the potential well of \( V_R \) located at \( \{ 2 \leq |x| \leq R \} \): Indeed, for \( R > 2 \)

\[ \int_{\{ 2 \leq |x| \leq R \}} |Q_R (x)|^2 dx \geq \int_{\{ |x-\zeta_R| \leq \frac{R-2}{2} \}} |Q_R (x)|^2 dx = \int_{\{ |x| \leq \frac{R-2}{2} \}} |Q (x)|^2 dx \]
and \(\|Q\|_2 = 1\), so
\[
\lim_{R \to \infty} \int_{\{2 \leq |x| \leq R\}} |Q_R(x)|^2 \, dx = 1.
\]

**Step 1** (Variational Principle). For all \(R\), by the variational principle,
\[
e(V_R) \leq \mathcal{E}_{V_R}(Q_R) = e(0) - \int_{\mathbb{R}^3} V_R(x) |Q_R(x)|^2 \, dx.
\]

By the above Lemma, there is a radial function \(\rho_R \in H^1(\mathbb{R}^3)\) with \(\|\rho_R\|_2 = 1\) and \(\mathcal{E}_{V_R}(\rho_R) = e^{\text{rad}}(V_R)\). Hence the claimed inequality in (2.10) will follow if we can prove for large,\n\[
\mathcal{E}_{V_R}(Q_R) < \mathcal{E}_{V_R}(\rho_R).
\]

**Step 2** (Proof by Contradiction). Suppose (2.10) is not true. Then there is a sequence \(\{R_n\}_{n=1}^\infty\) where \(R_n \to \infty\) as \(n \to \infty\) and \(\mathcal{E}_{V_{R_n}}(Q_{R_n}) \geq \mathcal{E}_{V_{R_n}}(\rho_{R_n})\), i.e.
\[
e(0) - \int_{\mathbb{R}^3} V_{R_n}(x) |Q_{R_n}(x)|^2 \, dx \geq \mathcal{E}_0(\rho_{R_n}) - \int_{\mathbb{R}^3} V_{R_n}(x) |\rho_{R_n}(x)|^2 \, dx.
\]

Then, since \(e(0) \leq \mathcal{E}_0(\rho_{R_n})\),
\[
0 \leq \mathcal{E}_0(\rho_{R_n}) - e(0) \leq \int_{\mathbb{R}^3} V_{R_n}(x) |\rho_{R_n}(x)|^2 \, dx - \int_{\mathbb{R}^3} V_{R_n}(x) |Q_{R_n}(x)|^2 \, dx.
\]

We recall that \(0 \leq V_{R_n}(x) \leq 1\) and \(V_{R_n}(x) = 1\) when \(2 \leq |x| \leq R_n\). By Hölder’s inequality,
\[
\int_{\{2 \leq |x| \leq R_n\}} |Q_{R_n}(x)|^2 \, dx \leq \int_{\mathbb{R}^3} V_{R_n}(x) |Q_{R_n}(x)|^2 \, dx \leq 1.
\]

Then, by our observation in (2.8),
\[
\lim_{n \to \infty} \int_{\mathbb{R}^3} V_{R_n}(x) |Q_{R_n}(x)|^2 \, dx = 1.
\]

Furthermore, by the inequalities in (2.11) and Hölder’s inequality,
\[
\int_{\mathbb{R}^3} V_{R_n}(x) |Q_{R_n}(x)|^2 \, dx \leq \int_{\mathbb{R}^3} V_{R_n}(x) |\rho_{R_n}(x)|^2 \, dx \leq 1.
\]

We conclude from (2.12) that
\[
\lim_{n \to \infty} \int_{\mathbb{R}^3} V_{R_n}(x) |\rho_{R_n}(x)|^2 \, dx = 1.
\]

We deduce from (2.12), (2.13) and the inequalities in (2.11) that
\[
\lim_{n \to \infty} \mathcal{E}_0(\rho_{R_n}) = e(0).
\]

Moreover, \(\|\rho_{R_n}\|_2 = 1\) and \(V_{R_n}(x) = 0\) when \(|x| \leq 1\), so
\[
\int_{\{|x| \leq 1\}} |\rho_{R_n}(x)|^2 \, dx = 1 - \int_{\{|x| > 1\}} |\rho_{R_n}(x)|^2 \, dx \leq 1 - \int_{\mathbb{R}^3} V_{R_n}(x) |\rho_{R_n}(x)|^2 \, dx.
\]
We then conclude from (2.13) that
\begin{equation}
\lim_{n \to \infty} \int_{\{|x| \leq 1\}} |\rho_{R_n}(x)|^2 \, dx = 0.
\end{equation}

**Step 3** (Conclusion). Recall \( \rho_R \in H^1(\mathbb{R}^3) \), \( \|\rho_R\|_2 = 1 \) and \( E_{\nu_R}(\rho_R) = e^{\text{rad}}(V_R) \). Seeking a contradiction, we have shown (see (2.14) and (2.13)) that for some \( R_n \to \infty \) as \( n \to \infty \), the sequence of radial functions \( \{\rho_{R_n}\}_{n=1}^\infty \) is vanishing on the unit ball while also minimizing for the Free Pekar Problem in (2.5). Moreover, we recall a result of E.H. Lieb (Theorem 10 in [Lb1977]) that this minimization problem in (2.5) admits a symmetric decreasing minimizer \( Q \in H^1(\mathbb{R}^3) \), which is unique up to translation.

Since \( \{\rho_{R_n}\}_{n=1}^\infty \) is minimizing for the problem in (2.5), by a standard argument ([Lb1977]) using Sobolev’s and Young’s inequalities,
\begin{equation}
\|\rho_{R_n}\|_{H^1} < C
\end{equation}
for all \( n \). Then there is a subsequence, which (with an abuse of notation) we also denote by \( \{\rho_{R_n}\}_{n=1}^\infty \), and some \( \rho \in H^1(\mathbb{R}^3) \) where
\begin{equation}
\rho_{R_n} \rightharpoonup \rho \text{ in } H^1(\mathbb{R}^3).
\end{equation}
We tabulate some immediate observations about \( \rho \): \( \{\rho_{R_n}\}_{n=1}^\infty \) is radial, so the weak limit \( \rho \) is radial almost everywhere. Moreover, by the weak lower semicontinuity of the \( L^2 \)-norm,
\begin{equation}
\|\rho\|_2 \leq \liminf_{n \to \infty} \|\rho_{R_n}\|_2 = 1
\end{equation}
and
\begin{equation}
\|\nabla \rho\|_2 \leq \liminf_{n \to \infty} \|\nabla \rho_{R_n}\|_2.
\end{equation}
Finally, since the subsequence \( \{\rho_{R_n}\}_{n=1}^\infty \) vanishes on the unit ball (see (2.15)), by the Rellich-Kondrashov theorem (Theorem 8.6 in [LL2001]),
\begin{equation}
\int_{\{|x| \leq 1\}} |\rho(x)|^2 \, dx = \lim_{n \to \infty} \int_{\{|x| \leq 1\}} |\rho_{R_n}(x)|^2 \, dx = 0.
\end{equation}
We shall argue that this weak limit \( \rho \)– an a.e. radial function vanishing on the unit ball (see (2.20))–is in fact a minimizer for the Free Pekar Problem in (2.5); appealing to Lieb’s uniqueness result, we then have a contradiction. The main task is to show
\begin{equation}
\int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\rho_{R_n}(x)|^2 |\rho_{R_n}(y)|^2}{|x-y|} \, dx \, dy \longrightarrow \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\rho(x)|^2 |\rho(y)|^2}{|x-y|} \, dx \, dy.
\end{equation}
From the positivity of the Coulomb energy (Theorem 9.8 in [LL2001]),
\begin{equation}
\left| \left( \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\rho_{R_n}(x)|^2 |\rho_{R_n}(y)|^2}{|x-y|} \, dx \, dy \right)^{\frac{1}{2}} - \left( \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\rho(x)|^2 |\rho(y)|^2}{|x-y|} \, dx \, dy \right)^{\frac{1}{2}} \right|
\end{equation}
\begin{equation}
\leq \left( \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|(\rho_{R_n} - \rho)(x)|^2 |(\rho_{R_n} - \rho)(y)|^2}{|x-y|} \, dx \, dy \right)^{\frac{1}{2}}.
\end{equation}
Since $\rho_{R_n}, \rho$ are radial (we abuse notation by writing $\rho_{R_n}(r) = \rho_{R_n}(x)$ with $r = |x|$), by Newton’s Theorem (Theorem 9.7 in [LL2001]),
\[
\int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|(\rho_{R_n} - \rho)(x)|^2 |(\rho_{R_n} - \rho)(y)|^2}{|x - y|} dx dy
\]
\[
= (4\pi)^2 \int_0^\infty |(\rho_{R_n} - \rho)(s)|^2 \left( |(\rho_{R_n} - \rho)(r)|^2 \min\left\{ r^{-1}, s^{-1} \right\} r^2 dr \right) s^2 ds
\]
\[
\leq (4\pi)^2 \left( \int_0^\infty |(\rho_{R_n} - \rho)(r)|^2 s^2 ds \right) \left( \int_0^\infty \frac{|(\rho_{R_n} - \rho)(r)|^2}{r} r^2 dr \right)
\]
\[
\leq 16\pi \left( \int_0^\infty \frac{|(\rho_{R_n} - \rho)(r)|^2}{r} r^2 dr \right)
\]  
\[\text{(2.23)}\]

From Strauss’ Radial Lemma ([Ss1977]; see also (2.3)) and the bounds in (2.16), (2.18) and (2.19),
\[
|(\rho_{R_n} - \rho)(r)| \leq \frac{\sqrt{2} |S|^2 |(\rho_{R_n} - \rho)(r)|}{r} < C \quad \text{when } r > 2.
\]  
\[\text{(2.24)}\]

Denoting $B_M(0)$ to be a ball of radius $M$ centered at the origin, by (2.24) and Hölder’s inequality,
\[
\int_0^\infty \frac{|(\rho_{R_n} - \rho)(r)|^2}{r} r^2 dr \leq \frac{\sqrt{M}}{2\sqrt{\pi}} \|\rho_{R_n} - \rho\|^2_{L^4(B_M(0))} + \frac{C \|\rho_{R_n} - \rho\|^2_{L^4(B_M(0))}}{2\sqrt{\pi}} \left( \int_M^\infty \frac{|(\rho_{R_n} - \rho)(r)|^2}{r^2} dr \right)^\frac{1}{2}
\]
\[
\leq \frac{\sqrt{M}}{2\sqrt{\pi}} \|\rho_{R_n} - \rho\|^2_{L^4(B_M(0))} + \frac{C}{\sqrt{\pi M}}
\]
\[\text{(2.25)}\]

Above, $M$ can be chosen arbitrarily large. Furthermore, by (2.17) and the Rellich-Kondrashov theorem (Theorem 8.6 in [LL2001]), $\|\rho_{R_n} - \rho\|_{L^4(B_M(0))} \to 0$ for all $M$. Therefore, the desired convergence in (2.21) follows from (2.22), (2.23) and (2.25).

Since $\|\rho\|_2 \leq 1$ (see (2.18)) and $e(0) < 0$ (Lemma 1(i) in [Lb1977]),
\[
\mathcal{E}_0(\rho) \geq \mathcal{E}_0 \left( \frac{\rho}{\|\rho\|_2} \right) \|\rho\|_2^2 \geq e(0) \|\rho\|_2^2 \geq e(0).
\]  
\[\text{(2.26)}\]

Also, by (2.14), (2.19) and (2.21),
\[
e(0) = \lim_{k \to \infty} \mathcal{E}_0(\rho_{R_n}) \geq \mathcal{E}_0(\rho).
\]  
\[\text{(2.27)}\]

We deduce from (2.26) and (2.27) that the weak limit $\rho$ is a minimizer for the Free Pekar Problem in (2.3):
\[
\|\rho\|_2 = 1 \quad \text{and} \quad \mathcal{E}_0(\rho) = e(0).
\]  
\[\text{(2.28)}\]

By Lieb’s uniqueness result (Theorem 10 in [Lb1977]),
\[
\rho(x) = Q(x - a) \quad \text{for some } a \in \mathbb{R}^3,
\]
\[\text{(2.29)}\]
where \( Q \) is symmetric decreasing about the origin. But \( \rho \) is a.e. radial, so \( a = 0 \) in (2.29) necessarily. Alas, the minimizer \( \rho \) with \( \| \rho \|_2 = 1 \) is symmetric decreasing about the origin, and yet \( \rho(x) = 0 \) for a.e. \( |x| \leq 1 \) (see (2.20)); we have a contradiction. \( \square \)

Theorem 1 now follows.

3. The Rotational Average

As explained in the introduction, we first need to differentiate the the map \( \delta \mapsto e(V + \delta Z) \) for radial test potentials \( Z \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \).

**Theorem 6.** Let the potential \( V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \) be nonnegative, vanishing at infinity and not almost everywhere identically-zero. For a function \( W \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \) and a real parameter \( \delta \), consider the perturbed Pekar energy

\[
(3.1) \quad e(V + \delta W) = \inf_{\|u\|_2 = 1} \mathcal{E}_{V + \delta W}(u) := \inf_{\|u\|_2 = 1} \left\{ \mathcal{E}_V(u) - \delta \int_{\mathbb{R}^3} W(x)|u(x)|^2 dx \right\},
\]

where

\[
\mathcal{E}_V(u) = \int_{\mathbb{R}^3} |\nabla u|^2 dx - \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|u(x)^2|u(y)|^2}{|x - y|} dx dy - \int_{\mathbb{R}^3} V(x)|u(x)|^2 dx.
\]

If the minimization problem for the Pekar energy \( e(V) = \inf\{\mathcal{E}_V(u) : \|u\|_2 = 1\} \) admits a minimizer \( u_V \) that is unique up to rotations, then for all radial functions \( Z \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \) the map \( \delta \mapsto e(V + \delta Z) \) is differentiable at \( \delta = 0 \) and

\[
(3.2) \quad \frac{d}{d\delta} \bigg|_{\delta=0} e(V + \delta Z) = -\int_{\mathbb{R}^3} Z(x)|u_V(x)|^2 dx.
\]

**Proof.** For \( W \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \), by a standard argument ([Lb1977], [LL2001]) using Sobolev’s and Young’s inequalities, there exist constants \( 0 < c_1 < 1 \) and \( c_2 > 0 \) such that for all \( u \in H^1(\mathbb{R}^3) \) with \( \|u\|_2 = 1 \) and \( |\delta| \) sufficiently small,

\[
(3.3) \quad \mathcal{E}_{V + \delta W}(u) \geq c_1 \|\nabla u\|_2^2 - c_2.
\]

Therefore,

\[
(3.4) \quad e(V + \delta W) > -\infty.
\]

We deduce from (3.2) that for \( W \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \) (and \( |\delta| \) sufficiently small), the perturbed problem in (3.1) admits an approximate minimizer \( u_\delta \in H^1(\mathbb{R}^3) \) with \( \|u_\delta\|_2 = 1 \) satisfying

\[
(3.5) \quad \mathcal{E}_{V + \delta W}(u_\delta) \leq e(V + \delta W) + \delta^2.
\]

We denote the set of minimizers for the Pekar energy as \( \mathcal{M} := \{u \in H^1(\mathbb{R}^3) : \|u\|_2 = 1 \text{ and } \mathcal{E}_V(u) = e(V)\}. \) For any \( \tilde{u} \in \mathcal{M} \), by the variational principle,

\[
(3.6) \quad e(V + \delta W) \leq \mathcal{E}_{V + \delta W}(\tilde{u}) = e(V) - \delta \int_{\mathbb{R}^3} W(x)|\tilde{u}(x)|^2 dx.
\]

Likewise, for an approximate minimizer \( u_\delta, \|u_\delta\|_2 = 1 \) satisfying (3.5),

\[
(3.7) \quad e(V) \leq \mathcal{E}_V(u_\delta) = \mathcal{E}_{V + \delta W}(u_\delta) + \delta \int_{\mathbb{R}^3} W(x)|u_\delta(x)|^2 dx \leq e(V + \delta W) + \delta^2 + \delta \int_{\mathbb{R}^3} W(x)|u_\delta(x)|^2 dx.
\]
Let $\delta > 0$. For a perturbation $W \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and an approximate minimizer $u_\delta$, $\|u_\delta\|_2 = 1$ in (3.5), by the inequalities in (3.6) and (3.7),

$$
(3.8) \quad - \int_{\mathbb{R}^3} W(x)|u_\delta(x)|^2 dx - \delta \leq \frac{e(V + \delta W) - e(V)}{\delta} \leq \left( \sup_{u \in \mathcal{M}} \int_{\mathbb{R}^3} W(x)|u(x)|^2 dx \right).
$$

When $\delta < 0$, the inequalities in (3.8) are merely reversed:

$$
(3.9) \quad - \int_{\mathbb{R}^3} W(x)|u_\delta(x)|^2 dx - \delta \geq \frac{e(V + \delta W) - e(V)}{\delta} \geq \left( \inf_{u \in \mathcal{M}} \int_{\mathbb{R}^3} W(x)|u(x)|^2 dx \right).
$$

By our uniqueness assumption, $\mathcal{M} = \langle u_V(\mathcal{R} x) : \mathcal{R} \in SO(3) \rangle$. Furthermore, with radial functions $Z \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, by a change of variable,

$$
(3.10) \quad \int_{\mathbb{R}^3} Z(x)|u_V(\mathcal{R} x)|^2 dx = \int_{\mathbb{R}^3} Z(x)|u_V(x)|^2 dx
$$

for all $\mathcal{R} \in SO(3)$. Then, for radial perturbations, the rightmost quantities in the inequalities (3.8) and (3.9) are equal. Hence (with $Z$ radial) the claimed differentiability of the map $\delta \mapsto e(V + \delta W)$ at $\delta = 0$ will follow from our observation in (3.10) and the inequalities in (3.8) and (3.9) if we can prove the convergence result stated below:

For radial $Z \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, let $u_\delta$ with $\|u_\delta\|_2 = 1$ be an approximate minimizer as defined in (3.5) above for the perturbed energy $e(V + \delta Z)$. Then, for any sequence $\{\delta_n\}_{n=1}^\infty$ where $|\delta_n| > 0$ and $\delta_n \to 0$ as $n \to \infty$, the corresponding sequence of approximate minimizer $\{u_{\delta_n}\}_{n=1}^\infty$ satisfies

$$
(3.11) \quad \lim_{n \to \infty} \int_{\mathbb{R}^3} Z(x)|u_{\delta_n}(x)|^2 dx = \int_{\mathbb{R}^3} Z(x)|u_V(x)|^2 dx.
$$

We observe that $\{u_{\delta_n}\}_{n=1}^\infty$ is minimizing for the problem $e(V) = \inf \{ \mathcal{E}_V(u) : \|u\|_2 = 1 \}$. Then, by Lions’ concentration compactness argument, every subsequence $\{u_{\delta_{n_k}}\}$ has a sub-subsequence $\{u_{\delta_{n_{k_l}}}\}$ converging strongly in $H^1(\mathbb{R}^3)$ to some function in $\mathcal{M} = \langle u_V(\mathcal{R} x) : \mathcal{R} \in SO(3) \rangle$. We deduce from our observation in (3.10) that

$$
\lim_{l \to \infty} \int_{\mathbb{R}^3} Z(x)|u_{\delta_{n_{k_l}}}(x)|^2 dx = \int_{\mathbb{R}^3} Z(x)|u_V(\mathcal{R} x)|^2 dx = \int_{\mathbb{R}^3} Z(x)|u_V(x)|^2 dx.
$$

We are now ready to prove Theorem 2.

Proof of Theorem 2. For any $W \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ we denote its rotational average $\langle W \rangle = \int_{SO(3)} W(\mathcal{R} x) d\gamma(\mathcal{R})$. Note that $\langle W \rangle \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. As explained at the end of the introduction, using the variational principle and (3.11), we arrive at the relations

$$
\frac{e(V_R + \delta \langle W \rangle) - e(V_R)}{\delta} \leq \liminf_{a \to \infty} - \frac{1}{a^3} \int_{\mathbb{R}^3} \|\Psi_{V_R}^a\|^2_2 \left( \frac{x}{a} \right) \langle W \rangle(x) dx,
$$

and

$$
\frac{e(V_R + \delta \langle W \rangle) - e(V_R)}{\delta} \geq \limsup_{a \to \infty} - \frac{1}{a^3} \int_{\mathbb{R}^3} \|\Psi_{V_R}^a\|^2_2 \left( \frac{x}{a} \right) \langle W \rangle(x) dx.
$$
Using Fubini’s theorem, a simple change of variable and that the electron density $\|\Psi^V_\alpha\|^2 (x)\frac{df}{d\delta} \bigg|_{\delta=0} e(V + \delta \langle W \rangle) = -\int_{\mathbb{R}^3} |u_{VR}(x)|^2 \langle W \rangle (x) dx = -\int_{\mathbb{R}^3} \left( \int_{SO(3)} |u_{VR}(Rx)|^2 d\gamma(R) \right) W(x) dx.$ \hfill $\Box$

**Appendix A. Existence and Uniqueness of a Ground State**

We describe the main ideas in [GLL2001] and [Ha2000] for arguing the existence of a unique ground-state wave function:

**Proposition 7.** Fix $\alpha > 0$. If the Schrödinger operator $\mathbf{p}^2 - \alpha^2 V(\alpha x)$ has a negative energy bound state in $L^2 (\mathbb{R}^3)$, i.e., there is an eigenfunction $\zeta \in L^2 (\mathbb{R}^3)$ and $\eta > 0$ so that

\[
(\mathbf{p}^2 - \alpha^2 V(\alpha x)) \zeta(x) = -\eta \zeta(x),
\]

then there exists a normalized function $\Psi^V_\alpha$ in $L^2 (\mathbb{R}^3) \otimes F$ satisfying

\[
H^V_\alpha \Psi^V_\alpha = E^V (\alpha) \Psi^V_\alpha.
\]

The existence of a negative energy bound state of the operator $\mathbf{p}^2 - \alpha^2 V(\alpha x)$ can be used to show that the Fröhlich Hamiltonian $H^V_\alpha$ satisfies the binding condition (cf. Theorem 3.1 in [GLL2001])

\[
E^V (\alpha) < E^{V=0} (\alpha).
\]

With the Rellich-Kondrashov theorem and the binding inequality in (A.1), the above proposition can be established along the lines of the argument provided in [GLL2001]. In order to see that the ground state is unique, we use the well-known Schrödinger representation of the phonon Fock space $F$, which is naturally identified with the $L^2$ space over a probability measure space $(Q, \mu)$ (see p. 185 in [Sp2004]). We denote the unitary operator

\[
\vartheta : L^2 (\mathbb{R}^3) \otimes F \mapsto L^2 (\mathbb{R}^3 \otimes Q, dx \times d\mu).
\]

The identification in (A.2) of $F$ with an $L^2$ space opens up the possibility of establishing the uniqueness of the ground state via the classical route of positivity improvement: on a $\sigma$–finite measure space $(\chi, \nu)$, a bounded operator $B$ on $L^2 (\chi, \nu)$ is positivity improving if $\langle f_1, B f_2 \rangle_{L^2 (\chi, \nu)} > 0$ for all positive $f_1$ and $f_2$ in $L^2 (\chi, \nu)$ (and a function $f \in L^2 (\chi, \nu)$ is positive if $f \geq 0$ a.e. and $f \neq 0$ a.e.). Armed with the Schrödinger representation and the notion of positivity improvement defined above, uniqueness can be shown along the lines of Hiroshima’s argument in [Ha2000]:

\[
\Psi^V_\alpha = \Psi^V_\alpha (x).\]
Proposition 8. Fix $\alpha > 0$, and let the external potential $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ satisfy the conditions of Proposition 1 above. Writing $V = V_+ - V_-$, suppose $\alpha^2 V_+ (\alpha x)$ is relatively form bounded with respect to the operator $p^2$ with form bound strictly less than one; that is, for some $0 < a < 1$ there exists $c_\alpha > 0$ such that for all $\xi \in H^1(\mathbb{R}^3)$,

\begin{equation}
\alpha^2 \int_{\mathbb{R}^3} V_+ (\alpha x) |\xi(x)|^2 \, dx \leq a \|\nabla \xi\|_2^2 + c_\alpha \|\xi\|_2^2.
\end{equation}

Then the ground-state wave function $\Psi^V_\alpha$ of the Fröhlich Hamiltonian $H^V_\alpha$ is unique.

Let $\vartheta$ be the unitary operator as given in (A.2). When the external potential $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ satisfies the condition in (A.3), it is possible to show using the functional integral formula for the heat kernel that the operator $\vartheta e^{-iH^V_\alpha \, \vartheta^{-1}}, \ t > 0$ is positivity improving [Ha2000]. It then follows that the ground state of $\vartheta H^V_\alpha \vartheta^{-1}$ is unique (see p.191 in [Sp2004]). Since $\vartheta$ is unitary, the ground state of $H^V_\alpha$ is therefore also unique.

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