Pekar's Ansatz and the Ground-State Symmetry of a Bound Polaron

Rohan Ghanta

Georgia Institute of Technology

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The Polaron Model

- In 1937 H. Fröhlich proposed a model–known today as the Fröhlich polaron–of an electron interacting with the quantized optical modes (phonons) of an ionic crystal (Proc. R. Soc. Lond. A, **160** (1937)).
- We consider a Fröhlich polaron bound in an external electric potential (impurity in a crystal).
- The Hilbert space associated with the system is $\mathscr{H} = L^2(\mathbb{R}^3) \otimes \mathscr{F}$, where

$$\mathscr{F} := \bigoplus_{n \geq 0} \otimes_s^n L^2(\mathbb{R}^3)$$

is a symmetric (phonon) Fock space over $L^2(\mathbb{R}^3)$.

Fröhlich Hamiltonian

It is described by the Hamiltonian

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

- $\mathbf{p} = -i\nabla_x$ is the electron momentum
- $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ is nonnegative and vanishes at infinity
- $a_k^\dagger$ and a_k are creation and annihlation operators on $\mathscr{F}$ satisfying $[a_k, a_{k'}^\dagger] = \delta(k - k')$
- $\alpha > 0$ is the electron-phonon coupling parameter

The Ground State

The Fröhlich Hamiltonian is

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

- The **ground-state energy** is

$$E_\alpha^F(V) = \inf_{\|\Psi\|_{\mathscr{H}}=1} \left(\Psi, H_\alpha^V \Psi \right)$$

- A normalized function in $\mathscr{H}$ that achieves the ground-state energy is called a **ground-state wave function**.

Existence and Uniqueness of a Ground State

The Fröhlich Hamiltonian is

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

Fix $\alpha > 0$. Suppose the external potential satisfies the following two conditions:

1. $\mathbf{p}^2 - \alpha^2 V(\alpha x)$ has a negative energy bound state in $L^2(\mathbb{R}^3)$, and
2. $\alpha^2 V(\alpha x)$ is relatively form-bounded with respect to $\mathbf{p}^2$ with form bound strictly less than one.

Then there exists a **unique** ground-state wave function $\Psi_\alpha^V \in \mathscr{H}$.

Pekar's *Produkt-Ansatz*

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$$E_\alpha^F(V) = \inf_{\|\Psi\|_{\mathscr{H}}=1} \left(\Psi, H_\alpha^V \Psi \right)$$

The electron-phonon interaction term in the Hamiltonian makes it difficult to calculate the ground-state energy of the polaron.

S.I. Pekar's Ansatz (Issledovaniya po Elektronnoi Teorii Kirstallov. Gostekhizdat, Moskow, 1951)

When α is large, the ground-state wave function is a product of a normalized electronic wave function in $L^2(\mathbb{R}^3)$ and a normalized coherent state in Fock space:

$$\Psi(x,\cdot) := \phi(x)\Phi(\cdot).$$

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$$\Psi(x,\cdot) := \phi(x)\Phi(\cdot).$$

$$\Phi = \prod_k \exp\left(-\frac{|z(k)|^2}{2} + z(k)a_k^\dagger\right)|0\rangle$$

- $|0\rangle$ is the vacuum in $\mathscr{F}$,
- $z(k) \in L^2(\mathbb{R}^3)$.
- $a_k\Phi = z(k)\Phi$ and $\langle\Phi,\Phi\rangle_{\mathscr{F}} = 1$.

Pekar's *Produkt-Ansatz*

Note: $\Phi = \prod_k \exp\left(-\frac{|z(k)|^2}{2} + z(k) a_k^\dagger\right)|0\rangle$ and $a_k \Phi = z(k)\Phi$.

Writing $\hat{\rho_\phi}(k) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{ik\cdot x} |\phi|^2 dx$, we calculate with Pekar's *ansatz*:

$$\left\langle \phi\Phi, H_\alpha^V \phi\Phi \right\rangle$$

$$= \int_{\mathbb{R}^3} |\nabla\phi|^2 dx - \alpha^2 \int_{\mathbb{R}^3} |\phi|^2 V(\alpha x)\, dx$$

$$+ \int_{\mathbb{R}^3} dk \left[|z(k)|^2 - 2\sqrt{\alpha\pi} \frac{\hat{\rho_\phi}(k)}{|k|} z(k) - 2\sqrt{\alpha\pi} \frac{\overline{\hat{\rho_\phi}(k)}}{|k|} \overline{z(k)} \right]$$

$$= \int_{\mathbb{R}^3} |\nabla\phi|^2 dx - \alpha^2 \int_{\mathbb{R}^3} |\phi|^2 V(\alpha x)\, dx$$

$$+ \int_{\mathbb{R}^3} \left(\left| z(k) - 2\sqrt{\alpha\pi} \frac{\overline{\hat{\rho_\phi}(k)}}{|k|} \right|^2 - 4\pi\alpha \frac{|\hat{\rho_\phi}(k)|^2}{|k|^2} \right) dk$$

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Pekar's *Produkt-Ansatz*

- It follows that

$$E_\alpha^F(V) \leq \inf_{\|\phi\|_2 = \|\Phi\|_{\mathscr{F}} = 1} \left\langle \phi\Phi, H_\alpha^V \phi\Phi \right\rangle$$

$$= \alpha^2 \left(e^P(V) \right),$$

where $e^P(V)$ given by the **Pekar minimization problem**:

$$e^P(V) :=$$

$$\inf_{\|\phi\|_2=1} \left\{ \int_{\mathbb{R}^3} \left(|\nabla \phi|^2 - |\phi|^2 V(x) \right) dx - \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\phi(x)|^2 |\phi(y)|^2}{|x-y|} \, dx \, dy \right\}.$$

- P.L. Lions showed that the Pekar minimization problem admits a minimizer (Ann. Inst. H. Poin. Non-Linear. **1**, 1984).

Pekar's "Ground State"

Pekar's Product State

Let $\varphi_V(x)$ be a minimizer for the Pekar energy $e^P(V)$. For α large, the "ground-state wave function" is

$$\alpha^{\frac{3}{2}}\varphi_V(\alpha x) \times \Phi_\alpha^V,$$

where

$$\Phi_\alpha^V = \prod_k \exp\left(-\frac{\left|z_\alpha^V(k)\right|^2}{2} + z_\alpha^V(k) a_k^\dagger\right)|0\rangle$$

and

$$z_\alpha^V(k) = \frac{2\sqrt{\alpha\pi}}{|k|(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{ik\cdot x}\left|\alpha^{\frac{3}{2}}\varphi_V(\alpha x)\right|^2 dx.$$

Exact Ground-State Energy in the Strong-Coupling Limit

Recall that $E_{\alpha}^{F}(V) \leq \alpha^{2}\left(e^{P}(V)\right)$, where

$$e^{P}(V) = \inf_{\|\phi\|_2=1}\left\{\int_{\mathbb{R}^3}\left(|\nabla\phi|^2 - |\phi|^2 V(x)\right)dx - \iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|\phi(x)|^2|\phi(y)|^2}{|x-y|}\,dx\,dy\right\}.$$

However, it was shown by M.D. Donsker and S.R.S. Varadhan that Pekar's upper bound is in fact exact in the strong-coupling limit (Comm. Pure. Appl. Math. **36**, 1983):

Ground-State Energy

$$\lim_{\alpha\to\infty}\frac{E_{\alpha}^{F}(V)}{\alpha^{2}} = e^{P}(V).$$

A simple proof was later given by E.H. Lieb and L.E. Thomas (Comm. Math. Phys. **183**, 1995).

What about the Ground-State Wave Function?

Pekar's Product State

Let $\varphi_V(x)$ be a minimizer for the Pekar energy $e^P(V)$. For α large, the "ground-state wave function" is

$$\alpha^{\frac{3}{2}}\varphi_V(\alpha x)\times\Phi_\alpha^V,$$

where

$$\Phi_\alpha^V=\prod_k\exp\left(-\frac{\left|z_\alpha^V(k)\right|^2}{2}+z_\alpha^V(k)a_k^\dagger\right)|0\rangle$$

and

$$z_\alpha^V(k)=\frac{2\sqrt{\alpha\pi}}{|k|(2\pi)^{3/2}}\int_{\mathbb{R}^3}e^{ik\cdot x}\left|\alpha^{\frac{3}{2}}\varphi_V(\alpha x)\right|^2dx.$$

If Pekar Minimizer is Unique...

Adapting an argument of E.H. Lieb and B. Simon in Thomas-Fermi theory (Adv. Math. **23**(1), 1977), we know:

Convergence of Electron Density

Suppose the Pekar minimization problem for the energy $e^P(V)$ admits a **unique** minimizer φ_V. Then for all $W \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$,

$$\lim_{\alpha\to\infty} \frac{1}{\alpha^3} \int_{\mathbb{R}^3} \|\Psi_\alpha^V\|_{\mathscr{F}}^2 \left(\frac{x}{\alpha}\right) W(x)\, dx = \int_{\mathbb{R}^3} |\varphi_V(x)|^2\, W(x)\, dx.$$

But...

What if the minimizers for the Pekar energy $e^P(V)$ are not unique?

A Discrepancy in Spherical Symmetry

Mexican Hat-type Potential

Let $R > 2$. Consider the potential $V_R \in C_c^\infty(\mathbb{R}^3)$, where $0 \leq V_R \leq 1$ and

$$V_R(x) = \begin{cases} 0 & \text{when} \quad |x| \leq 1 \\ 1 & \text{when} \quad 2 \leq |x| \leq R \\ 0 & \text{when} \quad |x| \geq R+1 \end{cases} .$$

- For all $\alpha > 0$ and $R > 2$, the ground-state $\Psi_\alpha^{V_R}$ is unique and its electron density $\|\Psi_\alpha^{V_R}\|_{\mathscr{F}}^2(x)$ is therefore a **radial** function!

Nonradiality of Pekar Minimizers

For R large, the Pekar problem for the energy $e^P(V_R)$ admits only **nonradial** minimizers.

A Discrepancy in Spherical Symmetry

Nonradiality of Pekar Minimizers (RG)

For R large, the Pekar problem for the energy $e^P(V_R)$ admits only **nonradial** minimizers.

- If $\varphi_{V_R}(x)$ is a minimizer, then $\varphi_{V_R}(\mathscr{R}x)$ is also a minimizer for all $\mathscr{R} \in SO(3)$.
- The **radial** ground-state electron density $\|\Psi_\alpha^{V_R}\|^2_{\mathscr{F}}(x)$ **cannot converge weakly** to a nonradial minmimizer $\varphi_{V_R}(x)$.

Assuming the Minimizers are Unique up to Rotation...

Convergence to Rotational Average

Let R be large enough so that the minimization problem for $e^P(V_R)$ admits only nonradial minimizers, and assume that the nonradial minimizer $\varphi_{V_R}(x)$ is unique up to rotation. Let γ be the Haar measure on $SO(3)$. Then, for all $W \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$

$$\lim_{\alpha\to\infty} \frac{1}{\alpha^3} \int_{\mathbb{R}^3} \|\Psi_\alpha^{V_R}\|_{\mathscr{F}}^2 \left(\frac{x}{\alpha}\right) W(x)dx = \int_{\mathbb{R}^3} \left[\int_{SO(3)} \left|\varphi_{V_R}(\mathscr{R}x)\right|^2 d\gamma(\mathscr{R})\right] W(x)\, dx$$