On the Global Minimum of the Energy–Momentum relation for the Polaron

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Remarks and outline

1. our result, inspired by Gerlach–Löwen, met the one of Polzer
2. we use more pedestrian operator techniques (which should be powerful enough, we show that in fact they are)
3. motivation – localization and symmetry breaking
4. statement and some insight into the guts of the proof
5. fresh news from the many–body physics community that are of interest in this context
6. is Pekar over? (with K. Jachymski – many thanks to the NCN for the financial support)

Elementary example

Consider a system of N non-relativistic quantum particles interacting via isotropic pair potentials $v_{ij}(|x_i - x_j|)$:

$$H_N = -\sum_{i=1}^{N} \frac{1}{2m_i}\Delta_{x_i} + \sum_{i<j} v_{ij}(|x_i - x_j|). \tag{1}$$

Now this Hamiltonian, defined on (a dense subspace of) $\otimes_{i=1}^{N} L^2(\mathbb{R}^3)$, has no ground state, just because 0 is the infimum of the spectrum of $-\Delta$ on $\mathbb{R}^3$ but not an eigenvalue.

Separation of the center of mass.

$$\begin{aligned} R = & \quad \tfrac{1}{M_t}\textstyle\sum_{i=1}^{N} m_i x_i \\ y_i = & \quad x_i - x_1, \quad i = 2, \ldots, N \end{aligned}$$

with $M_t = \sum_{i=1}^{N} m_i$ the total mass of the system. Then

$$H_N = -\frac{\Delta_R}{2M} + \sum_{i=2}^{N}\left(\frac{-\Delta_{y_i}}{2m_i} + v_{1,i}(y_i)\right) + \sum_{i,j=2}^{N} \frac{\nabla_{y_i}\nabla_{y_j}}{m_1} + \sum_{2=i<j\leq N} v_{ij}(y_i - y_j).$$

Thus there is no ground state of the whole as above, as the center of mass is separated from the rest ot the Hamiltonian and behaves as a free particle. This is attributed to translation invariance.

- It is known that under certain circumstances, ground states are degenerate and do not exhibit the same symmetry as the Hamiltonian (ex.: the Ising model).
- A question arises if translation symmetry can be broken in this way in field–theoretic models, where one cannot just simply separate out the motion of the center of mass due to the fluctuating particle number.
- In the physics literature, there has been one popular candidate for translation symmetry breaking.

The Fröhlich Hamiltonian

Quantum particle interacting with a phonon field.

$$\mathbb{H} = -\frac{1}{2m}\Delta_x + \int_{\mathbb{R}^d} \epsilon(k) a_k^\dagger a_k dk + \sqrt{\alpha} \int_{\mathbb{R}^d} \left(v(k) a_k e^{ik\cdot x} + \overline{v(k)} a_k^\dagger e^{-ik\cdot x} \right) dk.$$

- $v(k) \in L^2(\mathbb{R}^d)$ - *form factor*; $\epsilon(k) > 0$ - *dispersion relation*,
- $[a_k, a_q^\dagger] = \delta(k - q)$,
- Domain $\subset L^2(\mathbb{R}^d) \otimes \mathcal{F}$, $\mathcal{F} = \bigoplus_{n=0}^{\infty} L^2_{\mathrm{sym}}(\mathbb{R}^{dn})$
- $\alpha > 0$ coupling constant.

Fröhlich 1937, classical counterpart Landau 1933, Feynman's path-integral approach 1955, first rigorous paper Lieb–Yamazaki 1958.

- Study important for the understanding of transport pheonomena in **semiconductors, polymers, nanostructrues, ultracold gases** and presumably also **high-temperature superconductors**.

The Fröhlich polaron

- Continuum approximation
- $v(k) = \frac{1}{\sqrt{2}\pi}\frac{1}{|k|}$, charge-dipole interaction
- $\epsilon(k) = 1$ (optical phonons)

$$\mathbb{H} = -\Delta_x + \underbrace{\int_{\mathbb{R}^3} a_y^\dagger a_y \; dy + \sqrt{\alpha}\int_{\mathbb{R}^3} \frac{a_y^\dagger + a_y}{|x-y|^2} dy}_{\text{Oscillators in constant external potential}}$$

H. Fröhlich, *Theory of electrical breakdown in ionic crystals*, Proc. R. Soc. Lond. A **160**, 230-241 (1937).

Landau 1932: translation invariance breaking in the form of a localization transition suggested in a one–page paper.

The Hamiltonian does *not* commute with the particle number operator $N = \int dk a_k^\dagger a_k$, and thus the number of particles is not a good quantum number - it fluctuates. However, it does commute with the *total momentum*:

$$[\mathbb{H}, -i\nabla_x + P_f] = 0 \tag{2}$$

$$P_f = \int dk \;\, k \;\, a_k^\dagger a_k \tag{3}$$

(the field momentum), and is hence translationally invariant.

Translation invariance and LLPT

We have translation invariance, but cannot really "separate the center of mass". We can, however, fix the total momentum of the system.

- Lee-Low-Pines transformation

$$e^{iP_f x} a_k^\dagger e^{-iP_f x} = e^{ikx} a_k^\dagger$$

After the transformation, $\mathbb{H}$ turns into

$$\mathbb{H} = \frac{1}{2m}(-i\nabla_x - P_f)^2 + \int_{\mathbb{R}^d} \epsilon(k) a_k^\dagger a_k dk + \sqrt{\alpha} \int_{\mathbb{R}^d} \left(v(k) a_k + \overline{v(k)} a_k^\dagger \right) dk.$$

and thus $\mathbb{H}$ unitarily equivalent to $\int dP |P\rangle\langle P| \otimes \mathbb{H}_P$ with

$$\mathbb{H}_P = \frac{1}{2m}(P - P_f)^2 + \int_{\mathbb{R}^d} \epsilon(k) a_k^\dagger a_k dk + \sqrt{\alpha} \int_{\mathbb{R}^d} \left(v(k) a_k + \overline{v(k)} a_k^\dagger \right) dk.$$

Energy-momentum relation

$$E(P) = \inf \operatorname{spec} \mathbb{H}_P$$

(ground-state energy at fixed total momentum P).

The semiclassical counterpart of the quantum problem is given by the electronic Pekar functional

$$\mathcal{E}_\alpha^{\mathrm{Pek}}(\psi) = \frac{1}{2m}\int |\nabla\psi(x)|^2 - \alpha \iint |\psi(x)|^2 \frac{1}{|x-y|} |\psi(y)|^2 dxdy$$

Effectively, the polarization acts back on the electron in the form of a Coulomb potential.

- Pekar energy:

$$E^{\mathrm{Pek}}(\alpha) = \inf_{\psi \in L^2(\mathbb{R}^d), \|\psi\|_2 = 1} \mathcal{E}_\alpha^{\mathrm{Pek}}(\psi).$$

- It is known that $E_0/E^{\mathrm{Pek}}(\alpha) \to 1$ as $\alpha \to \infty$ (also for a certain class of regular form factors). On the other hand, $\mathcal{E}_\alpha^{\mathrm{Pek}}(\psi)$ possesses a manifold of ground states – localization and translation symmetry breaking occurs at the semiclassical level. This observation supported the idea of localization also for the full quantum model for α large enough.

The question is related to the properties of the energy–momentum relation. Heuristically, suppose that the set of global minima of $E(P)$, $\mathcal{M}$ has a non–zero Lebesgue measure, and construct the wave packet

$$\Psi = \int_{P \in \mathcal{M}} dP \lambda(P) e^{iPx} |\varphi_P\rangle \tag{4}$$

where $|\varphi_P\rangle$ is a ground state of $\mathbb{H}_P$, and $\lambda(P)$ is some square-integrable function. Then Ψ is square integrable and describes a localized state of the system, and

$$\mathbb{H}\Psi = \int_{P \in \mathcal{M}} dP \lambda(P) e^{iPx} \mathbb{H}_P |\varphi_P\rangle = E\Psi \tag{5}$$

and Ψ would be a localized function - a ground state of $\mathbb{H}$, breaking the translational symmetry, just as in the classical model.

Statements

We disprove this possibility in the folllowing

Theorem (Lampart-Mitrouskas-M 2022)

In the Fröhlich polaron model describing an electron with the induced polarization (quantum) field, it holds that for all $\alpha \geq 0$ and all P with $P \neq 0$,

$$E(0) < E(P). \tag{6}$$

- Proof is based on the idea of employing an auxiliary Hamiltonian, which traces back to Gerlach and Löwen 1988. We benefited from the progress in the analysis of the Fröhlich model in the math physics literature since then, most notably Moeller 2006.

Ideas behind the proof

Let Q be chosen such that $\min_P E(P) = E(Q)$. Assume that in fact $Q \neq 0$, and consider the original LLP-transformed Hamiltonian

$$\mathbb{H}_l = \frac{(-i\nabla_x - P_f)^2}{2m} + \int a_y^\dagger a_y dy + \sqrt{\alpha} \int \frac{a_y^\dagger + a_y}{|y|^2} dy \tag{7}$$

on $L^2([0,l]^3) \otimes \mathcal{F}$, where $l > 0$ is chosen s.t. $Q \in \left(\frac{2\pi}{l}\mathbb{Z}\right)^3$. Then $\mathbb{H}_l$ has a block decomposition

$$\mathbb{H}_l = \bigoplus_{P \in \left(\frac{2\pi}{l}\mathbb{Z}\right)^3} |P\rangle\langle P| \otimes \mathbb{H}_P \tag{8}$$

and – what is crucial – has a ground state $L^{-3/2} e^{iQx} \otimes \varphi_Q$. Now if $Q \neq 0$, then the ground state is necessarily degenerate by rotation invariance.

Let $\alpha > 0$. Then for all $\lambda > -\inf \mathrm{spec H_l}$ the resolvent of $(H_l + \lambda)^{-1}$ is positivity improving with respect to the cone

$$\mathcal{C} := \{\Psi \in L^2([0,l]^3) \otimes \mathcal{F} | \quad \forall n \in \mathbb{N}_0 : (-1)^n \Psi(x, y_1, \cdots y_n) \geq 0\}. \quad (9)$$

Recall that a (Hilbert) *cone* K is a set of elements of a Hilbert space such that K is closed and

1. $\langle v|u\rangle \geq 0$ for all $u, v \in K$;
2. for all w in the Hilbert space, there exist $u, v \in K$ such that $w = u - v$ and u and v are orthogonal.

Moreover, a bounded operator A is

1. positivity preserving w.r.t. K if $Au \in K$ for all $u \in K$;
2. positivity improving if $\langle Au|v\rangle > 0$ for any $u, v \in K\backslash\{0\}$.

Note that with our choice of cone, the interaction energy is negative for all $\Psi \in \mathcal{C}$.

Assume that A is positive definite and has a maximal eigenvalue e with the corresponding eigenvector w, and that it is positivity improving with respect to some cone K. Then w must have multiplicity one.

By the definition of a cone, we can write $w = w_+ - w_-$ where w_+, w_- are in the cone K. Then

$$
\begin{aligned}
e &= \langle w, Aw \rangle \\
&= \langle w_+, Aw_+ \rangle + \langle w_-, Aw_- \rangle - 2 \underbrace{\langle w_-, Aw_+ \rangle}_{\geq 0} \\
&\leq \langle (w_+ + w_-), A(w_+ + w_-) \rangle \leq e,
\end{aligned} \tag{10}
$$

since e is the largest eigenvalue and $\|w_+ + w_-\| = \|w\| = 1$. We must thus have equality in (10), so

$$
\langle w_-, Aw_+ \rangle = 0. \tag{11}
$$

Since A improves positivity this implies that either w_+ or w_- are equal to zero, i.e. $w \in K$ or $-K$. Now assume there exist two orthogonal real eigenfunctions $\Phi, \Psi \in \ker(A - e)$. By changing signs if necessary, we may assume that $\Phi, \Psi \in K \setminus \{0\}$. Then

$$
\langle \Phi, \Psi \rangle = e^{-1} \langle \Phi, A\Psi \rangle > 0, \tag{12}
$$

a contradiction, so e is a simple eigenvalue.

Corollary: $E(Q)$ must then be a simple eigenvalue. But $E(-Q)$ is also an eigenvalue by rotation invariance, which contradicts $Q \neq 0$. Hence, $Q = 0$.

Caution: what is essential here is that there exists Q such that $E(Q) = \inf_P E(Q)$, and that such an $E(Q)$ must be an eigenvalue. This follows from the fact that for models with UV cutoff λ one has

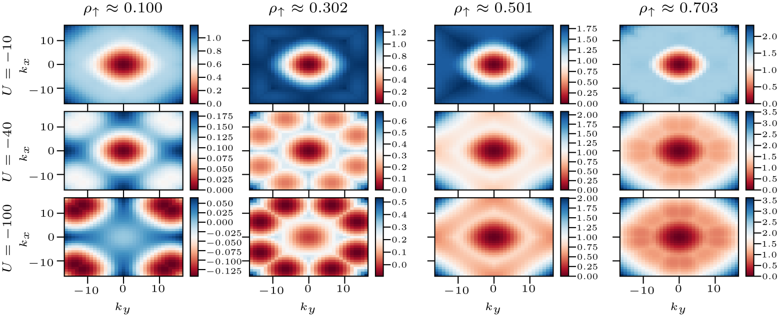
1. $\inf \mathrm{ess\ spec} \mathbb{H}^{\lambda}_{\mathrm{P}} = \mathrm{E}_{\lambda}(0) + 1$
2. $\lim_{|P| \to \infty} |E_{\lambda}(P) - \inf \mathrm{ess\ spec}\ \mathbb{H}^{\lambda}_{\mathrm{P}}| = 0$

and from the norm resolvent convergence of the regularized Hamiltonians to the original hamiltonian of our problem.

News from the physicists

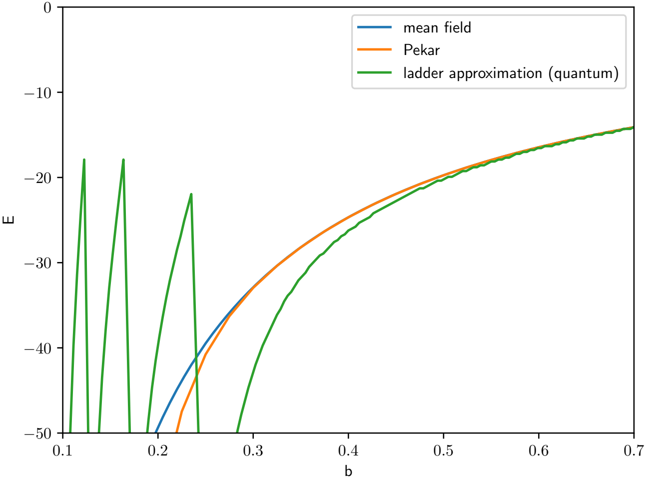
1. Should one regard $E(0) < E(P)$ as obvious?

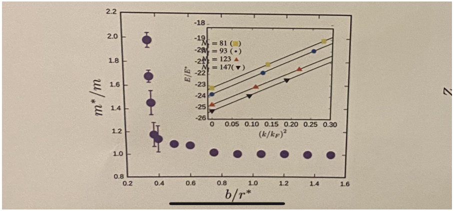
$$H_{FH} = -t \sum_{x,y:|x-y|=1} \left(b_x^\dagger b_y + a_x^\dagger a_y \right) + U \sum_x b_x^\dagger b_x a_x^\dagger a_x \tag{13}$$

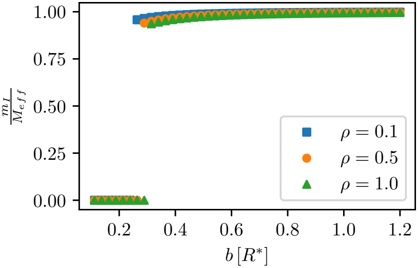


Results by G. Pascual (private communication)

2. Should one ignore Pekar localization altogether?







Monte Carlo results (upper) by L.P Ardila (private communication)