The polaron at strong coupling

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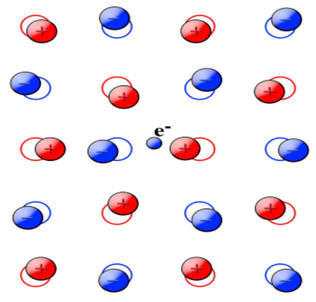
The Polaron

Model of a chargerd particle interacting with the quantized phonons of a polar crystal.

Polarization proportional to the electric field created by the charged particle.



In the **large polaron**, the electron is spread over distances much larger than the crystal spacing. Thus, the polarization field is modelled as a **continuous** quantum field.

The Fröhlich Model

Model of a charged particle interacting with the quantized phonons of a polar crystal.

Polarization proportional to the electric field created by the charged particle.

On $L^2(\mathbb{R}^3, dx) \otimes \mathcal{F}$ (with $\mathcal{F}$ the bosonic Fock space over $L^2(\mathbb{R}^3)$)

$$\mathfrak{H}_\alpha = -\Delta_x + \sqrt{\alpha} \int_{\mathbb{R}^3} \frac{1}{|x-y|^2} (a_y^* + a_y)\, dy + \int_{\mathbb{R}^3} a_y^* a_y \, dy$$

with **coupling constant** $\alpha > 0$.

The bosonic creation and annihilation operators satisfy the usual bosonic CCR

$$[a_y, a_x^*] = \delta(y-x) \qquad [a_y, a_x] = 0.$$

Note: Since $y \mapsto |y|^{-2}$ is not in $L^2(\mathbb{R}^2)$, $\mathfrak{H}_\alpha$ is not defined on the domain of $\mathfrak{H}_0$. It can be defined as a quadric form, however.

The Energy-Momentum Relation

The Fröhlich Hamiltonian is **translation invariant**, i.e., it commutes with the total momentum operator

$$P_{\mathrm{tot}} = -i\nabla_x + \int_{\mathbb{R}^3} a_y^*(-i\nabla_y)a_y \, dy$$

Hence there is a **fiber-integral** decomposition $\mathfrak{H}_\alpha = \int_{\mathbb{R}^3}^{\oplus} \mathfrak{H}_\alpha(P)\, dP$ with

$$\mathfrak{H}_\alpha(P) \cong \left(P - \int_{\mathbb{R}^3} a_y^*(-i\nabla_y)a_y \, dy\right)^2 + \sqrt{\alpha}\int_{\mathbb{R}^3} \frac{1}{|y|^2}(a_y^* + a_y)\, dy + \int_{\mathbb{R}^3} a_y^* a_y \, dy$$

acting on $\mathcal{F}$ only. The energy-momentum spectrum is defined as $(P, \sigma(\mathfrak{H}_\alpha(P)) \subset \mathbb{R}^4$ with the infimum at fixed P called the **energy-momentum relation**

$$E_\alpha(P) = \inf \sigma(\mathfrak{H}_\alpha(P)).$$

In the absence of interaction, $E_0(P) = \min\{P^2, 1\}$ and $\sigma_{\mathrm{ess}}(\mathfrak{H}_0(P)) = [1, \infty)$.

By the HVZ theorem **(Møller 2006)**: $\sigma_{\mathrm{ess}}(\mathfrak{H}_\alpha(P)) = [E_\alpha(0) + 1, \infty)$.

The semiclassical Pekar Functional

The semiclassical approximation amounts to replacing $a_y^* \mapsto \overline{\varphi}(y)$ and $a_y \mapsto \varphi(y)$ with $\varphi \in L^2(\mathbb{R}^3)$. This leads to

$$\mathcal{E}(\psi, \varphi) = \int_{\mathbb{R}^3} |\nabla \psi(x)|^2 dx + 2 \int_{\mathbb{R}^6} \frac{|\psi(x)|^2 \mathrm{Re}\varphi(y)}{|x-y|^2} dx dy + \int_{\mathbb{R}^3} |\varphi(y)|^2 dy.$$

Minimizing with respect to the classical field $\varphi \in L^2(\mathbb{R}^3)$ gives the **Pekar functional**

$$\mathcal{E}^{\mathrm{Pek}}(\psi) = \min_{\varphi} \mathcal{E}(\psi, \varphi) = \int_{\mathbb{R}^3} |\nabla \psi(x)|^2 dx - \int_{\mathbb{R}^6} \frac{|\psi(x)|^2 |\psi(y)|^2}{|x-y|} dx dy.$$

Lieb (1977) proved that there exists a minimizer of $\mathcal{E}^{\mathrm{Pek}}(\psi)$ with $\|\psi\|_2 = 1$ that it unique up to translations ("self-trapping"). We shall write ψ^{Pek} and φ^{Pek}.

Lenzmann (2009) showed that the Hessian at a minizer has only three trivial zero-modes due to the translational symmetry. ("Gold-stone modes")

Asymptotics of the Ground State Energy

Let $e^{\mathrm{Pek}} < 0$ denote the Pekar energy $\min_{\|\psi\|_2=1} \mathcal{E}^{\mathrm{Pek}}(\psi)$.

Using the probabilistic path integral formulation of the problem (Feynman 1955), **Donsker** and **Varadhan** (1983) proved the validity of the Pekar approximation for the ground state energy

$$\lim_{\alpha\to\infty} \alpha^{-2} \inf \sigma(\mathfrak{H}_\alpha) = e^{\mathrm{Pek}}.$$

Lieb and **Thomas** (1997) used operator techniques to obtain the quantitative bound

$$\alpha^2 e^{\mathrm{Pek}} \geq \inf \sigma(\mathfrak{H}_\alpha) \geq \alpha^2 e^{\mathrm{Pek}} - O(\alpha^{9/5})$$

for large α.

The upper bound follows from a simple product ansatz $\psi^{\mathrm{Pek}} \otimes W(\varphi^{\mathrm{Pek}})\Omega$.

Quantum fluctuations

What to expect for the quantum corrections? Consider

$$\mathcal{F}(\varphi) = \min_{\|\psi\|_2=1} \mathcal{E}(\psi,\varphi) = \inf \sigma\Big(-\Delta + 2\mathrm{Re}\varphi * |\cdot|^{-2}\Big) + \int_{\mathbb{R}^3} |\varphi(y)|^2 dy$$

and expand around a minimizer φ^{Pek}

$$\mathcal{F}(\varphi^{\mathrm{Pek}} + \varepsilon\varphi) \approx \mathcal{F}(\varphi^{\mathrm{Pek}}) + \varepsilon^2 \,\mathrm{Hess}|_{\varphi^{\mathrm{Pek}}}\mathcal{F}(\varphi) + o(\varepsilon^2).$$

The Hessian is given in terms of a quadratic form on $L^2(\mathbb{R}^3)$

$$\mathrm{Hess}|_{\varphi^{\mathrm{Pek}}}\mathcal{F}(\varphi) = \sum_{i,j} \Big(S_{ij}\big(\overline{\varphi_i}\varphi_j + \varphi_i\overline{\varphi_j}\big) + T_{ij}\big(\varphi_i\varphi_j + \overline{\varphi_i}\,\overline{\varphi_j}\big)\Big)$$

for some real numbers S_{ij}, T_{ij} and $\varphi(y) = \sum_i \varphi_i u_i(y)$. With this we define the quadratic Fock space operator

$$\mathbb{H} = \sum_{i,j} \Big(S_{ij}\big(a_i^* a_j + a_i a_j^*\big) + T_{ij}\big(a_i a_j + a_i^* a_j^*\big)\Big).$$

This motivates the prediction (Bogoliubov 1949, Allcock 1963)

$$\inf \sigma(\mathfrak{H}_\alpha) = \alpha^2 e^{\mathrm{Pek}} + \inf \sigma(\mathbb{H}) + o(1) \quad \text{as} \quad \alpha \to \infty.$$

Effective Mass

One can use the semiclassical approximation to arrive at the Landau–Pekar prediction

$$m_\alpha = \alpha^4 m^{\mathrm{Pek}} \quad \text{with} \quad m^{\mathrm{Pek}} = \frac{2}{3}\int_{\mathbb{R}^3} |\nabla \varphi^{\mathrm{Pek}}|^2 dy$$

for the **effective mass** defined by $E_\alpha(P) = E_\alpha(0) + P^2/(2m_\alpha) + o(P^2)$ as $P \to 0$.

Putting all together, we can thus expect that the energy-momentum relations satisfies

$$E_\alpha(P) = \alpha^2 e^{\mathrm{Pek}} + \inf \sigma(\mathbb{H}) + \frac{P^2}{2\alpha^4 m^{\mathrm{Pek}}} + o(1)$$

as $\alpha \to \infty$ for all $|P| \lesssim \alpha^2\sqrt{2m^{\mathrm{Pek}}}$.

The restriction $|P| \lesssim \alpha^2\sqrt{2m^{\mathrm{Pek}}}$ comes from $E_\alpha(P) \leq E_\alpha(0) + 1$ for any $P \in \mathbb{R}^3$ due to $\sigma_{\mathrm{ess}}(\mathfrak{H}_\alpha(P)) = [E_\alpha(0) + 1, \infty)$.

Main Results

Theorem [M., Myśliwy, Seiringer, Forum Sigma 2023]: As $\alpha \to \infty$

$$E_\alpha(P) \leq \alpha^2 e^{\mathrm{Pek}} + \inf \sigma(\mathbb{H}) + \min\left\{ \frac{P^2}{2\alpha^4 m^{\mathrm{Pek}}}, 1 \right\} + O(\alpha^{-1/2+\varepsilon}).$$

The proof is based on a trial state estimate for $\mathfrak{H}_\alpha(P)$.

A corresponding lower bound was proved by **Brooks** and **Seiringer** (2022).

Combining both results immediately verifies the Bogoliubov–Allcock prediction

$$\inf \sigma(\mathfrak{H}_\alpha) = \alpha^2 e^{\mathrm{Pek}} + \inf \sigma(\mathbb{H}) + o(1)$$

and shows that the inverse global curvature of $E_\alpha(P)$ agrees with the Landau–Pekar mass

$$\lim_{P \to 0} \lim_{\alpha \to \infty} \frac{1}{2} \frac{P^2}{E_\alpha(\alpha^2 P) - E_\alpha(0)} = m^{\mathrm{Pek}}.$$

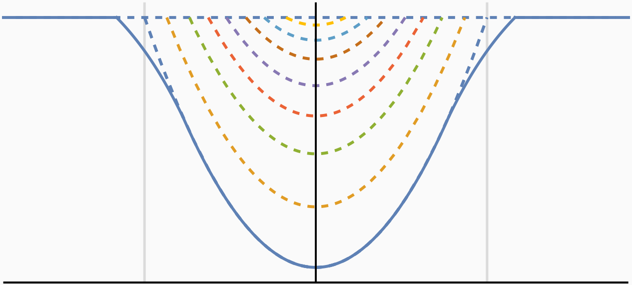
However, it does not say anything about the reversed order of the limits.

Excited States

Does $(P, \sigma(\mathfrak{H}_\alpha(P)))$ contain more discrete eigenvalues than $E_\alpha(P)$?

The upper bound construction can be generalized to prove the existence of **excited bound states** for large α.

Theorem [M., Seiringer 2022]: For $|P| \lesssim \alpha^2$, $\lim_{\alpha\to\infty} |\sigma_{\text{disc}}(\mathfrak{H}_\alpha(P))| = \infty$.



The result is in contrast to small α where $\sigma_{\text{disc}}(\mathfrak{H}_\alpha(0)) = \{E_\alpha(0)\}$ **(Seiringer 2022)**.

The confined Polaron Model

For a bounded region $\Omega \subset \mathbb{R}^3$, let $\Omega_\alpha = \frac{1}{\alpha}\Omega$. We now consider the **confined** polaron model

$$\mathfrak{H}_{\Omega,\alpha} = -\Delta_{\Omega_\alpha} + \sqrt{\alpha} \int_{\Omega_\alpha} v(x,y)(a_y^* + a_y)\, dy + \int_{\Omega_\alpha} a_y^* a_y \, dy$$

defined on $L^2(\Omega_\alpha) \otimes \mathcal{F}(L^2(\Omega_\alpha))$.

Here, Δ_{Ω_α} is the Dirichlet–Laplacian on $L^2(\Omega_\alpha)$ and $v(x,y) = (-\Delta_{\Omega_\alpha})^{-1/2}(x,y)$.

$\mathfrak{H}_{\Omega,\alpha}$ is not translation-invariant and has only discrete spectrum. Also, the corresponding semiclassical energy functional has unique minimizers $\psi^{\mathrm{Pek}}, \varphi^{\mathrm{Pek}}$.

Frank and **Seiringer** (CPAM, 2020) proved the Bogoliubov–Allcock prediction

$$\inf \sigma(\mathfrak{H}_{\Omega,\alpha}) = \alpha^2 e_\Omega^{\mathrm{Pek}} + \inf \sigma(\mathbb{H}_\Omega) + o(1) \quad \text{as} \quad \alpha \to \infty.$$

for α-independent e_Ω^{Pek} and $\inf \sigma(\mathbb{H}_\Omega)$.

Our next result provides an asymptotic expansion in α^{-1} for all eigenvalues.

Asymptotic Expansion for Eigenvalues

Theorem [Brooks, M. 2023]: Let $\mathscr{E}_\alpha^{(n)}$ and $E_0^{(n)}$ denote the nth eigenvalues of $\mathfrak{H}_{\Omega,\alpha}$ and $\mathbb{H}_\Omega$, respectively. There exists a sequence $(E_\ell^{(n)})_{\ell\geq 1}$ such that for every $b \geq 1$

$$\mathscr{E}_\alpha^{(n)} = \alpha^2 e_\Omega^{\text{Pek}} + \sum_{\ell=0}^{b} \frac{1}{\alpha^\ell} E_\ell^{(n)} + O(\alpha^{-b-1}).$$

The coefficients are defined in terms of a two-fold perturbation expansion.

For the proof, we construct approximate eigenstates that satisfy

$$\left\| \left(\mathfrak{H}_{\Omega,\alpha} - \alpha^2 e_\Omega^{\text{Pek}} - \frac{1}{\alpha^2} \sum_{\ell=0}^{b} \frac{1}{\alpha^\ell} E_\ell^{(n)} \right) \Psi^{(b)} \right\| = O(\alpha^{-b-1})$$

and additionally show that no others eigenvalues exist.

If $E_0^{(n)}$ is non-degenerate, the remainder is bounded by $C^b b!/\alpha^{b+1}$, which is reminiscent of Borel–summability. However, we can not prove Borel–summability due to the lack of a suitable analytic continuation of $\mathscr{E}_\alpha^{(n)}$.

Summary

- We investigate the energy-momentum spectrum for the Fröhlich polaron model in the strong coupling limit
- On the natural scale $P \sim \alpha^2$, the energy-momentum relation $E_\alpha(P)$ is a parabola determined by the semiclassical Pekar mass $\alpha^4 m^{\text{Pek}}$.
- The number of excited energy bands between $E_\alpha(P)$ and $E_\alpha(P) + 1$ diverges in the limit $\alpha \to \infty$.
- For the confined polaron, we derive an asymptotic expansion of each eigenvalue in inverse powers of α^{-1}.
- Corresponding results can be obtained for the time-dependent problem, deriving the **Landau–Pekar equations** from the Schrödinger equation of the Fröhlich Hamiltonian in the strong-coupling limit [Leopold, M., Rademacher, Schlein, Seiringer, PAA 2021].