The Polaron at Strong Coupling

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THE POLARON

Model of a charged particle (electron) interacting with the (quantized) phonons of a polar crystal. **Polarization** proportional to the electric field created by the charged particle.
The Fröhlich Model

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

$$H_\alpha = -\Delta - \sqrt{\alpha} \int_{\mathbb{R}^3} \frac{1}{|k|} \left( e^{ikx} a_k + e^{-ikx} a_k^\dagger \right) dk + \int_{\mathbb{R}^3} a_k^\dagger a_k dk$$

with $\alpha > 0$ the coupling strength. The creation and annihilation operators satisfy the usual CCR

$$[a_k, a_l] = 0, \quad [a_k, a_l^\dagger] = \delta(k - l)$$

This models a large polaron, where the electron is spread over distances much larger than the lattice spacing.

Note: Since $k \mapsto |k|^{-1}$ is not in $L^2(\mathbb{R}^3)$, $H_\alpha$ is not defined on the domain of $H_0$. It can be defined as a quadratic form, however.

Similar models of this kind appear in many places in physics, e.g., the Nelson model, spin-boson models, etc., and are used as toy models of quantum field theory.
**Strong Coupling Units**

The Fröhlich model allows for an “exact solution” in the strong coupling limit $\alpha \to \infty$. Changing variables

$$x \to \alpha^{-1} x, \quad a_k \to \alpha^{-1/2} a_\alpha^{-1} k$$

we obtain

$$\alpha^{-2} H_\alpha \cong \hbar_\alpha := -\Delta - \int_{\mathbb{R}^3} \frac{1}{|k|} \left( a_k e^{ikx} + a^\dagger_k e^{-ikx} \right) dk + \int_{\mathbb{R}^3} a^\dagger_k a_k \, dk$$

where the CCR are now $[a_k, a^\dagger_l] = \alpha^{-2} \delta(k - l)$.

Hence $\alpha^{-2}$ is an effective Planck constant and $\alpha \to \infty$ corresponds to a classical limit.

The classical approximation amounts to replacing $a_k$ by a complex-valued function $z_k$. We write it as a Fourier transform

$$z_k = \int_{\mathbb{R}^3} (\varphi(x) + i\pi(x)) e^{-ikx} \, dk$$
The Pekar Functional(s)

The classical approximation leads to the **Pekar functional**

\[
\mathcal{E}(\psi, \varphi, \pi) = \int_{\mathbb{R}^3} |\nabla \psi(x)|^2 dx - 2 \int_{\mathbb{R}^6} \frac{|\psi(x)|^2 \varphi(y)}{|x-y|^2} dx dy + \int_{\mathbb{R}^3} (\varphi(x)^2 + \pi(x)^2) dx
\]

Minimizing with respect to \( \varphi \) and \( \pi \) gives

\[
\mathcal{E}^P(\psi) = \min_{\varphi, \pi} \mathcal{E}(\psi, \varphi, \pi) = \int_{\mathbb{R}^3} |\nabla \psi(x)|^2 dx - \int_{\mathbb{R}^6} \frac{|\psi(x)|^2 |\psi(y)|^2}{|x-y|} dx dy
\]

**Lieb** (1977) proved that there exists a minimizer of \( \mathcal{E}^P(\psi) \) (with \( \|\psi\|_2 = 1 \)) and it is **unique** up to translations and multiplication by a phase.

In particular, the classical approximation leads to **self-trapping** of the electron due to its interaction with the polarization field.

Let \( e^P < 0 \) denote the **Pekar energy**

\[
e^P = \min_{\|\psi\|_2=1} \mathcal{E}^P(\psi)
\]
Asymptotics of the Ground State Energy

Donsker and Varadhan (1983) proved the validity of the Pekar approximation for the ground state energy:

$$\lim_{\alpha \to \infty} \inf \text{spec } h_\alpha = e^P$$

They used the (Feynman 1955) path integral formulation of the problem, leading to a study of the path measure

$$\exp \left( \alpha \int_{\mathbb{R}} ds \frac{e^{-|s|}}{2} \int_0^T \frac{dt}{|\omega(t) - \omega(t + s)|} \right) d\mathbb{W}^T(\omega)$$

as $T \to \infty$, where $\mathbb{W}^T$ denotes the Wiener measure of closed paths of length $T$.

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

$$e^P \geq \inf \text{spec } h_\alpha \geq e^P - O(\alpha^{-1/5})$$

for large $\alpha$. Note that the upper bound follows from a simple product ansatz.
Quantum Fluctuations

What is the leading order correction of $\inf \operatorname{spec} h_\alpha$ compared to $e^P$? With

$$\mathcal{F}^P(\varphi) = \min_{\psi, \pi} \mathcal{E}(\psi, \varphi, \pi) = \inf \operatorname{spec} \left( -\Delta - 2\varphi \ast |x|^{-2} \right) + \int_{\mathbb{R}^3} \varphi(x)^2 dx$$

we expand around a minimizer $\varphi^P$

$$\mathcal{F}^P(\varphi) \approx e^P + \langle \varphi - \varphi^P | H^P | \varphi - \varphi^P \rangle + O(\|\varphi - \varphi^P\|_2^3)$$

with $H^P$ the Hessian at $\varphi^P$. We have $0 \leq H^P \leq 1$, and $H^P$ has exactly 3 zero-modes due to translation invariance (Lenzmann 2009).

Reintroducing the field momentum and studying the resulting system of harmonic oscillators leads to the conjecture

$$\inf \operatorname{spec} h_\alpha = e^P + \frac{1}{2\alpha^2} \operatorname{Tr} \left( \sqrt{H^P} - 1 \right) + o(\alpha^{-2})$$

predicted in the physics literature (Allcock 1963).
A Theorem for a Confined Polaron

Allcock’s conjecture was recently proved for a confined polaron with Hamiltonian

\[
\mathfrak{h}_{\alpha, \Omega} = -\Delta_{\Omega} - \int_{\Omega} (-\Delta_{\Omega})^{-1/2}(x, y) (a_{y} + a^\dagger_{y}) \, dy + \int_{\Omega} a^\dagger_{y} a_{y} \, dy
\]

for (nice) bounded sets \(\Omega \subset \mathbb{R}^3\). Assuming coercivity of the corresponding Pekar functional

\[
\mathcal{E}_{\Omega}^P(\psi) = \int_{\Omega} |\nabla \psi(x)|^2 \, dx - \int_{\Omega^2} |\psi(x)|^2 (-\Delta_{\Omega})^{-1}(x, y)|\psi(y)|^2 \, dx \, dy
\]

i.e.,

\[
\mathcal{E}_{\Omega}^P(\psi) \geq \mathcal{E}_{\Omega}^P(\psi_{\Omega}^P) + K_{\Omega} \min_{\theta} \int_{\Omega} |\nabla (\psi(x) - e^{i\theta} \psi_{\Omega}^P(x))|^2 \, dx
\]

for some \(K_{\Omega} > 0\) (which can be proved for \(\Omega\) a ball [FeliciangeliS19]), one has

**Theorem [FrankS19]:** As \(\alpha \to \infty\)

\[
\inf \text{spec} \mathfrak{h}_{\alpha, \Omega} = e_{\Omega}^P + \frac{1}{2\alpha^2} \text{Tr} \left( \sqrt{H_{\Omega}^P} - 1 \right) + o(\alpha^{-2})
\]
**Effective Mass**

The Fröhlich Hamiltonian $H_\alpha$ is **translation invariant** and commutes with the **total momentum**

$$P = -i \nabla_x + \int_{\mathbb{R}^3} k a_k^\dagger a_k \, dk$$

Hence there is a fiber-integral decomposition $H = \int_{\mathbb{R}^3} H^P \, dP$. In fact,

$$H^P_\alpha \equiv \left( P - \int_{\mathbb{R}^3} k a_k^\dagger a_k \, dk \right)^2 - \sqrt{\alpha} \int_{\mathbb{R}^3} \frac{1}{|k|} \left( a_k + a_k^\dagger \right) \, dk + \int_{\mathbb{R}^3} a_k^\dagger a_k \, dk$$

(acting on $\mathcal{F}$ only). With $E_\alpha(P) = \inf \text{spec } H^P_\alpha$, the **effective mass** $m \geq 1/2$ is defined as

$$\frac{1}{m} := 2 \lim_{P \to 0} \frac{E_\alpha(P) - E_\alpha(0)}{|P|^2}$$

A simple argument based on the Pekar approximation suggests $m \sim \alpha^4$ as $\alpha \to \infty$. The best rigorous result so far is

**Theorem [LiebS19]:** $\lim_{\alpha \to \infty} m = \infty$
SUMMARY AND OPEN PROBLEMS

We derived the **quantum corrections** to the (classical) Pekar asymptotics of the ground state energy of a confined polaron, and showed that the polaron’s **effective mass** diverges in the strong coupling limit.

Many open problems remain:

- Quantum corrections to the Pekar approximation in the unconfined case $\Omega = \mathbb{R}^3$
- Divergence rate of the effective mass, conjectured to satisfy
  \[
  \lim_{\alpha \to \infty} \frac{m}{\alpha^4} = \frac{8\pi}{3} \int_{\mathbb{R}^3} |\psi^{\text{Pek}}(x)|^4 \, dx
  \]
- The Pekar approximation can also be applied in a dynamic setting. It should be possible to derive the corresponding **time-dependent Pekar equations** from the Schrödinger equation with the Fröhlich Hamiltonian.

Recent partial results by Frank & Schlein, Frank & Gang and Griesemer, as well as [Leopold, Rademacher, Schlein, S, 2019].
Ideas in the Proof

Theorem [FrankS19]: As $\alpha \to \infty$

$$\inf \text{spec } h_{\alpha,\Omega} = e_\Omega^P + \frac{1}{2\alpha^2} \text{Tr} \left( \sqrt{H_\Omega^P} - 1 \right) + o(\alpha^{-2})$$

- electron in instantaneous ground state of potential generated by (fluctuating) field
- $\varphi \not\in L^2$, hence not close to $\varphi^P$; need ultraviolet cutoff $\Lambda$
- quantify effect of cutoff using commutator method of [Lieb, Yamazaki, 1958]:

$$\int_{|k|>\Lambda} \frac{e^{ikx}}{|k|} a_k dk = \left[ -i \nabla_x, \int_{|k|>\Lambda} \frac{k e^{ikx}}{|k|^3} a_k dk \right]$$

- we apply, in fact, three commutators, and a Gross transformation, to conclude that the ground state energy is affected at most by $\Lambda^{-5/2}$
- IMS localization in Fock space, use Hessian close to $\varphi^P +$ global coercivity
**Ideas in the Proof**

**Theorem [LiebS19]:** \( \lim_{\alpha \to \infty} m = \infty \)

- decomposing the **Pekar product ansatz** into fibers suggests for the fiber ground states \( \Phi_P \)

\[
\Phi_P \approx \hat{\psi}_\alpha^{\text{Pek}} (P - P_f) e^{a^\dagger (\varphi^{\text{Pek}})} |\Omega\rangle \approx \Phi_0 + P \cdot \frac{\nabla \hat{\psi}_\alpha^{\text{Pek}} (-P_f)}{\hat{\psi}_\alpha^{\text{Pek}} (-P_f)} \Phi_0
\]

- use this as a **trial state** for \( H_P \), with \( \Phi_0 \) the actual ground state of \( H_0 \), yielding

\[
\frac{1}{2m} \leq 1 + \langle \Phi_0 | \mathcal{O}_\alpha | \Phi_0 \rangle
\]

for some explicit operator \( \mathcal{O}_\alpha \) built from \( P_f \) and \( H_0 \).

- Prove that \( \lim_{\alpha \to \infty} \langle \Phi_0 | \mathcal{O}_\alpha | \Phi_0 \rangle = -1 \) by suitably **perturbing** \( H \) and redoing the Lieb-Thomas proof with perturbation terms.