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The Polaron at Strong Coupling

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Mean-field and other effective models in mathematical physics

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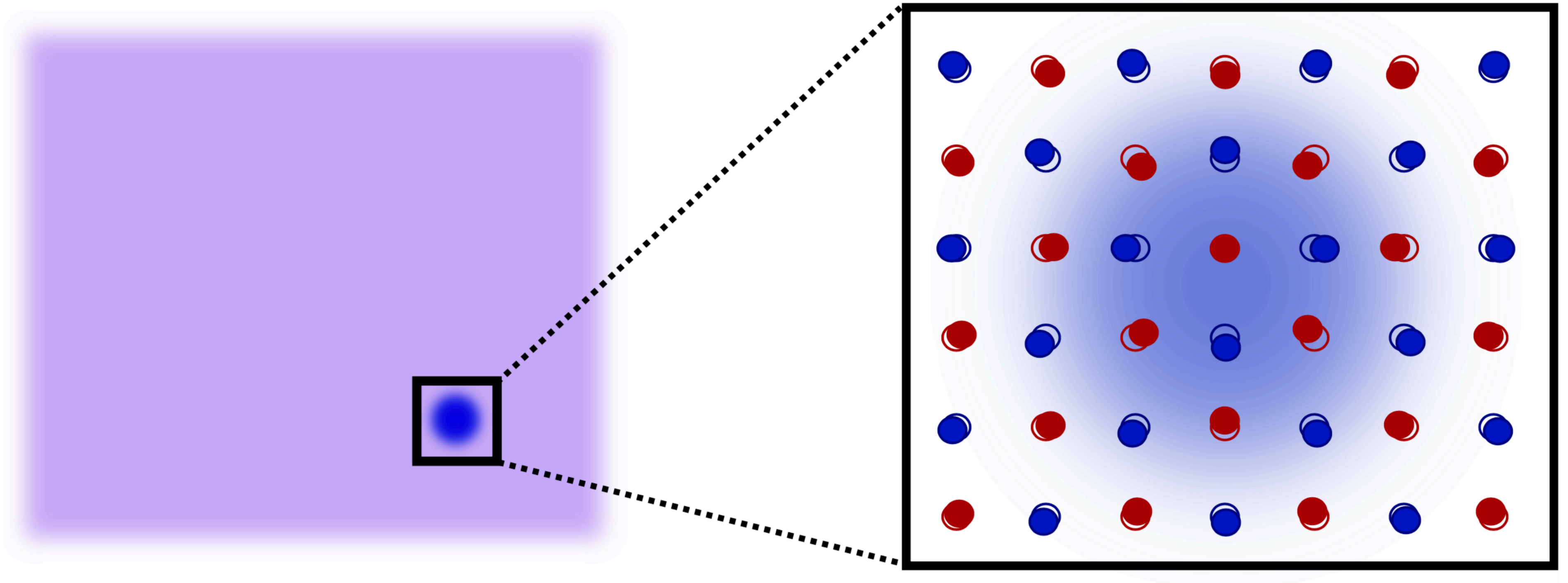
The Polaron

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 $L^2(\mathbb{R}^3)$),

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

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

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

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_α 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

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

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

Hence α^{-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

$$z_k = \int_{\mathbb{R}^3} \left(\varphi(x) + i\pi(x) \right) e^{-ikx} dk$$

The Pekar Functional(s)

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

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

Minimizing with respect to φ and π gives

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

Lieb (1977) proved that there exists a minimizer of $\mathcal{E}^{\mathrm{P}}(\psi)$ (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 $e^{\mathrm{P}} < 0$ denote the **Pekar energy**

$$e^{\mathrm{P}} = \min_{\|\psi\|_2=1} \mathcal{E}^{\mathrm{P}}(\psi)$$

Asymptotics of the Ground State Energy

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

$$\lim_{\alpha\to\infty} \inf \operatorname{spec} \mathfrak{h}_\alpha = e^{\mathrm{P}}$$

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

$$e^{\mathrm{P}} \geq \inf \operatorname{spec} \mathfrak{h}_\alpha \geq e^{\mathrm{P}} - O(\alpha^{-1/5})$$

for large α. Note that the upper bound follows from a simple product ansatz.

Quantum Fluctuations

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

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

we expand around a minimizer φ^{P}

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

with H^{P} the **Hessian** at φ^{P}. We have $0 \leq H^{\mathrm{P}} \leq \mathbb{1}$, 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**

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

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

$$\mathfrak{h}_{\alpha,\Omega} = -\Delta_\Omega - \int_\Omega (-\Delta_\Omega)^{-1/2}(x,y)\left(a_y + a_y^\dagger\right) dy + \int_\Omega a_y^\dagger a_y \, dy$$

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

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

i.e.,

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

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

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

$$\inf \operatorname{spec} \mathfrak{h}_{\alpha,\Omega} = e_\Omega^{\mathrm{P}} + \frac{1}{2\alpha^2} \mathrm{Tr}\left(\sqrt{H_\Omega^{\mathrm{P}}} - \mathbb{1}\right) + o(\alpha^{-2})$$

Effective Mass

The Fröhlich Hamiltonian H_α 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 $H = \int_{\mathbb{R}^3}^{\oplus} H_\alpha^P\, dP$. In fact,

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

(acting on $\mathcal{F}$ only). With $E_\alpha(P) = \inf \operatorname{spec} H_\alpha^P$, 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]:

$$\lim_{\alpha \to \infty} m = \infty$$

Further Results and Open Problems

- With **Frank**, **Lieb** and **Thomas** we have studied the many-polaron problem (where an additional Coulomb repulsion between the electrons has to be taken into account).

  We investigated polaron **binding** due to the effective attraction via the polarization field, and the resulting question of **stability** of the system for large particle number.

- 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] (**next talk**)