Ubiquity of bound states for the strongly coupled polaron

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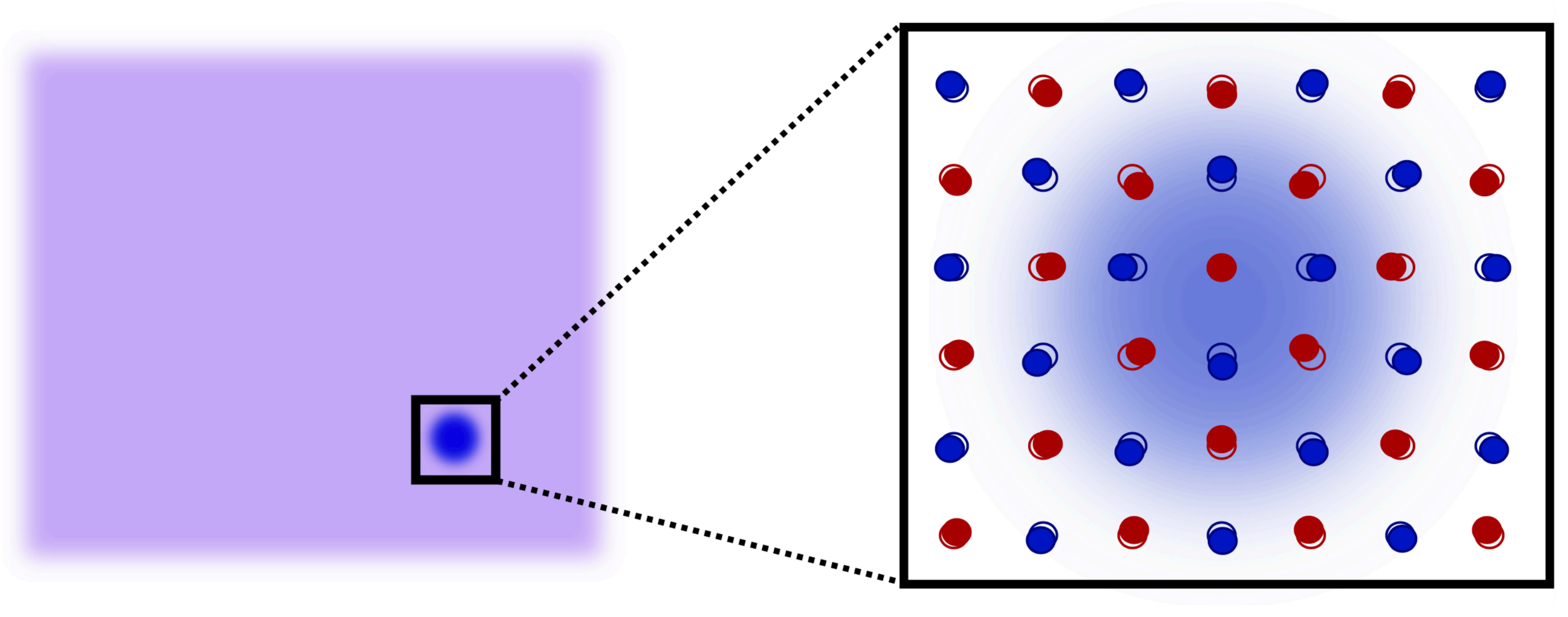
The Polaron

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

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.

On $L^2(\mathbb{R}^3) \otimes \mathcal{F}$ (with $\mathcal{F} = \bigoplus_{n\geq 0} L^2_{\rm sym}(\mathbb{R}^{3n})$ the bosonic Fock space over $L^2(\mathbb{R}^3)$),

$$\mathfrak{H}_\alpha = -\Delta - \sqrt{\alpha}\, \Phi(v_x) + \mathbb{N} \quad , \quad v_x(y) = \frac{1}{|x-y|^2}$$

with $\alpha > 0$ the coupling strength and $\Phi(f) = a(f) + a^\dagger(f)$. The creation and annihilation operators satisfy the usual **CCR**

$$[a(f), a(g)] = 0 \quad , \quad [a(f), a^\dagger(g)] = \langle f | g \rangle$$

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

Note: Since $y \mapsto |y|^{-2}$ is not in $L^2(\mathbb{R}^3)$, $\mathfrak{H}_\alpha$ is not defined on the domain of $\mathfrak{H}_0$. It can be defined as a quadratic form, however.

Energy–Momentum Spectrum and Effective Mass

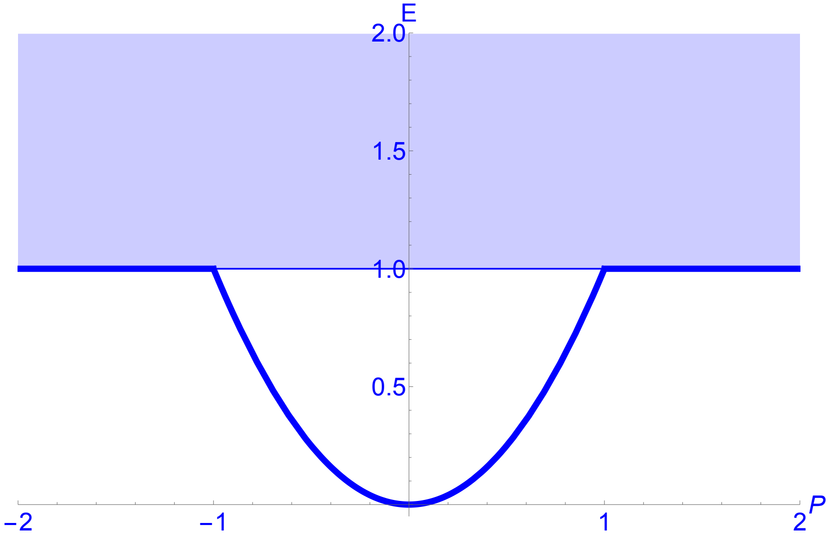
The Fröhlich Hamiltonian $\mathfrak{H}_\alpha$ is **translation invariant** and commutes with the **total momentum** $P = -i\nabla_x + P_f$, $P_f = d\Gamma(-i\nabla_y)$. Hence there is a fiber-integral decomposition $\mathfrak{H}_\alpha = \int_{\mathbb{R}^3}^{\oplus} \mathfrak{H}_\alpha^P \, dP$. In fact,

$$\mathfrak{H}_\alpha^P \cong (P - P_f)^2 - \sqrt{\alpha}\,\Phi(v) + \mathbb{N} \qquad \text{(acting on } \mathcal{F} \text{ only)}$$

Energy–momentum spectrum $(P, \sigma(\mathfrak{H}_\alpha^P))$, with infimum

$$E_\alpha(P) = \inf \operatorname{spec} \mathfrak{H}_\alpha^P$$

Note: $\sigma_{\text{ess}}(\mathfrak{H}_\alpha^P) = [E_\alpha(0) + 1, \infty)$ for any P. In the absence of interaction ($\alpha = 0$), $E_0(P) = \min\{|P|^2, 1\}$, and $\sigma_{\text{ess}}(\mathfrak{H}_0^P) = [1, \infty)$.



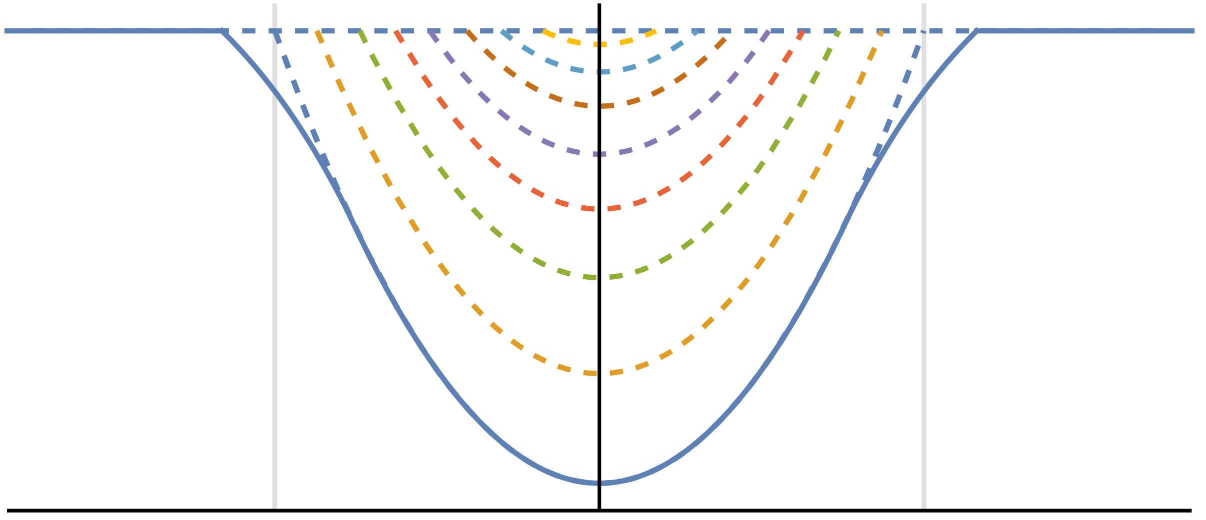
The **effective mass** m_{eff} of the polaron is defined by

$$E_\alpha(P) = E_\alpha(0) + P^2/(2m_{\text{eff}}) + o(P^2) \quad \text{as } P \to 0.$$

Excited States

Our main result concerns the existence of additional spectrum in the gap $(E_\alpha(0), E_\alpha(0)+1)$, i.e., **excited states**. They exist for large α:

THEOREM [Mitrouskas, S. 2023]: For $|P| \ll \alpha^2$, $\lim_{\alpha\to\infty} |\sigma_{\rm disc}(\mathfrak{H}_\alpha^P)| = \infty$



This is in contrast to the case of small α:

THEOREM [S. 2023]: For α small enough, $\sigma_{\rm disc}(\mathfrak{H}_\alpha^0) = \{E_\alpha(0)\}$

Excitation Energies

We actually give **upper bounds** on excited eigenvalues, in terms of a Bogoliubov-type Hamiltonian constructed from the classical **Landau–Pekar** functional (to be explained below).

THEOREM [Mitrouskas, S. 2023]: The nth min-max value $\mu_n(\mathfrak{H}_\alpha^P)$ satisfies

$$\mu_n(\mathfrak{H}_\alpha^P) \leq \alpha^2 e^{\mathrm{Pek}} + \frac{1}{2}\mathrm{Tr}\left(\sqrt{H^{\mathrm{Pek}}} - 1\right) + \Lambda_n + \frac{P^2}{2\alpha^4 m^{\mathrm{LP}}} + O(\alpha^{-1/2+\varepsilon})$$

as $\alpha \to \infty$, where $\Lambda_n < 1$ is the nth eigenvalue of $d\Gamma(\sqrt{H_{\perp 0}^{\mathrm{Pek}}})$.

The result then follows in combination with the following **lower bound** on the ground state energy:

THEOREM [Brooks, S. 2023]:

$$E_\alpha(0) \geq \alpha^2 e^{\mathrm{Pek}} + \frac{1}{2}\mathrm{Tr}\left(\sqrt{H^{\mathrm{Pek}}} - 1\right) + O(\alpha^{-1/29+\varepsilon})$$

The Classical Pekar Functional

The **classical approximation** amounts to replacing $a(f)$ by $\int \overline{f(y)}\varphi(y)dy$ for a complex-valued function φ. This leads to

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

Lieb (1977) proved that there exists a minimizer $\{\psi^{\mathrm{Pek}},\varphi^{\mathrm{Pek}}\}$ of $\mathcal{E}^{\mathrm{Pek}}$ (with $\|\psi\|_2 = 1$) and it is **unique** up to translations and multiplication by a phase. (**"self-trapping"**)

Lenzmann (2009) showed that the Hessian at a minimizer has only trivial **zero-modes** due to the symmetries.

Based on a **traveling wave** ansatz, one arrives at the **Landau–Pekar** prediction

$$m_{\mathrm{eff}} = \frac{2}{3}\int |\nabla\varphi^{\mathrm{Pek}}|^2 = \alpha^4 m^{\mathrm{Pek}}$$

for the polaron's effective mass, now known to be valid as $\alpha\to\infty$ [Brooks, S., 2024].

Asymptotics of the Ground State Energy

Denote the **Pekar energy** by $\alpha^2 e^{\mathrm{Pek}} = \min_{\|\psi\|_2=1} \mathcal{E}^{\mathrm{Pek}}(\psi,\phi) < 0$. **Donsker and Varadhan** (1983) proved the validity of the Pekar approximation for the ground state energy:

$$\lim_{\alpha\to\infty} \alpha^{-2} \inf \operatorname{spec} \mathfrak{H}_\alpha = e^{\mathrm{Pek}}$$

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

$$\exp\left(\alpha\pi^3 \int_{\mathbb{R}} ds \frac{e^{-|s|}}{2} \int_0^T \frac{dt}{|\omega(t)-\omega(t+s)|}\right) d\mathbb{W}^T(\omega)$$

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

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

for large α. Upper bound follows from a simple product ansatz $\psi^{\mathrm{Pek}} \otimes W(\varphi^{\mathrm{Pek}})\Omega$.

Quantum Fluctuations

What is the **leading order correction** of $\inf \operatorname{spec} \mathfrak{H}_\alpha$ compared to $\alpha^2 e^{\mathrm{Pek}}$? With

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

we expand around a minimizer φ^{Pek}

$$\mathcal{F}^{\mathrm{Pek}}(\varphi) \approx \alpha^2 e^{\mathrm{Pek}} + \langle \varphi - \varphi^{\mathrm{Pek}} | H^{\mathrm{Pek}} | \varphi - \varphi^{\mathrm{Pek}} \rangle + O(\|\varphi - \varphi^{\mathrm{Pek}}\|_2^3)$$

with H^{Pek} the **Hessian** at φ^{Pek}. We have $0 \leq H^{\mathrm{Pek}} \leq \mathbb{1}$, and H^{Pek} has exactly **3 zero-modes** due to translation invariance (Lenzmann 2009).

Re-introducing the field momentum and studying the resulting system of harmonic oscillators leads to the **prediction** (Allcock 1963)

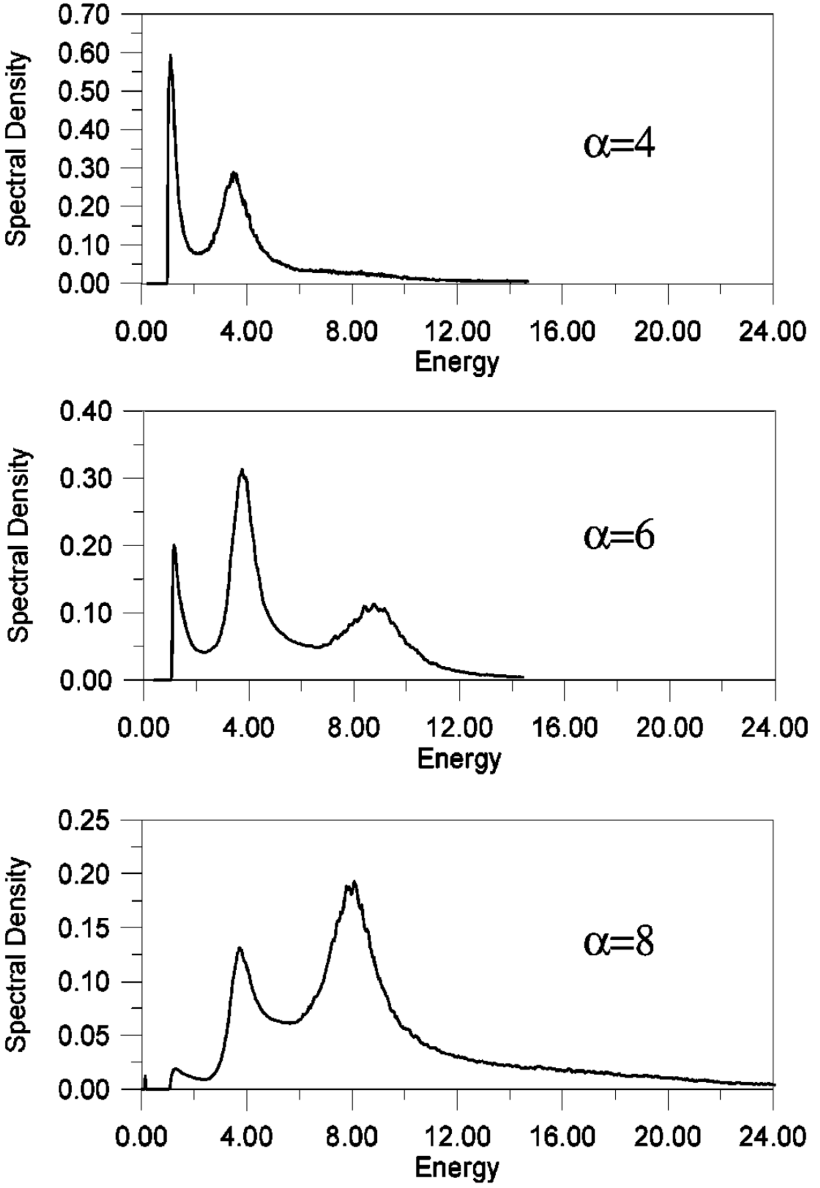
$$\inf \operatorname{spec} \mathfrak{H}_\alpha = \alpha^2 e^{\mathrm{Pek}} + \frac{1}{2}\operatorname{Tr}\left(\sqrt{H^{\mathrm{Pek}}} - \mathbb{1}\right) + o(1) \quad \text{as } \alpha \to \infty$$

Numerics

Previous **numerical investigations** up to $\alpha \approx 8$ have not shown a sign of the excited states.

Diagrammatic quantum Monte Carlo study by [Mishchenko et al. 2000] of the **spectral density** defined by

$$\langle \Omega | e^{-t\mathfrak{H}_\alpha^0} | \Omega \rangle = \int_0^\infty e^{-t(E_\alpha(0)+\lambda)} d\mu(\lambda)$$

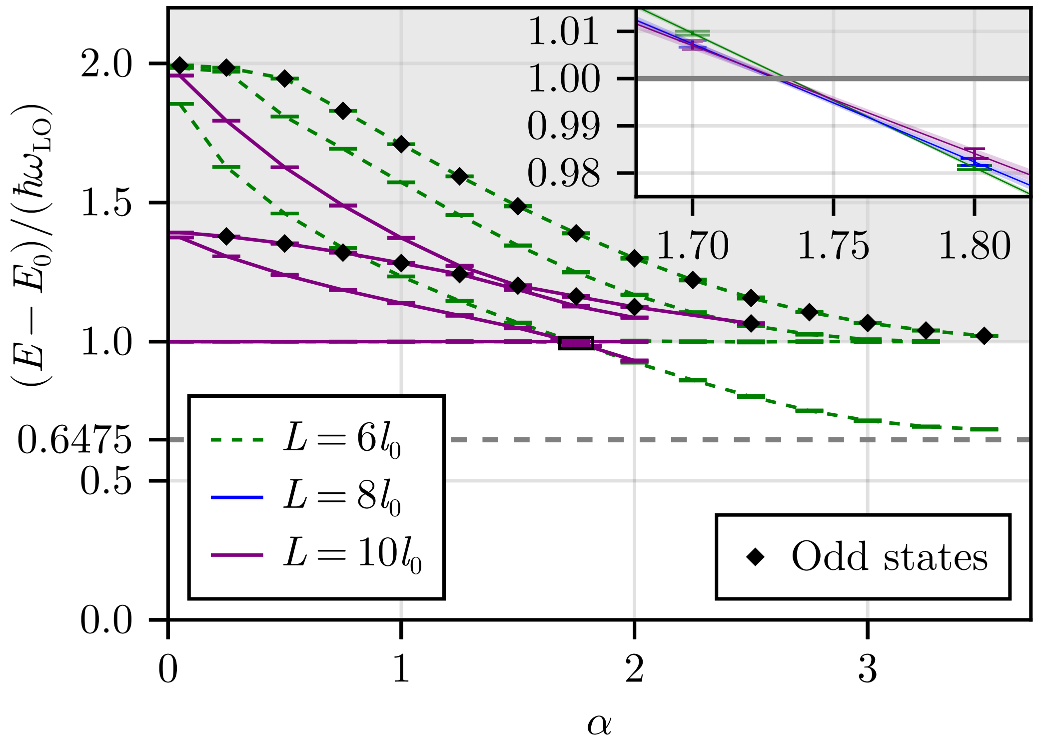


Numerics for a model in one dimension

For the Fröhlich model in **one dimension**, defined on $L^2(\mathbb{R}) \otimes \mathcal{F}(L^2(\mathbb{R}))$ as

$$\mathfrak{H}_\alpha = -\partial_x^2 - \sqrt{\alpha}\,\Phi(v_x) + \mathbb{N} \quad , \quad v_x(y) = \delta(x-y)$$

recent numerical investigations [Brand et al. 2025] have shown that the critical value for the appearance of the first bound state is $\alpha_c \approx 1.73$.



Conclusions

- We investigate the **energy–momentum spectrum** for the Fröhlich polaron model.
- In the strong coupling limit, we show that the number of **bound states** of $\mathfrak{H}_\alpha^{P=0}$ below the essential spectrum $[E_\alpha(0)+1,\infty)$ diverges as $\alpha \to \infty$.
- We derive upper bounds on the min-max values of $\mathfrak{H}_\alpha^P$, which display a two-term asymptotics corresponding to the **classical approximation** and **quantum fluctuations** about the classical limit.
- In combination with a corresponding **lower bound** on the absolute ground state energy, this proves the existence of many excited eigenvalues at large coupling.
- It remains an **open problem** to determine (numerically) the critical coupling constant for the appearance of the first excited state.
- For a corresponding **one-dimensional model**, the numerics shows that $\alpha_c \approx 1.73$.