The Strongly Coupled Polaron on a Torus

Quantum Corrections to the Pekar Asymptotics

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joint work with Robert Seiringer

From Equilibrium Phenomena Towards Open Quantum Systems,
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Physical and Mathematical Introduction

The Polaron Model - Physical Introduction

Physical picture:

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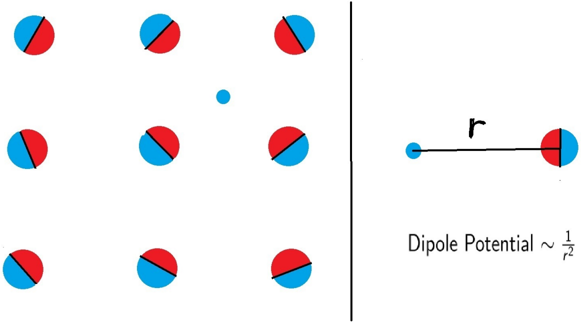

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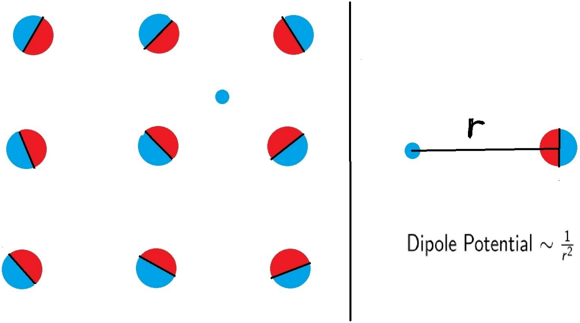

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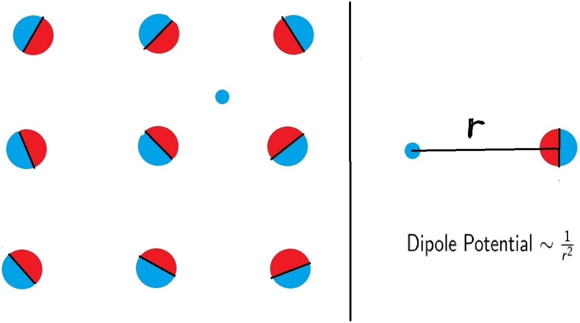

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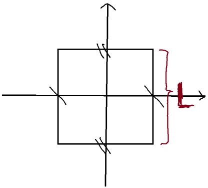
Phonons: name used to refer to the quantum field of excitations induced by the electron.

We work on $\mathbb{T}_L^3 := [-L/2, L/2]^3$.
L is a parameter of the problem.



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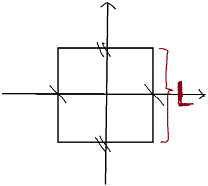

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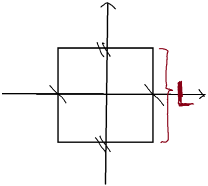

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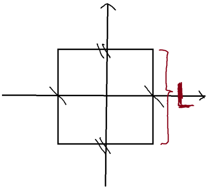

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State Space: $\mathcal{H} = \underbrace{L^2(\mathbb{T}_L^3)}_{\text{electron}} \otimes \underbrace{\mathcal{F}}_{\text{phonons}}$, where $\mathcal{F}$ is the **bosonic Fock space** over $L^2(\mathbb{T}_L^3)$.

The Mathematical Model: Fröhlich Hamiltonian

If the wavelength of the electron is much larger than the lattice spacing, the Polaron is described by the **Fröhlich Hamiltonian**[1], defined on $\mathcal{H}$ by:

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Here a_α and $a_\alpha^\dagger$ satisfy the **rescaled** CCR:

$$[a_\alpha(f), a_\alpha^\dagger(g)] = \alpha^{-2} \langle f|g\rangle \xrightarrow{\alpha\to\infty} 0.$$

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We are interested in the expansion of **ground state energy** of the system in the limit $\boxed{\alpha \to \infty}$, i.e. the α-expansion of

$$\boxed{E_L := \inf_{\Psi\in\mathcal{H}} \langle\Psi|H_{\alpha,L}|\Psi\rangle}$$

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Classical Functional(s) and Pekar Asymptotics

We introduce the **classical functional(s)** corresponding to the Fröhlich Hamiltonian

$$\mathcal{G}_L(\psi,\varphi) := \|\varphi\|_2^2 + \langle\psi|\overbrace{-\Delta_L + \underbrace{V_\varphi}_{-2(-\Delta_L)^{-1/2}\varphi}}^{h_\varphi}|\psi\rangle$$

$$\mathcal{E}_L(\psi) := \inf_\varphi \mathcal{G}_L(\psi,\varphi) = \mathcal{G}_L(\psi,(-\Delta_L)^{-1/2}|\psi|^2) = \langle\psi|-\Delta_L|\psi\rangle - \left\langle|\psi|^2\middle|(-\Delta_L)^{-1}\middle||\psi|^2\right\rangle$$

$$\mathcal{F}_L(\varphi) := \inf_\psi \mathcal{G}_L(\psi,\varphi) = \mathcal{G}_L(\underbrace{\psi_\varphi}_{\text{g.s. of } h_\varphi},\varphi) = \|\varphi\|_2^2 + \text{inf spec}\, h_\varphi$$

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Pekar Asymptotics states that

$$E_L = e_L + o_\alpha(1)$$

where

$$e_L = \inf_{\psi,\varphi} \mathcal{G}_L(\psi,\varphi) = \inf_{\psi} \mathcal{E}_L(\psi) = \inf_{\varphi} \mathcal{F}_L(\varphi)$$

Our Results and General Overview

Results - Properties of the Classical Functionals on $\mathbb{T}_L^3$

If we define $\mathcal{M}_L^{\mathcal{E}}$ and $\mathcal{M}_L^{\mathcal{F}}$ to be the set of minimizers of the functional $\mathcal{E}_L$ and $\mathcal{F}_L$ respectively, we can prove the following.

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If we define $\mathcal{M}_L^{\mathcal{E}}$ and $\mathcal{M}_L^{\mathcal{F}}$ to be the set of minimizers of the functional $\mathcal{E}_L$ and $\mathcal{F}_L$ respectively, we can prove the following.

Theorem (F., Seiringer 2020)

There exists $0 < L_1 < \infty$ and a universal and positive constant κ s.t. for $L > L_1$ there exists $0 < \psi_L \in C^\infty(\mathbb{T}_L^3)$, such that $\psi_L^y \neq \psi_L$ for any $0 \neq y \in \mathbb{T}_L^3$ and

$$\boxed{\mathcal{M}_L^{\mathcal{E}} = \{e^{i\theta}\psi_L^y \mid \theta \in [0, 2\pi),\ y \in \mathbb{T}_L^3\}} \quad \Rightarrow \quad \mathcal{M}_L^{\mathcal{F}} = \left\{\varphi_L^y \mid y \in \mathbb{T}_L^3\right\}$$

finally, for any normalized $f \in L^2(\mathbb{T}_L^3)$

$$\boxed{\mathcal{E}_L(f) - e_L \geq \kappa\, \mathrm{dist}^2_{H^1}\left(\mathcal{M}_L^{\mathcal{E}}, f\right)} \quad \Rightarrow \quad \mathcal{F}_L(\varphi) - e_L \geq \inf_{y \in \mathbb{T}_L^3} \langle \varphi - \varphi_L^y | B | \varphi - \varphi_L^y \rangle$$

$$\text{with} \quad B = \mathbb{1} - (\mathbb{1} + \kappa'(-\Delta_L)^{-1/2})^{-1}$$

Results - Second order Expansion of GSE on $\mathbb{T}^3_L$

Theorem (F., Seiringer 2020)

For any $L > L_1$ and any $\varphi_L \in \mathcal{M}_L^{\mathcal{F}}$, as $\alpha \to \infty$

$$E_L = \inf \operatorname{spec} H_{\alpha,L} = e_L - \frac{1}{2\alpha^2} \operatorname{Tr}\left(\mathbb{1} - \sqrt{D^2\mathcal{F}_L(\varphi_L)}\right) + o(\alpha^{-2}),$$

more precisely, the bounds

$$-C_L\alpha^{-1/7} \leq \alpha^2(E_L - e_L) + \frac{1}{2}\operatorname{Tr}\left(\mathbb{1} - \sqrt{D^2\mathcal{F}_L(\varphi_L)}\right) \leq C_L\alpha^{-2/11}$$

hold for some $C_L > 0$ and α sufficiently large.

Overview of Known Results

	Ω Dirichlet b.c.	$\mathbb{T}^3_L(L > L_1)$	$\mathbb{R}^3$
Class. Fun.	✓ (only for B_R)[2]	✓	✓[3]
GSE expansion (order I)	✓[4]	✓	✓[5]
GSE expansion (order II)	✓[4]	✓	

[2] Dario Feliciangeli and Robert Seiringer. "Uniqueness and non-degeneracy of minimizers of the Pekar functional on a ball". In: *SIAM Journal on Mathematical Analysis* 52.1 (2020), pp. 605–622

[3] Elliott H Lieb. "Existence and uniqueness of the minimizing solution of Choquard's nonlinear equation". In: *Studies in Applied Mathematics* 57.2 (1977), pp. 93–105

[3] Enno Lenzmann. "Uniqueness of ground states for pseudorelativistic Hartree equations". In: *Analysis & PDE* 2.1 (2009), pp. 1–27

[4] Rupert L. Frank and Robert Seiringer. "Quantum Corrections to the Pekar Asymptotics of a Strongly Coupled Polaron". In: *Communications on Pure and Applied Mathematics* (2021)

[5] Monroe D Donsker and SR Srinivasa Varadhan. "Asymptotics for the polaron". In: *Communications on Pure and Applied Mathematics* 36.4 (1983), pp. 505–528

[5] Elliott H Lieb and Lawrence E Thomas. "Exact ground state energy of the strong-coupling polaron". In: *Condensed Matter Physics and Exactly Soluble Models*. Springer, 1997, pp. 311–321

Thanks for your attention