The energy-momentum relation of the Fröhlich polaron

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Quantissima in the Serenissima IV

August 2022

Based on joint work with J. Lampart, K. Myśliwy and R. Seiringer

The Fröhlich polaron

An electron moving through a continuous polarizable medium.

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

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

with coupling constant $\alpha > 0$ and the bosonic creation and annihilation operators satisfying the usual CCR

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

It is well understood that H_α defines a self-adjoint semi-bounded operator.

Mainly interested in the limit $\alpha \to \infty$. This corresponds to

- strong coupling
- semi-classical regime (the field becomes classical)
- adiabatic decoupling (similarly as in Born–Oppenheimer theory).

Note: Rescaling all lengths by $1/\alpha$ one finds $H_\alpha \cong \alpha^2 \tilde{H}_\alpha$ with

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

Energy-momentum relation

Due to translation invariance H_α commutes with the total momentum

$$P_{\text{tot}} = -i\nabla_x + P_f \quad \text{with} \quad P_f = d\Gamma(-i\nabla).$$

Hence there is a direct integral decomposition

$$H_\alpha \cong \int_{\mathbb{R}^3}^{\oplus} H_\alpha(P)\, dP$$

with fiber Hamiltonian

$$\boxed{H_\alpha(P) = \frac{1}{2}(P - P_f)^2 + \sqrt{\alpha}\int_{\mathbb{R}^3} \frac{1}{|y|^2}(a_y^* + a_y)\, dy + \int_{\mathbb{R}^3} a_y^* a_y\, dy}$$

Note: $H_\alpha(P)$ acts on $\mathcal{F}$ and describes the system at total momentum P.

The energy-momentum relation is defined as

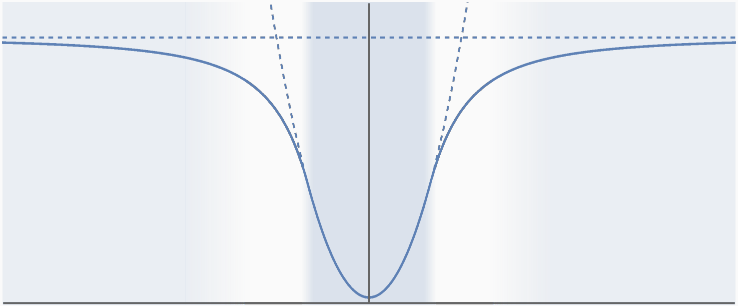
$$P \mapsto E_\alpha(P) := \inf \sigma(H_\alpha(P)).$$

Effective mass $M_\alpha^{\text{eff}} := 1/E_\alpha^{''}(0)$.

Energy-momentum relation

For $\alpha = 0$ one finds $E_0(P) = \min\{\frac{P^2}{2}, 1\}$

For $\alpha > 0$ the expectation from physics is that $E_\alpha(P)$ looks like



Two characteristic regimes

- $E_\alpha(P) \approx E_\alpha(0) + \frac{1}{2M_\alpha^{\mathrm{eff}}} P^2$ for all $P^2 \ll 2M_\alpha^{\mathrm{eff}}$ (quasi-particle regime)
- $E_\alpha(P) \longrightarrow \inf \sigma_{\mathrm{ess}}(H_\alpha(P))$ as $|P| \to \infty$ (radiation regime)

Note: $\sigma_{\mathrm{ess}}(H_\alpha(P)) = [E_\alpha(0) + 1, \infty)$ as shown by Møller 06

Qualitative results

A non-complete list of known qualitative results

- $E_\alpha(0) \leq E_\alpha(P)$ (L. Gross 72)
- Domain of analyticity in P and α (J. Fröhlich 74, Spohn 88)
- Monotonicity and concavity of $|P| \to E_\alpha(|P|)$ (Polzer 22)

Our first result proves that $P = 0$ is the unique global minimum.

Theorem (Lampart–M–Myśliwy 22) For all $\alpha \geq 0$ and $P \in \mathbb{R}^3$

$$E_\alpha(0) < E_\alpha(P).$$

Based on a Perron–Frobenuis argument (motivated by Gerlach–Löwen 91)

In the probabilistic framework this was also shown by Dybalski–Spohn 20 (under a certain technical assumption) and Polzer 22

Corollary: The Fröhlich Hamiltonian H_α does not have a ground state. In particular there is no self-trapping at finite α.

Quantitative estimates for large α

From Donsker–Varadhan 83 and Lieb–Thomas 97 we know that

$$E_\alpha(0) = \alpha^2 e^{\mathrm{Pek}} + o(\alpha^2) \quad \text{as} \quad \alpha \to \infty$$

with $e^{\mathrm{Pek}} < 0$ the infimum of the semi-classical Pekar energy functional.

Our next result gives a parabolic upper bound on $E_\alpha(P) = \inf \sigma(H_\alpha(P))$

Theorem (M–Myśliwy–Seiringer 22) There exists a $C > 0$ such that

$$E_\alpha(P) \leq \alpha^2 e^{\mathrm{Pek}} + \tfrac{1}{2}\mathrm{Tr}_{L^2}(\sqrt{H^{\mathrm{Pek}}} - 1) + \frac{1}{2\alpha^4 M^{\mathrm{Pek}}} P^2 + C\alpha^{-\frac{1}{2}}$$

for all $|P| \lesssim \alpha^2$, where

- $0 \leq H^{\mathrm{Pek}} \leq 1$ is an explicit operator on $L^2(\mathbb{R}^3)$
- $M^{\mathrm{Pek}} = \frac{2}{3}\|\nabla\varphi\|_2^2$ is the semi-classical effective mass (Lan–Pek 48)

A similar lower bound for $E_\alpha(0)$ was obtained by Brooks–Seiringer, hence

$$E_\alpha(0) = \alpha^2 e^{\mathrm{Pek}} + \tfrac{1}{2}\mathrm{Tr}_{L^2}(\sqrt{H^{\mathrm{Pek}}} - 1) + o(1).$$

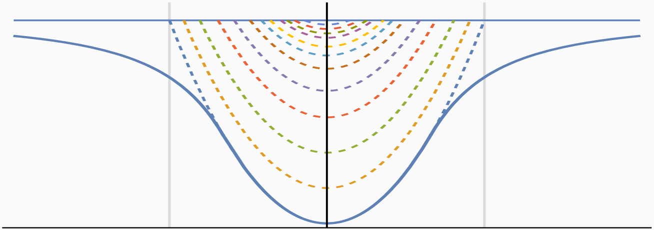
Excited bound states

Our last result concerns the existence of excited energy bands below the essential spectrum $\sigma_{\mathrm{ess}}(H_\alpha(P)) = [E_\alpha(0) + 1, \infty)$.

Theorem (M–Myśliwy–Seiringer, in prep.) Let $\sigma_{\mathrm{disc}}(H_\alpha(P))$ be the discrete part of the spectrum of $H_\alpha(P)$. There exists a $\zeta \in (0,1)$ such that

$$|\sigma_{\mathrm{disc}}(H_\alpha(P))| \xrightarrow{\alpha\to\infty} \infty \quad \text{for all} \quad |P| \lesssim \alpha^{2-\zeta}$$

Based on upper bounds for the min-max values of $H_\alpha(P)$



The existence of excited energy bands was previously not known. In fact there are predictions that such excited bound states would not exist.

Summary

- $P \mapsto E_\alpha(P)$ attains its unique global minimum at $P = 0$
- Optimal parabolic upper bound for $E_\alpha(P)$ for large α
- Number of excited energy bands diverges as $\alpha \to \infty$

Many open problems

- Matching parabolic lower bound for $E_\alpha(P)$
- Asymptotic formulas for the excited energy bands
- Does $E_\alpha(P)$ enter the essential spectrum for large $|P|$?
- Large α limit of the effective mass $M_\alpha^{\text{eff}} \sim \alpha^4 M^{\text{Pek}}$ (Volker's talk)

Thank you for your attention