

Monotonicity of the Polaron Energy

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1 The Fröhlich Hamiltonian for a single polaron

The Fröhlich Hamiltonian for a single polaron is given by

$$H_\Lambda = -\frac{1}{2}\Delta - \sqrt{\alpha} \int_{|k| \leq \Lambda} dk \frac{1}{|k|} [e^{ik \cdot x} a(k) + e^{-ik \cdot x} a(k)^*] + N_f,$$
$$N_f = \int_{\mathbb{R}^3} dk a(k)^* a(k).$$

$a(k), a(k)^*$ are annihilation- and creation operators, respectively. These satisfy the standard commutation relations:

$$[a(k), a(k')^*] = \delta(k - k'), \quad [a(k), a(k')] = 0 = [a(k)^*, a(k')^*].$$

The Hamiltonian H_Λ lives in the Hilbert space $L^2(\mathbb{R}^3) \otimes \mathfrak{F}$, where \mathfrak{F} is the Fock space over $L^2(\mathbb{R}^3)$:

$$\mathfrak{F} = \bigoplus_{n=0}^{\infty} L_s^2(\mathbb{R}^{3n}).$$

$L_s^2(\mathbb{R}^{3n})$ is the set of all symmetric vectors in $L^2(\mathbb{R}^{3n})$:

$$L_s^2(\mathbb{R}^{3n}) = \left\{ \varphi \in L^2(\mathbb{R}^{3n}) \mid \varphi(k_{\sigma(1)}, \dots, k_{\sigma(n)}) = \varphi(k_1, \dots, k_n) \text{ a.e. } \forall \sigma \in \mathfrak{S}_n \right\},$$

where \mathfrak{S}_n is the permutation group on $\{1, \dots, n\}$. $\Lambda > 0$ is the ultraviolet cutoff and $\alpha > 0$ is the coupling strength. By the Kato-Rellich theorem, H_Λ is semibounded self-adjoint operator on $\text{dom}(-\Delta) \cap \text{dom}(N_f)$ for all $\alpha, \Lambda > 0$.

This Hamiltonian was introduced by H. Fröhlich [5] as a model of the large polaron. As to the physical background of this model, see [1, 4] and references therein. Readers can learn recent developments concerning mathematical analysis of the model from [3, 12] for example.

2 The Fröhlich Hamiltonian at a fixed total momentum

The total momentum operator is defined by

$$P_{\text{tot}} = -i\nabla + P_{\text{f}}, \quad P_{\text{f}} = \int_{\mathbb{R}^3} dk k a(k)^* a(k).$$

$P_{\text{tot},j}$, $j = 1, 2, 3$ is essentially self-adjoint. We denote its closure by the same symbol. Let \mathcal{U} be a unitary operator defined by

$$\mathcal{U} = \mathcal{F} e^{ix \cdot P_{\text{f}}},$$

where \mathcal{F} is the Fourier transformation: $(\mathcal{F}f)(p) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} f(x) e^{-ip \cdot x} dx$. Then we obtain

$$\mathcal{U} P_{\text{tot}} \mathcal{U}^* = \int_{\mathbb{R}^3}^{\oplus} P dP, \quad \mathcal{U} H_{\Lambda} \mathcal{U}^* = \int_{\mathbb{R}^3}^{\oplus} H_{\Lambda}(P) dP,$$

where

$$H_{\Lambda}(P) = \frac{1}{2}(P - P_{\text{f}})^2 - \sqrt{\alpha} \int_{|k| \leq \Lambda} dk \frac{1}{|k|} [a(k) + a(k)^*] + N_{\text{f}}.$$

$H_{\Lambda}(P)$ is the Hamiltonian at a fixed total momentum P . $H_{\Lambda}(P)$ is a semibounded self-adjoint operator acting in \mathfrak{F} .

3 Monotonicity of the polaron energy

Let $E_{\Lambda} = \inf \text{spec}(H_{\Lambda})$ and let $E_{\Lambda}(P) = \inf \text{spec}(H_{\Lambda}(P))$. In [10], we obtained the following theorems.

Theorem 3.1 $E_{\Lambda}(P)$ is monotonically decreasing in Λ for all $P \in \mathbb{R}^3$.

Theorem 3.2 $E_{\Lambda}(P)$ is strictly decreasing in Λ provided $|P| < \sqrt{2}$.

Remark 3.3 J. Møller obtained similar results for a regularized Hamiltonian [12]. In contrast, we employ the sharp cutoff function as a form factor. This makes mathematical analysis harder.

Theorem 3.4 E_{Λ} is strictly decreasing in Λ .

4 Uniqueness of the ground state

By Theorems 3.2 and 3.4, the ultraviolet cutoff has to be removed from the Hamiltonian because $E_{\Lambda=\infty}(P)$ is most stable energetically. As to the removal of ultraviolet cutoff, the following proposition is fundamental.

Proposition 4.1 [6, 13] *There exists a semibounded self-adjoint operator $H(P)$ such that $H_{\Lambda}(P)$ converges to $H(P)$ in the strong resolvent sense as $\Lambda \rightarrow \infty$.*

In this way, we can define the Hamiltonian without ultraviolet cutoff as a limiting operator. Our next problem is to investigate spectral properties of $H(P)$. In [7, 14], it was already proven that $H(P)$ has a ground state. Now a natural question arises. Is this ground state unique? The following theorem answers the question.

Theorem 4.2 $H(P)$ has a unique ground state provided $|P| < \sqrt{2}$.

Our main purpose in this note is to show how useful operator inequalities are when we prove above theorems. To this end, we will illustrate essential ideas of proofs of Theorems 3.1 and 4.2 as examples.

5 Proof of Theorem 3.1

5.1 Basic definitions

Definition 5.1 (i) The *Fröhlich cone* \mathfrak{F}_+ is a cone in \mathfrak{F} defined by

$$\mathfrak{F}_+ = \bigoplus_{n \geq 0} L_s^2(\mathbb{R}^{3n})_+,$$

$$L_s^2(\mathbb{R}^{3n})_+ = \{\psi \in L_s^2(\mathbb{R}^{3n}) \mid \psi(k_1, \dots, k_n) \geq 0 \text{ a.e.}\}$$

with $L_s^2(\mathbb{R}^0)_+ = \mathbb{R}_+$.

(ii) A bounded linear operator A in \mathfrak{F} is said to be *positivity preserving* if

$$A\mathfrak{F}_+ \subseteq \mathfrak{F}_+.$$

We denote this as $A \trianglerighteq 0$. This symbol was introduced by Miura [8].

(iii) If two linear operators A, B satisfy $A - B \trianglerighteq 0$, then we write this as $A \trianglerighteq B$.

5.2 Basic properties

Lemma 5.2 *We have the following.*

- (1) $\varphi, \psi \in \mathfrak{F}_+ \Rightarrow \langle \varphi, \psi \rangle \geq 0$.
- (2) If $A \trianglerighteq 0$ and $B \trianglerighteq 0$, then $AB \trianglerighteq 0$.
- (3) If $A \trianglerighteq 0$ and $B \trianglerighteq 0$, then $\alpha A + \beta B \trianglerighteq 0$ for all $\alpha, \beta \in \mathbb{R}_+$.
- (4) If $A \trianglerighteq B$, then $\langle \varphi, A\psi \rangle \geq \langle \varphi, B\psi \rangle$ for all $\varphi, \psi \in \mathfrak{F}_+$.

Proof. (1) is trivial.

$$(2) B\mathfrak{F}_+ \subseteq \mathfrak{F}_+ \Rightarrow AB\mathfrak{F}_+ \subseteq A\mathfrak{F}_+ \subseteq \mathfrak{F}_+ \Rightarrow AB \trianglerighteq 0.$$

$$(3) A, B \trianglerighteq 0 \Rightarrow \alpha A, \beta B \trianglerighteq 0 \Rightarrow \alpha A + \beta B \trianglerighteq 0.$$

$$(4) A \trianglerighteq B \Rightarrow (A - B)\psi \in \mathfrak{F}_+ \Rightarrow \langle \varphi, (A - B)\psi \rangle \geq 0. \quad \square$$

5.3 Second quantized operators

In case of unbounded operators, we modify the definition as follow: $A \trianglerighteq 0$ if and only if

$$A[\text{dom}(A) \cap \mathfrak{F}_+] \subseteq \mathfrak{F}_+.$$

Lemma 5.3 *If $f \in L^2(\mathbb{R}^3)_+$, then $a(f) \trianglerighteq 0$ and $a(f)^* \trianglerighteq 0$ hold.*

Proof. For $\psi = \oplus_{n \geq 0} \psi^{(n)} \in \text{dom}(a(f)) \cap \mathfrak{F}_+$, remark that $\psi^{(n)}(k_1, \dots, k_n) \geq 0$ a.e.. Thus

$$\left(a(f)\psi\right)^{(n)}(k_1, \dots, k_n) = \sqrt{n+1} \int_{\mathbb{R}^3} \underbrace{dk f(k)}_{\geq 0} \underbrace{\psi^{(n+1)}(k, k_1, \dots, k_n)}_{\geq 0} \geq 0.$$

This means that $a(f)$ preserves the positivity. \square

Lemma 5.4 *If ω is a positive function on \mathbb{R}^3 , then $e^{-td\Gamma(\omega)} \geq 0$ for all $t \geq 0$, where $d\Gamma(\omega) = \int_{\mathbb{R}^3} dk \omega(k) a(k)^* a(k)$.*

Proof. For $\psi = \oplus_{n \geq 0} \psi^{(n)} \in \mathfrak{F}_+$, one has

$$\left(e^{-td\Gamma(\omega)}\psi\right)^{(n)}(k_1, \dots, k_n) = \underbrace{e^{-t(\omega(k_1)+\dots+\omega(k_n))}}_{\geq 0} \underbrace{\psi^{(n)}(k_1, \dots, k_n)}_{\geq 0} \geq 0.$$

Thus $e^{-td\Gamma(\omega)}$ preserves the positivity. \square

5.4 Proof of Theorem 3.1: Step 1

Proposition 5.5 *For all $P \in \mathbb{R}^3, \beta \geq 0$ and $\Lambda \geq 0$, $e^{-\beta H_\Lambda(P)} \geq 0$ holds.*

Sketch of Proof. Write

$$H_\Lambda(P) = L(P) - V_\Lambda,$$

where

$$L(P) = \frac{1}{2}(P - P_f)^2 + N_f, \quad V_\Lambda = \sqrt{\alpha} \int_{|k| \leq \Lambda} dk \frac{1}{|k|} [a(k) + a(k)^*].$$

Note that

$$e^{-\beta L(P)} \geq 0, \quad V_\Lambda \geq 0.$$

By the Duhamel expansion, one has

$$\begin{aligned} e^{-\beta H_\Lambda(P)} &= \sum_{n=0}^{\infty} D_n, \\ D_n &= \int_0^\beta ds_1 \int_0^{\beta-s_1} ds_2 \cdots \int_0^{\beta-s_1-\dots-s_{n-1}} ds_n \\ &\quad \times e^{-s_1 L(P)} V_\Lambda e^{-s_2 L(P)} \cdots e^{-s_n L(P)} V_\Lambda e^{-(\beta-s_1-\dots-s_n)L(P)}. \end{aligned}$$

Remark

$$\underbrace{e^{-s_1 L(P)}}_{\geq 0} \underbrace{V_\Lambda}_{\geq 0} \underbrace{e^{-s_2 L(P)}}_{\geq 0} \cdots \underbrace{e^{-s_n L(P)}}_{\geq 0} \underbrace{V_\Lambda}_{\geq 0} \underbrace{e^{-(\beta-s_1-\dots-s_n)L(P)}}_{\geq 0} \geq 0.$$

Thus $D_n \geq 0$ for all n , which implies $\sum_{n=0}^{\infty} D_n \geq 0$, which implies $e^{-\beta H_\Lambda(P)} \geq 0$. \square

5.5 Proof of Theorem 3.1: Step 2

For each $\varepsilon > 0$, there is a normalized vector $\varphi_{\varepsilon,\Lambda} = \oplus_{n \geq 0} \varphi_{\varepsilon,\Lambda}^{(n)} \in \text{dom}(P_f^2) \cap \text{dom}(N_f)$ such that $\varphi_{\varepsilon,\Lambda}^{(n)}$ is real and

$$\langle \varphi_{\varepsilon,\Lambda}, H_\Lambda(P) \varphi_{\varepsilon,\Lambda} \rangle \leq E_\Lambda(P) + \varepsilon.$$

$\varphi_{\varepsilon,\Lambda}^{(n)}$ can be written as $\varphi_{\varepsilon,\Lambda}^{(n)} = \varphi_{\varepsilon,\Lambda}^{(n)+} - \varphi_{\varepsilon,\Lambda}^{(n)-}$, where $\varphi_{\varepsilon,\Lambda}^{(n)+}, \varphi_{\varepsilon,\Lambda}^{(n)-}$ are positive and negative part of $\varphi_{\varepsilon,\Lambda}^{(n)}$ respectively. Thus it holds that $\varphi_{\varepsilon,\Lambda}^{(n)\pm} \in L_s^2(\mathbb{R}^{3n})_+$ and $\langle \varphi_{\varepsilon,\Lambda}^{(n)+}, \varphi_{\varepsilon,\Lambda}^{(n)-} \rangle = 0$. We define

$$\begin{aligned} \varphi_{\varepsilon,\Lambda}^+ &= \bigoplus_{n \geq 0} \varphi_{\varepsilon,\Lambda}^{(n)+}, \quad \varphi_{\varepsilon,\Lambda}^- = \bigoplus_{n \geq 0} \varphi_{\varepsilon,\Lambda}^{(n)-}, \\ |\varphi_{\varepsilon,\Lambda}| &= \varphi_{\varepsilon,\Lambda}^+ + \varphi_{\varepsilon,\Lambda}^-. \end{aligned}$$

Note $\varphi_{\varepsilon,\Lambda} = \varphi_{\varepsilon,\Lambda}^+ - \varphi_{\varepsilon,\Lambda}^-$.

Lemma 5.6 *It holds that $\varphi_{\varepsilon,\Lambda} \in \text{dom}(|H_\Lambda(P)|^{1/2})$ and*

$$\langle \varphi_{\varepsilon,\Lambda}, H_\Lambda(P) \varphi_{\varepsilon,\Lambda} \rangle \geq \langle |\varphi_{\varepsilon,\Lambda}|, H_\Lambda(P) |\varphi_{\varepsilon,\Lambda}| \rangle.$$

Proof. Since $e^{-\beta H_\Lambda(P)} \geq 0$, we have

$$\begin{aligned} \langle \varphi_{\varepsilon,\Lambda}, e^{-\beta H_\Lambda(P)} \varphi_{\varepsilon,\Lambda} \rangle &= \underbrace{\langle \varphi_{\varepsilon,\Lambda}^+, e^{-\beta H_\Lambda(P)} \varphi_{\varepsilon,\Lambda}^+ \rangle + \langle \varphi_{\varepsilon,\Lambda}^-, e^{-\beta H_\Lambda(P)} \varphi_{\varepsilon,\Lambda}^- \rangle}_{\geq 0} \\ &\quad - \underbrace{\langle \varphi_{\varepsilon,\Lambda}^+, e^{-\beta H_\Lambda(P)} \varphi_{\varepsilon,\Lambda}^- \rangle + \langle \varphi_{\varepsilon,\Lambda}^-, e^{-\beta H_\Lambda(P)} \varphi_{\varepsilon,\Lambda}^+ \rangle}_{\leq 0} \\ &\leq \langle \varphi_{\varepsilon,\Lambda}^+, e^{-\beta H_\Lambda(P)} \varphi_{\varepsilon,\Lambda}^+ \rangle + \langle \varphi_{\varepsilon,\Lambda}^-, e^{-\beta H_\Lambda(P)} \varphi_{\varepsilon,\Lambda}^- \rangle \\ &\quad + \langle \varphi_{\varepsilon,\Lambda}^+, e^{-\beta H_\Lambda(P)} \varphi_{\varepsilon,\Lambda}^- \rangle + \langle \varphi_{\varepsilon,\Lambda}^-, e^{-\beta H_\Lambda(P)} \varphi_{\varepsilon,\Lambda}^+ \rangle \\ &= \langle |\varphi_{\varepsilon,\Lambda}|, e^{-\beta H_\Lambda(P)} |\varphi_{\varepsilon,\Lambda}| \rangle. \end{aligned}$$

Thus we arrive at

$$\langle \varphi_{\varepsilon,\Lambda}, e^{-\beta H_\Lambda(P)} \varphi_{\varepsilon,\Lambda} \rangle \leq \langle |\varphi_{\varepsilon,\Lambda}|, e^{-\beta H_\Lambda(P)} |\varphi_{\varepsilon,\Lambda}| \rangle.$$

Hence

$$\frac{1}{\beta} \left\langle \varphi_{\varepsilon,\Lambda}, \left(\mathbb{1} - e^{-\beta H_\Lambda(P)} \right) \varphi_{\varepsilon,\Lambda} \right\rangle \geq \frac{1}{\beta} \left\langle |\varphi_{\varepsilon,\Lambda}|, \left(\mathbb{1} - e^{-\beta H_\Lambda(P)} \right) |\varphi_{\varepsilon,\Lambda}| \right\rangle.$$

Taking $\beta \rightarrow +0$, we have the desired result. \square

5.6 Proof of Theorem 3.1: Step 3

Lemma 5.7 *If $\Lambda \leq \Lambda'$, we have $H_\Lambda(P) \geq H_{\Lambda'}(P)$.*

Proof. Define

$$\eta_{\Lambda',\Lambda}(k) = \frac{\chi_{\Lambda'}(k) - \chi_\Lambda(k)}{|k|} \geq 0,$$

where $\chi_\Lambda(k) = 1$ if $|k| \leq \Lambda$, $\chi_\Lambda(k) = 0$ otherwise. One has, by Lemma 5.3,

$$H_\Lambda(P) - H_{\Lambda'}(P) = \sqrt{\alpha} \left(\underbrace{a(\eta_{\Lambda',\Lambda})}_{\geq 0} + \underbrace{a(\eta_{\Lambda',\Lambda})^*}_{\geq 0} \right) \geq 0. \quad \square$$

5.7 Completion of proof of Theorem 3.1

We have

$$\begin{aligned}
E_\Lambda(P) + \varepsilon &\geq \langle \varphi_{\varepsilon, \Lambda}, H_\Lambda(P) \varphi_{\varepsilon, \Lambda} \rangle \\
&\geq \langle |\varphi_{\varepsilon, \Lambda}|, H_\Lambda(P) |\varphi_{\varepsilon, \Lambda}| \rangle \quad (\text{Lemma 5.6}) \\
&\geq \langle |\varphi_{\varepsilon, \Lambda}|, H_{\Lambda'}(P) |\varphi_{\varepsilon, \Lambda}| \rangle \quad (\text{Lemma 5.7}) \\
&\geq E_{\Lambda'}(P),
\end{aligned}$$

whenever $\Lambda' > \Lambda$. Note $\|\varphi\| = \||\varphi|\|$. Thus we conclude that $E_\Lambda(P) \geq E_{\Lambda'}(P)$.

6 Comments on Theorems 3.2 and 3.4

Proofs of Theorems 3.2 and 3.4 are much more difficult. In this note, we will not prove these theorems. Instead we only provide a list of essential ingredients for proofs. (As to complete proofs, see [9, 10, 11] for details.)

- (1) For all $\Lambda > 0$, $H_\Lambda(P)$ has a ground state provided $|P| < \sqrt{2}$.
- (2) The abstract Perron-Frobenius theorem (Theorem 7.2).
- (3) Positivity arguments and spectral properties of $H_\Lambda(P)$.

7 Idea of proof of Theorem 4.2

7.1 Basic definitions

We will try to explain basic ideas of proof of Theorem 4.2. To this end, we need some additional definitions.

Definition 7.1 (1) We say a vector $\varphi = \oplus_{n \geq 0} \varphi^{(n)} \in \mathfrak{F}_+$ is *strictly positive* if

$$\varphi^{(n)}(k_1, \dots, k_n) > 0 \quad a.e.$$

- (2) A bounded linear operator A is *positivity improving* if for each $\varphi \in \mathfrak{F}_+ \setminus \{0\}$, $A\varphi$ is strictly positive. We denote this as $A \triangleright 0$.

7.2 Perron-Frobenius-Faris theorem

Theorem 7.2 [2, 9] Let A be a positive self-adjoint operator on \mathfrak{F} . Suppose that $e^{-tA} \succeq 0$ for all $t \geq 0$ and $\inf \text{spec}(A)$ is an eigenvalue. Let P_A be the orthogonal projection onto the closed subspace spanned by eigenvectors associated with $\inf \text{spec}(A)$. Then the following are equivalent.

- (i) $\dim \text{ran}(P_A) = 1$ and $P_A \triangleright 0$.
- (ii) $e^{-tA} \triangleright 0$ for all $t > 0$.

By Theorem 7.2 and §6 (2), it suffices to show that $e^{-\beta H(P)} \triangleright 0$ for all $\beta > 0$. Remark that this is not so easy because $H(P)$ is defined by the limiting procedure.

7.3 Hamiltonian with a mild cutoff

For each $n \in \mathbb{N}$, let

$$\varrho_n(k) = e^{-k^2/n} > 0.$$

We introduce the Hamiltonian with a mild cutoff by

$$H_{\varrho_n}(P) = \frac{1}{2}(P - P_f)^2 - \sqrt{\alpha} \int_{\mathbb{R}^3} dk \frac{\varrho_n(k)}{|k|} [a(k) + a(k)^*] + N_f.$$

Proposition 7.3 *We have the following.*

- (1) $H_{\varrho_n}(P)$ converges to $H(P)$ in the strong resolvent sense as $n \rightarrow \infty$.
- (2) For all $n \in \mathbb{N}$ and $\beta > 0$, it holds that $e^{-\beta H_{\varrho_n}(P)} \triangleright 0$.

Proof. See [6, 9, 11]. \square

Proposition 7.4 *One has $e^{-\beta H_{\varrho_{n+1}}(P)} \succeq e^{-\beta H_{\varrho_n}(P)}$ for all $\beta \geq 0$ and $n \in \mathbb{N}$.*

Proof. By an argument similar to the proof of Lemma 5.7, we have $H_{\varrho_{n+1}}(P) \leq H_{\varrho_n}(P)$. In addition, $e^{-\beta H_{\varrho_n}(P)} \succeq 0$ for all $n \in \mathbb{N}$. This is equivalent to $(H_{\varrho_n}(P) + s)^{-1} \succeq 0$, since $(A + s)^{-1} = \int_0^\infty e^{-\lambda(A+s)} d\lambda$ and $e^{-\beta A} = s\text{-}\lim_{N \rightarrow \infty} (\mathbb{1} + \beta A/N)^N$. Thus we have

$$\begin{aligned} & (H_{\varrho_{n+1}}(P) + s)^{-1} - (H_{\varrho_n}(P) + s)^{-1} \\ &= \underbrace{(H_{\varrho_{n+1}}(P) + s)^{-1}}_{\succeq 0} \underbrace{(H_{\varrho_n}(P) - H_{\varrho_{n+1}}(P))}_{\succeq 0} \underbrace{(H_{\varrho_n}(P) + s)^{-1}}_{\succeq 0} \succeq 0. \end{aligned}$$

This completes the proof. \square

7.4 Completion of proof of Theorem 4.2

By Proposition 7.4, $e^{-\beta H_{\varrho_n}(P)}$ is monotonically increasing sequence of operators:

$$e^{-\beta H_{\varrho_N}(P)} \succeq e^{-\beta H_{\varrho_n}(P)}, \text{ whenever } N > n.$$

Taking the limit $N \rightarrow \infty$, we obtain

$$e^{-\beta H(P)} \succeq e^{-\beta H_{\varrho_n}(P)}$$

by Proposition 7.3 (1). Since the right hand side of the above improves the positivity by Proposition 7.3 (2), it follows that $e^{-\beta H(P)} \triangleright 0$ for all $\beta > 0$.

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