An Invitation to Path Measure Methods for Polaron Models

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Mathematical Challenges in Quantum Mechanics

Online PhD Lecture

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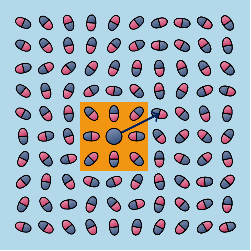
Motivation: The Fröhlich Polaron

The Fröhlich polaron (Fröhlich 1934) is an effective model for a charged particle moving through a dielectric crystal.



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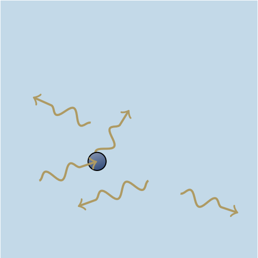

$$H_\lambda = -\frac{1}{2}\Delta + N + \lambda\varphi(v_x) \qquad \text{on } L^2(\mathbb{R}^3)\otimes\mathcal{F} \cong L^2(\mathbb{R}^3;\mathcal{F})$$

Fock Space: $\mathcal{F} = \bigoplus_{n=0}^{\infty} \mathcal{F}^{(n)}, \qquad \mathcal{F}^{(0)} = \mathbb{C},\ \mathcal{F}^{(n)} = L^2_{\mathrm{sym}}(\mathbb{R}^{3n})$

Particle Number Operator: $N \upharpoonright \mathcal{F}^{(n)} = n$

Field Operator: $\varphi(v) = \int_{\mathbb{R}^d} (\overline{v(k)}a_k + v(k)a_k^\dagger)dk$

$a_k f(k_1,\dots,k_n) = \sqrt{n+1} f(k,k_1,\dots,k_n)$ for $f \in \mathcal{F}^{(n+1)}$

$$v_x(k) = \mathrm{e}^{-\mathrm{i}kx}|k|^{-1}$$

Strong Coupling Limit $|\lambda| \to \infty$, a brief teaser.

Pekars Conjecture (1946): $\boxed{\inf \sigma(H_\lambda) = (2\pi)^2 |\lambda|^4 e_{\mathsf{P}} + \mathcal{O}(1)}$,

where $e_{\mathsf{P}} = \inf_\psi \int |\nabla \psi|^2 - \int\int \frac{|\psi(x)|^2 |\psi(y)^2}{|x-y|} \mathsf{d}(x,y)$.

Proof of leading order lower bound:

- Donsker, Varadhan 1987 – probabilistic techniques
- Lieb, Thomas 1997 – operator theoretic techniques

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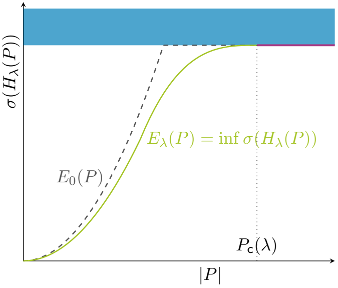
Translation Invariance:

$$H_\lambda \cong \int_{\mathbb{R}^3}^{\oplus} H_\lambda(P), H_\lambda(P) = \frac{1}{2}(P - P_{\mathsf{f}})^2 + N + \lambda\varphi(v_0)$$



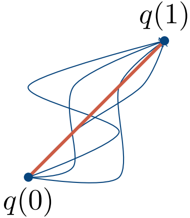
- Landau–Pekar Conjecture (1948) $m_{\mathsf{eff}}(\lambda) = (\partial_P^2 E(P)|_{P=0})^{-1} \cong |\lambda|^8 m_{\mathsf{LP}}$
  Betz, Polzer 2024, Bazaes, Mukherjee, Varadhan, Sellke 2024, Brooks, Seiringer 2022–
- Lower bounds on $P_{\mathsf{c}}(\lambda)$
  Polzer 2023, Mitrouskas, Myśliwy, Seiringer 2023
- $H_\lambda(P)$ has a ground state $\iff |P| < P_{\mathsf{c}}$
  Møller 2006, Polzer 2023

Goal of this Talk

Understand the connection between the ground state problem of quantum theory and probabilistic approaches.

What are path integrals?

The equations of motion in classical mechanics (Newton's laws of motion) can be derived from the stationary-action principle: a classical particle will always take the trajectory in which the action is stationary.



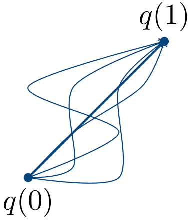
Action: $S[q] = \int_0^1 L(q, \dot{q}, t)\mathrm{d}t$

Example: $L(q, p, t) = \frac{1}{2}p^2$
(free particle)

What are path integrals?

Feynman (1942) formulated quantum mechanics in terms of (formal) integrals over all possible paths, weighted with the classical action.

$$\psi(x,1) \text{“}=\text{”} \int_{q(0)=x} \mathrm{e}^{\mathrm{i}S[q]}\psi_0(q(1))\mathrm{d}q \text{“}=\text{”} \int_{q(0)=x} \psi_0(q(1))\mathrm{d}\mathcal{P}(q)$$



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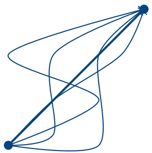

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Theorem (Cameron 1962).

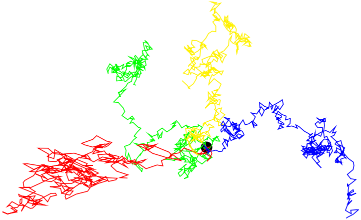
There exists no (complex) measure $\mathcal{P}$ on $\{f : [0,\infty) \to \mathbb{R}^n\}$ equipped with the σ-algebra generated by pointwise evaluations such that

$$\psi(x,t) = \int_{q(0)=x} \psi_0(q(t))\mathrm{d}\mathcal{P}(q) \qquad \text{solves} \qquad \mathrm{i}\partial_t\psi = -\Delta\psi,\ \psi(0) = \psi_0.$$

Path Measures for the Heat Equation

What happens if we take other path measures?

E.g., the Wiener measure (Wiener 1923) describing Brownian motion.



Brownian motion B_t

- $B_0 = x$
- B_t is almost surely continuous
- B_t has independent increments
- $B_t - B_s \sim \mathcal{N}(0, t-s)$

Using the Wiener measure, we obtain solutions to the free heat equation

$$\psi(x,t) = \mathbb{E}[\psi_0(B_t)|B_0 = x] \quad \Longrightarrow \quad \partial_t\psi = \frac{1}{2}\Delta\psi,\ \psi(x,0) = \psi_0(x).$$

Proof. $\psi(x,t) = \frac{1}{(2\pi t)^{d/2}} \int \mathrm{e}^{-|x-y|^2/2t}\psi_0(y)\mathrm{d}y$ ∎

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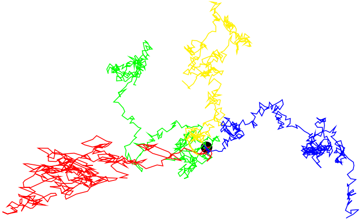

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Instead of solving the free Schrödinger equation, we now solve the free heat equation. Does this still work if we add an external potential?

Note: The above PDE solution immediately extends to the Hilbert space setting, i.e., $\left(\mathrm{e}^{t\frac{1}{2}\Delta} f\right)(x) = \mathbb{E}[f(B_t)|B_0 = x]$.

The Feynman–Kac Formula

Theorem (Kac 1951).

Assume $V : \mathbb{R}^d \to \mathbb{R}$ is continuous with compact support. Then for all $f \in L^2(\mathbb{R}^d)$ and almost all $x \in \mathbb{R}^d$

$$\left(\mathrm{e}^{-t(-\frac{1}{2}\Delta+V)} f\right)(x) = \mathbb{E}\left[\mathrm{e}^{-\int_0^t V(B_s)\mathrm{d}s} f(B_t) \middle| B_0 = x\right]$$

Proof. Apply the Trotter product formula

$$\mathrm{e}^{-t(-\frac{1}{2}\Delta+V)} f = \lim_{n\to\infty} \left(\mathrm{e}^{\frac{t}{n}\frac{1}{2}\Delta} \mathrm{e}^{-\frac{t}{n}V}\right)^n f = \lim_{n\to\infty} \mathbb{E}\left[\mathrm{e}^{-\sum_{j=1}^{n} V(B_{t\cdot\frac{j}{n}})} f(B_t) \middle| B_0 = x\right] \blacksquare$$

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How about other potentials or free particles?

- Our restrictive assumption on V can immediately be relaxed. The path measure $\mathbb{E}[\,\bullet\,\mathrm{e}^{-\int_0^t V(B_s)\mathrm{d}s}]$ can still be used in many singular settings.
- The free particle does not need to be non-relativistic (or on $\mathbb{R}^d$). Similar approaches work in many settings (discrete/relativistic/. . .).

How can we learn properties of quantum systems from solving the heat equation?

Assume we are given the Hilbert space $\mathcal{H}$ and a selfadjoint operator H. What can we learn about the spectrum of H from e^{-tH}?

Ground State (Energies)

A connection between semigroup and smallest spectral energies is obtained from spectral calculus.

Lemma (Bloch's formula).

Let $\psi \in \mathcal{H}$, $\|\psi\| = 1$. Then

$$E_0(\psi) = \inf \operatorname{supp} \langle \psi, \mathsf{E}_H(\cdot)\psi \rangle = -\lim_{t\to\infty} \frac{1}{t} \langle \psi, \mathsf{e}^{-tH}\psi \rangle,$$

where E_H is the spectral measure of H.

We can even go further and study eigenfunctions this way.

Theorem (Ground State Overlap).

$$\langle \psi, \mathsf{E}_H(\{E_0(\psi)\})\psi \rangle = \lim_{t\to\infty} \frac{\langle \psi, \mathsf{e}^{-tH}\psi \rangle^2}{\langle \psi, \mathsf{e}^{-2tH}\psi \rangle}$$

How can we ensure that this gives us the ground state energy and overlap?

Positive Cones in Hilbert Spaces

Definition.

Let $\mathfrak{P}$ be a self-dual convex cone in $\mathcal{H}$, i.e.,

$$\mathfrak{P} = \{x \in \mathcal{H} | \langle x, y \rangle \geq 0 \text{ for all } y \in \mathfrak{P}\}.$$

Let $\mathfrak{P}^+ = \{x \in \mathfrak{P} | \langle x, y \rangle > 0 \text{ for } y \in \mathfrak{P} \setminus \{0\}\}$ be strictly pos. elements.

- $B \in \mathcal{B}(\mathcal{H})$ is called positivity preserving if $B\mathfrak{P} \subset \mathfrak{P}$.
- $B \in \mathcal{B}(\mathcal{H})$ is called positivity improving if $B(\mathfrak{P} \setminus \{0\}) \subset \mathfrak{P}^+$.

Examples.

- $\mathcal{H} = L^2(\mathbb{R}^d)$, $\mathfrak{P} = \{f \geq 0 \text{ a.e.}\}$, $\mathfrak{P}^+ = \{f > 0 \text{ a.e.}\}$
- $\mathcal{H} = \mathcal{F}$, $\mathfrak{P} = \{\psi^{(n)} \geq 0 \text{ a.e. for all } n \in \mathbb{N}_0\}$

Theorem (Perron–Frobenius, Faris 1972).

If e^{-tH} is positivity improving for some (and hence all) $t > 0$ and if $\psi \in \mathfrak{P}$, then $E_0(\psi) = \inf \sigma(H)$ and $\dim \ker(H - E_0(\psi)) \leq 1$.

FKF: $\mathrm{e}^{-t(-\frac{1}{2}\Delta + V)} f(x) = \mathbb{E}[\mathrm{e}^{-\int_0^t V(B_s)\mathrm{d}s} f(B_t) | B_0 = x] > 0$ a.e. $x \in \mathbb{R}^d$

How can we make this toolbox available, when the potential V takes values in Fock space, e.g., for polaron models?

Polaron Models

$$H = -\frac{1}{2}\Delta + \mathsf{d}\Gamma(\omega) + \varphi(v_x) \qquad \text{on } L^2(\mathbb{R}^d;\mathcal{F})$$

$$H(P) = \frac{1}{2}(P - \mathsf{d}\Gamma(\hat{p}))^2 + \mathsf{d}\Gamma(\omega) + \varphi(v_0) \qquad \text{on } \mathcal{F}$$

- Fock Space: $\mathcal{F} = \bigoplus_{n=0}^{\infty} \mathcal{F}^{(n)}, \qquad \mathcal{F}^{(0)} = \mathbb{C},\ \mathcal{F}^{(n)} = L^2_{\mathsf{sym}}(\mathbb{R}^{dn})$
- Second Quantization Operator: $\mathsf{d}\Gamma(m) = \int m(k) a_k^\dagger a_k \mathsf{d}k$

$$\mathsf{d}\Gamma(m) \restriction \mathcal{F}^{(n)}(k_1,\dots,k_n) = m(k_1) + \cdots + m(k_n)$$

- Field Operator: $\varphi(v) = \int_{\mathbb{R}^d} (\overline{v(k)} a_k + v(k) a_k^\dagger)\mathsf{d}k$

$$a_k f(k_1,\dots,k_n) = \sqrt{n+1} f(k,k_1,\dots,k_n),\ f \in \mathcal{F}^{(n+1)}$$

$$a_k^\dagger f(k_1,\dots,k_n) = \frac{1}{\sqrt{n}} \sum_{\ell=1}^{n} \delta(k-k_\ell) f(k_1,\dots,\cancel{k_\ell},\dots,k_n),\ f \in \mathcal{F}^{(n-1)}$$

Polaron Models

$$H = -\frac{1}{2}\Delta + \mathrm{d}\Gamma(\omega) + \varphi(v_x) \qquad \text{on } L^2(\mathbb{R}^d; \mathcal{F})$$

$$H(P) = \frac{1}{2}(P - \mathrm{d}\Gamma(\hat{p}))^2 + \mathrm{d}\Gamma(\omega) + \varphi(v_0) \qquad \text{on } \mathcal{F}$$

Assumptions for H, $H(P)$ to define selfadjoint operators.

- $\omega : \mathbb{R}^d \to [0, \infty)$ measurable, positive almost everywhere
- $v_0, \omega^{-1/2} v_0 \in L^2(\mathbb{R}^d)$, $v_x(k) = \mathrm{e}^{-\mathrm{i}kx} v_0(k)$

Examples. (with ultraviolet cutoff coupling function χ)

- Fröhlich polaron: $\omega = 1$, $v_0(k) = \chi(k)|k|^{-1}$
  Fröhlich 1934: effective model for impurity in dielectric crystal
- Nelson model: $\omega(k) = |k|$, $v_0(k) = \chi(k)|k|^{-1/2}$
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Two Versions of Feynman–Kac Formulas for Polaron Models

$$H = -\frac{1}{2}\Delta + \mathsf{d}\Gamma(\omega) + \varphi(v_x) \qquad \text{on } L^2(\mathbb{R}^d;\mathcal{F})$$

$$H(P) = \frac{1}{2}(P - \mathsf{d}\Gamma(\hat{p}))^2 + \mathsf{d}\Gamma(\omega) + \varphi(v_0) \qquad \text{on } \mathcal{F}$$

Version 1: Euclidean Quantum Field Theory – A Recipe

- Map $\mathcal{F}$ to an L^2-space
- Model the free field $\mathsf{d}\Gamma(\omega)$ as an infinite-dimensional Gaussian process

$$\boxed{\langle \Phi, \mathsf{e}^{-tH}\Psi\rangle = \mathbb{E}_{B,\xi}\left[\overline{\Phi(B_0,\xi_0)}\mathsf{e}^{-\int_0^t \xi_s(v_{X_s})\mathsf{d}s}\Psi(X_t,\xi_t)\right]}$$

This formula is called a Feynman–Kac–Nelson formula and is attributed to Nelson 1964.

Formulas of this type have been studied by many people, amongst many others including Betz, Hiroshima, Minlos, Lőrinczi, Spohn, ...

Two Versions of Feynman–Kac Formulas for Polaron Models

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$$H(P) = \frac{1}{2}(P - \mathrm{d}\Gamma(\hat{p}))^2 + \mathrm{d}\Gamma(\omega) + \varphi(v_0) \qquad \text{on } \mathcal{F}$$

Version 2: Operator-Valued Potentials. Güneysu–Matte–Møller 2017

$$\mathrm{e}^{-tH}\psi(x) = \mathbb{E}\left[\mathrm{e}^{u_t}\mathrm{e}^{a^\dagger(U_t^+)}\mathrm{e}^{-t\mathrm{d}\Gamma(\omega)}\mathrm{e}^{a(U_t^-)}\psi(B_t)\middle| B_0 = x\right]$$

$$\mathrm{e}^{-tH(P)} = \mathbb{E}\left[\mathrm{e}^{u_t}\mathrm{e}^{a^\dagger(U_t^+)}\mathrm{e}^{-t\mathrm{d}\Gamma(\omega)}\mathrm{e}^{a(U_t^-)}\mathrm{e}^{\mathrm{i}(P-\mathrm{d}\Gamma(\hat{p}))\cdot B_t}\right]$$

with $U_t^+ = \int_0^t \mathrm{e}^{-s\omega} v_{B_s}\mathrm{d}s$, $U_t^- = \int_0^t \mathrm{e}^{-(t-s)\omega} v_{B_s}\mathrm{d}s$, $u_t = \int_0^t \langle U_s^- | v_{B_s}\rangle\, \mathrm{d}s$.

Reminder: $\mathrm{e}^{-t(-\frac{1}{2}\Delta + V)}f(x) = \mathbb{E}[\mathrm{e}^{-\int_0^t V(B_s)\mathrm{d}s} f(B_t) | B_0 = x]$

$$a(f) = \int \overline{f(k)} a_k \mathrm{d}k, \quad a^\dagger(f) = \int f(k) a_k^\dagger \mathrm{d}k,$$
$$\varphi(f) = a(f) + a^\dagger(f), \quad f \in L^2(\mathbb{R}^d)$$

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Remarks.

- $\mathrm{e}^{a^\dagger(U_t^+)}\mathrm{e}^{-t\mathrm{d}\Gamma(\omega)}\mathrm{e}^{a(U_t^-)}$ defines a $\mathcal{B}(\mathcal{F})$-valued stochastic process. This can be seen by expanding the exponentials with a and $a^\dagger$.
- GMM also applied this approach to more general models of non-relativistic quantum field theory, e.g., the Pauli–Fierz model.

The Ultraviolet Problem

$$H = -\frac{1}{2}\Delta + \mathrm{d}\Gamma(\omega) + \varphi(v_x) \qquad \text{on } L^2(\mathbb{R}^d; \mathcal{F})$$

The assumption $v_0, \omega^{-1/2} v_0 \in L^2(\mathbb{R}^d)$ is not satisfied for any of our examples if $\chi \equiv \lambda$.

Examples. (with ultraviolet cutoff coupling function χ)

- Fröhlich polaron: $\omega = 1$, $v_0(k) = \chi(k)|k|^{-1}$
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Problem

Pick a sequence $\chi_n(k) = \lambda 1_{|k|<n}$, define

$$H_n = -\tfrac{1}{2}\Delta + \mathrm{d}\Gamma(\omega) + \varphi(v_{x,n}) \qquad \text{on } L^2(\mathbb{R}^d; \mathcal{F})$$

and study the limit $n \to \infty$.

Removal of the UV Cutoff

$$e^{-tH_n}\psi(x) = \mathbb{E}\left[e^{u_{n,t}} e^{a^\dagger(U^+_{n,t})} e^{-t d\Gamma(\omega)} e^{a(U^-_{n,t})}\psi(B_t)\middle| B_0 = x\right]$$

- Construct $U^\pm_{\infty,t}$ and prove $U^\pm_{n,t} \to U^\pm_{\infty,t}$ (in appropriate sense).
- Construct $u_{\infty,t}$, eventually after substracting a self-energy contribution and prove $u_{n,t} \to u_{\infty,t}$.

- Fröhlich polaron: e^{-tH_n} converges in norm Lieb, Yamazaki 1958, Griesemer, Wünsch 2016, Lampart, Schmidt 2019
  Convergence to $u_t = \int_0^t \int_0^s e^{-(s-r)}|B_r - B_s|^{-1} dr ds$ Feynman 1955. H., Matte 2024
- Nelson model: $e^{-t(H_n - \inf\sigma(H_n))}$ converges in norm Nelson 1964, Griesemer, Wünsch 2018, Lampart, Schmidt 2019
  Gubinelli, Hiroshima, Lőrinczi 2014, Matte, Møller 2018
- Bose polaron: $e^{-t(H_n - \inf\sigma(H_n))}$ converges in norm Lampart 2020
- 2D Relativistic Nelson: Sloan 1973, Schmidt 2019, H., Matte 2023
- Spin Boson Model: Lonigro 2022, H., Lampart, Valentín Martín in preparation, Fröhlich, H. in prep.

Ground State Energy and Existence

$$\mathrm{e}^{-tH(P)} = \mathbb{E}\Big[\mathrm{e}^{u_t}\mathrm{e}^{a^\dagger(U_t^+)}\mathrm{e}^{-t\mathrm{d}\Gamma(\omega)}\mathrm{e}^{a(U_t^-)}\mathrm{e}^{\mathrm{i}(P-\mathrm{d}\Gamma(\hat{p}))\cdot B_t}\Big]$$

Vacuum Expectation of the Semigroup

$$\langle \Omega, \mathrm{e}^{-tH(P)}\Omega\rangle = \mathbb{E}\big[\mathrm{e}^{u_t}\mathrm{e}^{\mathrm{i}P\cdot B_t}\big], \quad u_t = \int_0^t\int_0^s \langle v_{X_s}, \mathrm{e}^{-(s-r)\omega}v_{X_r}\rangle\, \mathrm{d}r\mathrm{d}s$$

For the Fröhlich polaron, this is exactly why Donsker, Varadhan 1987 could study Feynman's expression for u_t to prove the Pekar conjecture.

Remark. Recall from Sec. 4 that $\mathrm{e}^{-tH(P)}$ should improve positivity, w.r.t. a suitable cone containing Ω. For $P \neq 0$ and after cutoff removal this becomes non-trivial! Miyao 2019, Lampart 2019, H., Hiroshima 2024

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Vacuum Expectation of the Semigroup

$$\langle \Omega, \mathrm{e}^{-tH(P)}\Omega\rangle = \mathbb{E}\big[\mathrm{e}^{u_t}\mathrm{e}^{\mathrm{i}P\cdot B_t}\big], \quad u_t = \int_0^t\int_0^s \langle v_{X_s}, \mathrm{e}^{-(s-r)\omega}v_{X_r}\rangle\,\mathrm{d}r\mathrm{d}s$$

For the Fröhlich polaron, this is exactly why Donsker, Varadhan 1987 could study Feynman's expression for u_t to prove the Pekar conjecture.

Remark. Recall from Sec. 4 that $\mathrm{e}^{-tH(P)}$ should improve positivity, w.r.t. a suitable cone containing Ω. For $P \neq 0$ and after cutoff removal this becomes non-trivial! Miyao 2019, Lampart 2019, H., Hiroshima 2024

This representation of the vacuum expectation has been used in the study of ground state existence, in the past and recently. Many of the cited authors as well as plenty more have contributed.

Thank you for the invitation
and the attention!