Effective Mass of the Polaron: a lower bound

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Joint work with Steffen Polzer (Geneva)

The Fröhlich Polaron

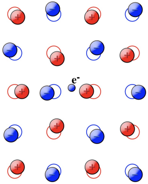

Image from Wikipedia

A charged particle in a polar crystal drags around a polarization cloud when moving.

It therefore appears to be heavier.

Its Hamiltonian is the self-adjoint operator in $L^2(\mathbb{R}^3) \otimes \mathcal{F}(L^2(\mathbb{R}^3))$ given by

$$H_\alpha = \frac{1}{2}p^2 + \int_{\mathbb{R}^3} \omega(k) a_k^* a_k \, \mathrm{d}k + \sqrt{\alpha} \int_{\mathbb{R}^3} \frac{\hat{\varrho}(k)}{\sqrt{2\omega(k)}} \left(\mathrm{e}^{\mathrm{i}k\cdot x} \, a_k + \mathrm{e}^{-\mathrm{i}k\cdot x} \, a_k^* \right) \mathrm{d}k.$$

The three terms are particle (kinetic) energy, field energy and interaction energy, respectively.

For the Fröhlich Hamiltonian, $\omega(k) = 1$ and $\frac{\hat{\varrho}(k)}{\sqrt{2\omega(k)}} = \frac{1}{\sqrt{2}\pi|k|}$.

The **coupling constant** α determines the strength of the interaction. We will be interested in large α.

The effective mass

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H commutes with the total momentum operator $p + P_\mathrm{f}$ with $P_\mathrm{f} = \int_{\mathbb{R}^3} k a_k^* a_k \,\mathrm{d}k$. Therefore, it is unitarily equivalent to the fiber Hamiltonian $\int_{\mathbb{R}^3}^{\oplus} H_\alpha(P)\mathrm{d}P$ with

$$H_\alpha(P) = \frac{1}{2}\big(P - P_\mathrm{f}\big)^2 + \int_{\mathbb{R}^3} \omega(k) a_k^* a_k \,\mathrm{d}k + \sqrt{\alpha} \int_{\mathbb{R}^3} \frac{\hat{\varrho}(k)}{\sqrt{2\omega(k)}} (a_k + a_k^*) \,\mathrm{d}k.$$

Set $E_\alpha(P) := \inf \mathrm{spec} H_\alpha(P) = E_{\alpha,\mathrm{r}}(|P|)$ by rotation invariance.

Corresponds to $p \mapsto \frac{1}{2m}p^2$ of a free particle of mass m.

The effective mass is given by $m_{\mathrm{eff}}(\alpha) = \frac{1}{E''_{\alpha,\mathrm{r}}(0)}$.

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Theorem [Lieb, Seiringer 2020]: $\lim_{\alpha\to\infty} m_\mathrm{eff}(\alpha) = \infty$.

Effective Mass and perturbed Brownian motion

For $T > 0$ define a probability measure on $C([0,\infty),\mathbb{R}^3)$ by

$$\mathbb{P}_T(\mathrm{d}X) = \frac{1}{Z_{\alpha,T}}\,\mathrm{e}^{\frac{\alpha}{2}\int_{-T}^{T}\mathrm{d}s\int_{-T}^{T}\mathrm{d}t\,\frac{\mathrm{e}^{-|t-s|}}{|X_t - X_s|}}\,\mathcal{W}^0(\mathrm{d}X).$$

$\mathcal{W}^0$ is the path measure of Brownian motion.

Intuition:

- attractive interaction; favours paths revisiting their past.
- expect: mean square displacement $\mathbb{E}_{\alpha,T}\big(|X_T|^2\big) < \mathbb{E}_{\alpha,T}\big(|X_T|^2\big) = 3T$ for $\alpha > 0$.
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Fact: if

$$\sigma^2(\alpha) = \lim_{T\to\infty}\frac{1}{3T}\mathbb{E}_{\alpha,T}\big(|X_T|^2\big).$$

exists, then the Polaron effective mass is given by $m_{\mathrm{eff}} = \frac{1}{\sigma^2(\alpha)}$.

(use Feynman-Kac formula, see [Feynman 55, Spohn 87, **Dybalski, Spohn 20**])

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Extracting information from the expression for $\mathbb{P}_T(\mathrm{d}X)$ is hard!

Main result

For $T > 0$ and $1 \leqslant \gamma < 2$ let

$$\mathbb{P}_T(\mathrm{d}X) = \frac{1}{Z_{\alpha,T}}\, \mathrm{e}^{\frac{\alpha}{2}\int_{-T}^{T}\mathrm{d}s\int_{-T}^{T}\mathrm{d}t\, v(X_t - X_s) g(t-s)}\, \mathcal{W}^0(\mathrm{d}X).$$

with

- $v(x) = |x|^{-\gamma}$ for $\gamma \in [1,2)$,
- $g \geqslant 0$, $\sup_{t \geqslant 0}(1+t)g(t) < \infty$,
  $\int_0^\infty g(s)\,\mathrm{d}s = 1$ and
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Theorem [B., Polzer 22]

$\sigma^2(\alpha) = \lim_{T \to \infty} \frac{1}{3T} \mathbb{E}_{\alpha,T}\left(|X_T|^2\right)$ exists, and there exists $C < \infty$ such that $\sigma^2(\alpha) \leqslant C\alpha^{-2/5}$ for all $\alpha > 0$.

Consequently, $m_{\mathrm{eff}}(\alpha) \geqslant C^{-1}\alpha^{2/5}$.

This is ten percent of the way up to $m_{\mathrm{eff}}(\alpha) \sim \alpha^4$.

Varadhans point process representation

Let $\Gamma_{\alpha,T}$ be the distribution of the PPP with intensity measure

$$\mu_{\alpha,T}(\mathrm{d}s\,\mathrm{d}t) = \alpha g(t-s) 1\!\!1_{\{0 \leqslant s<t \leqslant T\}}\,\mathrm{d}s\mathrm{d}t, \qquad c_{\alpha,T} := \mu_{\alpha,T}(\mathbb{R}^2).$$

Then for measurable $A \subset C([0,\infty),\mathbb{R}^3)$ we have

$$\mathbb{P}_T(A) = \frac{1}{Z_{\alpha,T}} \int_A \mathcal{W}(\mathrm{d}X)\, \mathrm{e}^{\alpha \iint_{0 \leqslant s<t \leqslant T} \mathrm{d}s\mathrm{d}t\, g(t-s) v(X_t - X_s)}$$

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$$= \frac{1}{Z_{\alpha,T}} \sum_{n=0}^{\infty} \frac{1}{n!} \int \mu_{\alpha,T}^{\otimes n}\Big(\prod_{i=1}^n \mathrm{d}s_i \mathrm{d}t_i\Big) \int_A \mathcal{W}(\mathrm{d}X) \prod_{i=1}^n v(X_{t_i} - X_{s_i})$$

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$$= \int \underbrace{\frac{\mathrm{e}^{c_{\alpha,T}}}{Z_{\alpha,T}} F(\xi)\Gamma_{\alpha,T}(\mathrm{d}\xi)}_{=\hat{\Gamma}_{\alpha,T}(\mathrm{d}\xi)} \underbrace{\frac{1}{F(\xi)}\mathbb{E}_{\mathcal{W}}\big(\mathbb{1}_A \prod_{(s,t)\in\mathrm{supp}(\xi)} v(X_t - X_s)\big)}_{=:\boldsymbol{P}_{\xi}(A)}$$

with $F(\xi) = \mathbb{E}_{\mathcal{W}}\big(\prod_{(s,t)\in\mathrm{supp}(\xi)} v(X_t - X_s)\big)$.

Point process and interval process

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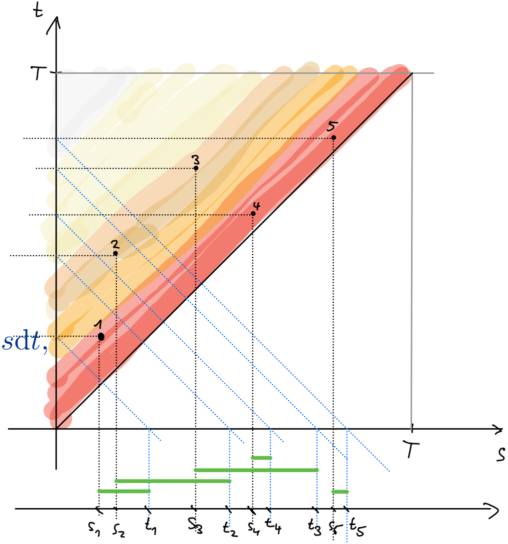

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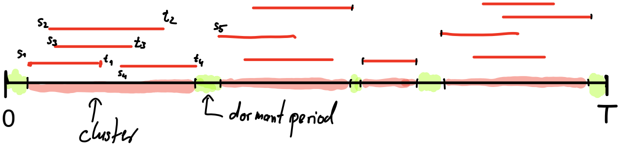
[Mukherjee, Varadhan 19] Generalized in [B., Polzer 21].

$\mathbb{P}_{\alpha,T}$ is a mixture of path measures, the mixing measure is the point process with distribution $\hat{\Gamma}_{\alpha,T}$, which can be seen as a collection of overlapping intervals.



$\boldsymbol{P}_\xi$ factorizes with respect to clusters (independent increments!).

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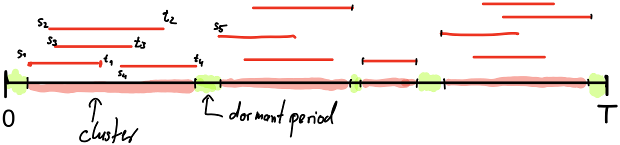

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Infinite volume limit and CLT can be deduced from this.

Mean square displacement: ideas

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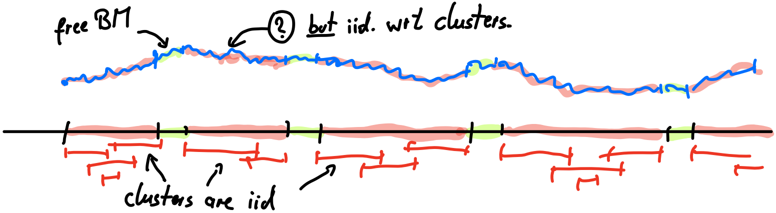

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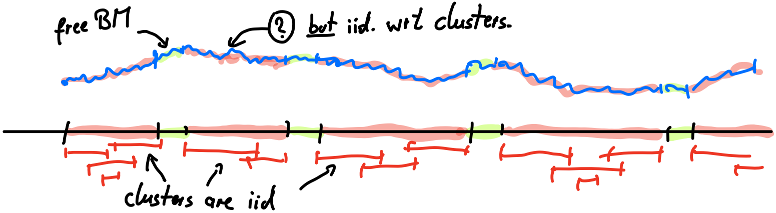

We need to estimate (from above) the mean square displacement per unit length in one typical cluster.

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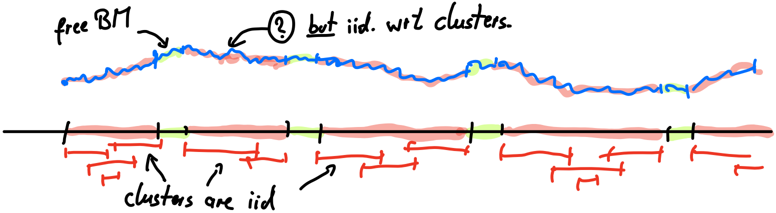

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For large α, clusters get longer and more densely populated. Getting information about them is still rather tricky!

Effective mass estimate: a shift of energy

Define $v_{\varepsilon}(x) = \dfrac{1}{|x|} + \varepsilon, \quad g(t) = \mathrm{e}^{-|t|}$

$$\mu_{\alpha,T}(\mathrm{d}s\,\mathrm{d}t) = \alpha g(t-s) 1\!\!1_{\{0 \leqslant s<t \leqslant T\}}\,\mathrm{d}s\mathrm{d}t, \qquad c_{\alpha,T} := \mu_{\alpha,T}(\mathbb{R}^2).$$

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Decompose this further: $v_{\varepsilon}(x) = \frac{1}{|x|} + \varepsilon = \int_{[0,\infty)} \nu_{\varepsilon}(\mathrm{d}u)\,\mathrm{e}^{-u^2|x|^2/2}$,

$$\nu_{\varepsilon} = \sqrt{2/\pi}\,\mathrm{d}u + \varepsilon \delta_0(\mathrm{d}u).$$

Then:

Effective mass: a variational formula

$$\mathbb{P}_{\alpha,T}(\mathrm{d}X) = \int \hat{\Gamma}^{\varepsilon}_{\alpha,T}(\mathrm{d}\xi) \int \kappa_{\varepsilon}(\xi, \mathrm{d}u) \boldsymbol{P}_{\xi,u}(\mathrm{d}X)$$

with $u \in \mathbb{R}^{|\xi|}$, the kernel

$$\kappa_{\varepsilon}(\xi, u) := \frac{\phi(\xi, u)}{F_{\varepsilon}(\xi)} {\nu_{\varepsilon}}^{|\xi|}(\mathrm{d}u), \quad \phi(\xi, u) = \mathbb{E}_{\mathcal{W}}\big(\mathrm{e}^{-\sum_{(s,t)\in\xi} u^2_{(s,t)}(X_t - X_s)^2}\big)$$

and Gaussian path measure

$$\boldsymbol{P}_{\xi,u}(\mathrm{d}X) = \frac{1}{\phi(\xi, u)} \mathrm{e}^{-\sum_{(s,t)\in\xi} u^2_{(s,t)}(X_t - X_s)^2} \mathcal{W}(\mathrm{d}X).$$

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$$\mathbb{P}_{\alpha,T}(\mathrm{d}X) = \int \hat{\Gamma}^{\varepsilon}_{\alpha,T}(\mathrm{d}\xi) \int \kappa_{\varepsilon}(\xi, \mathrm{d}u) \boldsymbol{P}_{\xi,u}(\mathrm{d}X)$$

with $u \in \mathbb{R}^{|\xi|}$, the kernel

$$\kappa_{\varepsilon}(\xi, u) := \frac{\phi(\xi, u)}{F_{\varepsilon}(\xi)} {\nu_{\varepsilon}}^{|\xi|}(\mathrm{d}u), \quad \phi(\xi, u) = \mathbb{E}_{\mathcal{W}}\Big(\mathrm{e}^{-\sum_{(s,t)\in\xi} u^2_{(s,t)}(X_t - X_s)^2} \Big)$$

and Gaussian path measure

$$\boldsymbol{P}_{\xi,u}(\mathrm{d}X) = \frac{1}{\phi(\xi, u)} \, \mathrm{e}^{-\sum_{(s,t)\in\xi} u^2_{(s,t)}(X_t - X_s)^2} \, \mathcal{W}(\mathrm{d}X).$$

We then have

$$\sigma^2_{\alpha,T} := \frac{1}{3T} \mathbb{E}_{\alpha,T}(|X_T - X_0|^2) = \int \hat{\Gamma}^{\varepsilon}_{\alpha,T}(\mathrm{d}\xi) \int \kappa_{\varepsilon}(\xi, \mathrm{d}u) \sigma^2_T(\xi, u),$$

where $\sigma^2_T(\xi, u) = \frac{1}{3T} \boldsymbol{E}_{\xi,u}(|X_T - X_0|^2) =$

$$= \frac{1}{T} \mathrm{dist}_{L^2}\big(B_{[0,T]}, \mathrm{span}\{u_{(s,t)}(B_t - B_s) + Z_{(s,t)} : (s,t) \in \xi\}\big)^2$$

Here B is a 1-dim BM and the $Z_{(s,t)}$ are $\mathcal{N}(0,1)$, iid indep. of B.

Effective mass: identifying a simple part of the point process

$$\sigma^2_{\alpha,T} = \int \hat{\Gamma}^{\varepsilon}_{\alpha,T}(\mathrm{d}\xi) \int \kappa_{\varepsilon}(\xi, \mathrm{d}u)\ \sigma^2_T(\xi, u),$$

with

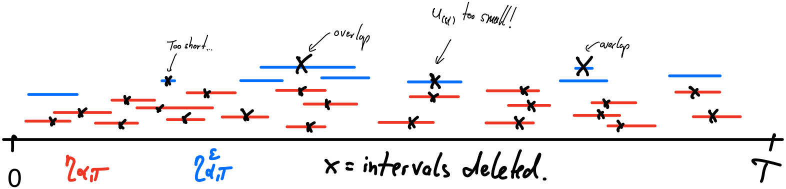
$$\sigma^2_T(\xi, u) = \frac{1}{T}\mathrm{dist}_{L^2}\big(B_{[0,T]}, \mathrm{span}\{u_{(s,t)}(B_t - B_s) + Z_{(s,t)} : (s,t) \in \xi\}\big)^2$$

Observation 1: deleting intervals (s,t) from ξ enlarges $\sigma^2_T(\xi, u)$. This is good, we want an upper bound for $\sigma^2_{\alpha,T}$. The same holds for decreasing some component of u.

Observation 2: $\hat{\Gamma}^{\varepsilon}_{\alpha,T}$ is a Cox process with driving measure $\mu_{\alpha,T}(\mathrm{d}s\mathrm{d}t) v_{\varepsilon}(X_t - X_s)$ with $X \sim \mathbb{P}_{\alpha,T}$, i.e. conditional on X the intensity measure is $\mu_{\alpha,T}(\mathrm{d}s\mathrm{d}t) v_{\varepsilon}(X_t - X_s)$.

Observation 3: $\hat{\Gamma}^{\varepsilon}_{\alpha,T}$ is the distribution of the independent sum $\eta_{\alpha,T} + \eta^{\varepsilon}_{\alpha,T}$ with $\eta_{\alpha,T} \sim \hat{\Gamma}^{0}_{\alpha,T}$ and $\eta^{\varepsilon}_{\alpha,T} \sim \Gamma_{\varepsilon\alpha,T}$. We understand $\Gamma_{\varepsilon\alpha,T}$ very well!

Effective mass: lower bound



Strategy:

1. We delete all intervals from (ξ, u) that
   - come from the process $\eta_{\alpha,T}$,
   - or are shorter than length 1,
   - or carry a mark less than $C(\alpha)$ (to be fixed later).
   - then we remove overlapping intervals.

   Since $\alpha \to \infty$ there are still plenty of intervals left.
2. We use stochastic domination to estimate the kernel $\kappa_\varepsilon(\xi, \mathrm{d}u)$ that *depends on the whole* ξ by a product kernel that marks all intervals independently with either 0 or $C(\alpha)$, with suitable probability for each one.
3. In the resulting configuration, $\sigma_T^2(\xi, u)$ can be computed. Optimizing $C(\alpha) = \alpha^{1/5}$ gives the result.

Thank you for listening!