The Gaussian Correlation Inequality and the Polaron

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$$d\widehat{\mathbb{P}}_{\alpha,T}(\mathrm{B}) \equiv \frac{1}{Z_{\alpha,T}} \exp\left(\alpha \int_0^T \int_0^T e^{-|t-s|} V(\|\mathrm{B}_t - \mathrm{B}_s\|)\, \mathrm{d}t\, \mathrm{d}s\right) d\mathbb{P}(\mathrm{B}),$$

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I will explain a **confinement** result upper bounding $\mathbb{E}^{\widehat{\mathbb{P}}_{\alpha,T}} \|B_T\|^2$.

Physically, this means we lower bound the *effective mass*

$$m_{\text{eff}}(\alpha) \equiv \mathbb{E}^{\widehat{\mathbb{P}}_{\alpha,T}} \left[\frac{3T}{\|B_T\|^2}\right].$$

1. Introduction to the Polaron
2. Royen's Gaussian Correlation inequality
3. Lower bounds on the effective mass

Start from a quantum mechanical Hamiltonian, an operator on $L^2(\mathbb{R}^3) \otimes \mathcal{F}(L^2(\mathbb{R}^3))$:

$$H = -\nabla_x^2/2 + \int_{\mathbb{R}^3} a_k^\dagger a_k \, \mathrm{d}k + \sqrt{\alpha} \int_{\mathbb{R}^3} \frac{e^{-ikx}}{|k|} a_k^\dagger \, \mathrm{d}k + \sqrt{\alpha} \int_{\mathbb{R}^3} \frac{e^{ikx}}{|k|} a_k \, \mathrm{d}k.$$

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H commutes with momentum. Each momentum $P \in \mathbb{R}^3$ has a ground state energy $E_\alpha(|P|)$.

- [Gross 72]: $E_\alpha(P) \geq E_\alpha(0)$.
- [Polzer 22]: $E_\alpha(P)$ is increasing in P, and strictly so at 0.
- Effective mass was originally defined by:

$$\frac{1}{2m_{\mathrm{eff}}(\alpha)} = \lim_{P \to 0} \frac{E_\alpha(P) - E_\alpha(0)}{P^2}.$$

Progress on the Effective Mass

Asymptotics of $E_\alpha(0)$ determined by [Donsker-Varadhan 83] using large deviations. Effective mass has required more time.

- [Landau-Pekar 1948]: predicted $m_{\text{eff}}(\alpha) \approx C_* \alpha^4$.
- [Lieb-Seiringer 17]: $\lim_{\alpha \to \infty} m_{\text{eff}}(\alpha) = \infty$.
- [Spohn 87, Dybalski-Spohn 20]: rigorous path integral definition of m_{eff}, assuming a functional CLT for $\widehat{\mathbb{P}}_{\alpha,T}$.
- [Mukherjee-Varadhan 21, Betz-Polzer 22a]: confirmation of functional CLT.
- [Betz-Polzer 22b]: $m_{\text{eff}}(\alpha) \geq c\alpha^{2/5}$.
- [Brooks-Seiringer 22 via Polzer 22]: $m_{\text{eff}}(\alpha) \leq C_* \alpha^4 + O(\alpha^{4-\varepsilon})$.

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Theorem (S 22)

As $\alpha \to \infty$, one has $m_{\text{eff}}(\alpha) \geq \frac{c\alpha^4}{(\log \alpha)^6}$.

Proved using ideas from high-dimensional geometry. The bounds now almost match.

Gaussian Domination for Concave Potentials

Given a centered Gaussian measure μ on a Banach space $\mathcal{X}$, consider the weighting

$$\mathrm{d}\mu_W(x) \propto e^{W(x)}\,\mathrm{d}\mu(x).$$

Many measures (e.g. Polaron) take this form.

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If W is <u>concave</u>:

- $\mathbb{E}^{x\sim\mu_W}[xx^\top] \preceq \mathbb{E}^{x\sim\mu}[xx^\top]$ (covariance shrinks).
- μ_W inherits Poincare/Log-Sobolev inequalities from μ_W [Bakry-Emery 85]:
- The optimal transport map $\mu \to \mu_W$ is 1-Lipschitz [Caffarelli 00].

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Moreover, suppose $W(x) = Q(x) + \widetilde{W}(x)$, where $Q, \widetilde{W}$ are concave and Q is **quadratic**.

- Then μ_W is dominated by $d\mu_Q \propto e^{Q(x)} d\mu(x)$, a "more confined" Gaussian than μ.

Non-Convexity of the Coulomb Interaction

Unfortunately this theory does not apply to the Polaron. Recall:

$$d\widehat{\mathbb{P}}_{\alpha,T}(B) \equiv \frac{1}{Z_{\alpha,T}} \exp\left(\alpha \int_0^T \int_0^T e^{-|t-s|} V(\|B_t - B_s\|)\, dt\, ds\right) d\mathbb{P}(B),$$

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However the interaction term makes the walk self-attractive. We certainly expect $\widehat{\mathbb{P}}_{\alpha,T}$ to be "dominated" by Brownian motion.

Formalizing this requires a **more flexible** notion of Gaussian domination.

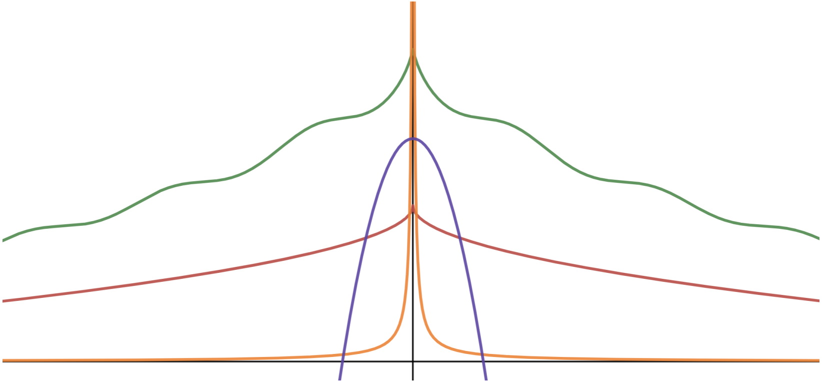
Symmetric Quasi-Concave Functions

Definition

$W : \mathcal{X} \to \mathbb{R}$ is symmetric quasi-concave if:

- $W(x) = W(-x)$.
- All super-level sets $S_\lambda = \{x \in \mathcal{X} \; : \; W(x) \geq \lambda\}$ are convex.

Examples for $\mathcal{X} = \mathbb{R}$:



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More general setup: probability measures

$$d\mu_W(x) \propto e^{W(x)} \, d\mu(x)$$

for $W : \mathcal{X} \to \mathbb{R}$ which is symmetric quasi-concave, or a sum/integral of such functions.

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The Polaron measure does take this form:

$$W(\mathrm{B}_{[0,T]}) = \int_0^T \int_0^T \frac{\alpha e^{-|t-s|}}{\|\mathrm{B}_t - \mathrm{B}_s\|} \mathrm{d}t\mathrm{d}s = \int_0^T \int_0^T W_{t,s}(\mathrm{B}_{[0,T]})\mathrm{d}t\mathrm{d}s.$$

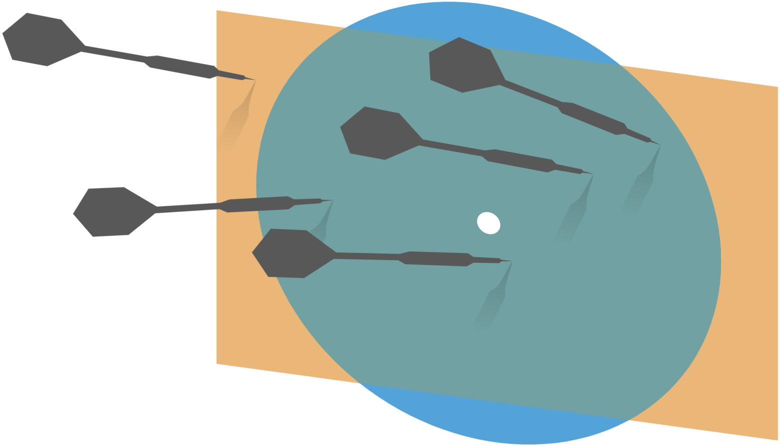
The **Gaussian correlation inequality** is a perfect tool for such situations.

Key Tool: Royen's Gaussian Correlation Inequality

Theorem (Royen 2014)

Let $\mu \in \mathcal{P}(\mathcal{X})$ be a centered Gaussian measure, and $K_1, K_2 \subseteq \mathcal{X}$ symmetric convex sets (i.e. $K_i = -K_i$). Then 1_{K_1} and 1_{K_2} have non-negative correlation under μ, i.e.

$$\mu(K_1 \cap K_2) \geq \mu(K_1)\mu(K_2).$$



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History (see 2017 Quanta article):

- Conjectured by [Dunnet-Sobel 55], [Gupta-Eaton-Perlman-Savage-Sobel 72].
- [Khatri 67, Sidak 67, Pitts 77, Schechtman-Schlumprecht-Zinn 98, Hargé 99]: special cases such as $\mathcal{X} = \mathbb{R}^2$.
- **[Royen 2014]**: brilliant solution (while brushing teeth!). Initially escapes attention.
- [Latała-Matlak 2015]: exposition of Royen's proof

Proof idea: for $x, y \overset{i.i.d.}{\sim} \mu$, equivalent to

$$\mathbb{P}[x \in K_1 \wedge x \in K_2] \geq \mathbb{P}[x \in K_1, y \in K_2].$$

Royen showed $f(t) = \mathbb{P}[x \in K_1 \;\wedge\; \sqrt{1-t}x + \sqrt{t}y \in K_2]$ is decreasing on $t \in [0,1]$.

Interpreting GCI as Gaussian Domination

GCI: if $K_1, K_2 \subseteq \mathcal{X}$ are symmetric convex, then

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By induction, if $K_1, \ldots, K_n \subseteq \mathcal{X}$ are symmetric convex:

$$\mu(K_1 \cap \cdots \cap K_n) \geq \mu(K_1 \cap \cdots \cap K_m) \cdot \mu(K_{m+1} \cap \cdots \cap K_n),$$

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By Fubini, if $f_1, \ldots, f_n : \mathcal{X} \to \mathbb{R}^+$ are symmetric quasi-concave,

$$\mathbb{E}^{\mu}[f_1 f_2 \ldots f_n] \geq \mathbb{E}^{\mu}[f_1 f_2 \ldots f_m] \cdot \mathbb{E}^{\mu}[f_{m+1} f_{m+2} \ldots f_n].$$

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Let's say $\nu \preceq \mu$ if $\frac{d\nu}{d\mu}$ is a limit of products of SQC functions. If μ is centered Gaussian:

$$\nu(K) = \mathbb{E}^{\mu}\left[\frac{d\nu}{d\mu} \cdot 1_K\right] \overset{\text{GCI}}{\geq} \mathbb{E}^{\mu}\left[\frac{d\nu}{d\mu}\right] \cdot \mu(K) = \mu(K)$$

for any symmetric convex set K. **This is a type of Gaussian domination.**

First Application to the Polaron

$\nu \preceq \mu$ if $\frac{d\nu}{d\mu}$ is a limit of <u>products of SQC functions</u>. If μ is centered Gaussian:

1. $\nu(K) \geq \mu(K)$ for symmetric convex K, by GCI.
2. By Fubini again, $\mathbb{E}^{\nu}[f] \geq \mathbb{E}^{\mu}[f]$ for symmetric convex f.
3. In particular,
$$\mathbb{E}^{\nu}[\|x\|^2] \geq \mathbb{E}^{\mu}[\|x\|^2].$$
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Immediate Polaron consequence: since $\widehat{\mathbb{P}}_{\alpha,T}(B) \preceq \mathbb{P}$, we have $m_{\mathrm{eff}}(\alpha) \geq 1$ via:

$$\mathbb{E}^{\widehat{\mathbb{P}}_{\alpha,T}}\|B_T\|^2 \leq \mathbb{E}^{\mathbb{P}_{\alpha,T}}\|B_T\|^2 = 3T.$$

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More refined uses of GCI will show interactions strictly decrease diffusivity.

Plan

1. Introduction to the Polaron
2. Royen's Gaussian Correlation inequality
3. Lower bounds on the effective mass
   - Initial attempt: $\frac{\sqrt{\alpha}}{\log^C T}$
   - Improvement: $\frac{\alpha^2}{\log^C T}$
   - T-independence: $\frac{\alpha^2}{\log^C \alpha}$
   - Final step: $\frac{\alpha^4}{\log^C \alpha}$

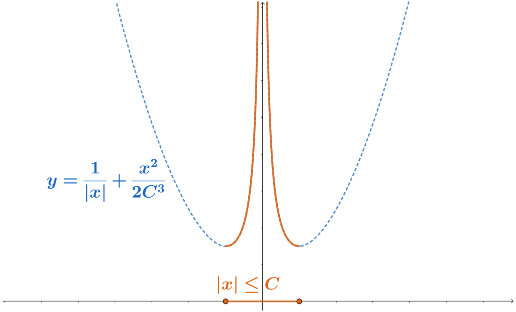
Attempt at Improvement

So far, we have only used that $V(r) = \frac{1}{r}$ is symmetric and monotone. However:

- Interaction decays exponentially in time, so only $|t-s| \leq 1$ should be needed.
- If $|t-s| \leq 1$, we have $\mathbb{P}[\|B_t - B_s\| \leq C] \geq 0.999$ for Brownian motion.
- V is **more monotone** on **small distances**. The function

$$r \mapsto \frac{1}{|r|} + \frac{r^2}{2C^3}$$

is symmetric and quasi-concave on $r \in [-C, C]$.



Attempt at Improvement

$r \mapsto \frac{1}{|r|} + \frac{r^2}{2C^3}$ is symmetric and quasi-concave on $|r| \leq C$.

Fixing t, s with $|t - s| \leq 1$, suppose we magically **KNEW** $\|B_t - B_s\| \leq C$. Then

$$W_{t,s} = \frac{e^{|t-s|}}{\|B_t - B_s\|} + \frac{\|B_t - B_s\|^2}{2eC^3}$$

would behave as a symmetric quasi-concave function.

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would behave as a symmetric quasi-concave function.

This would imply an improved Gaussian domination $\widehat{\mathbb{P}}_{\alpha,T} \preceq \widetilde{\mathbb{P}}_{\alpha,T}$, where

$$\widetilde{\mathbb{P}}_{\alpha,T} \equiv \frac{1}{\widetilde{Z}_{\alpha,T}} \exp\left(\alpha \int_0^T \int_0^T \mathbb{1}\{|t-s| \leq 1\} \cdot \frac{-\|\mathrm{B}_t - \mathrm{B}_s\|^2}{10C^3}\, \mathrm{d}t\, \mathrm{d}s\right) \mathrm{d}\mathbb{P}(\mathrm{B}).$$

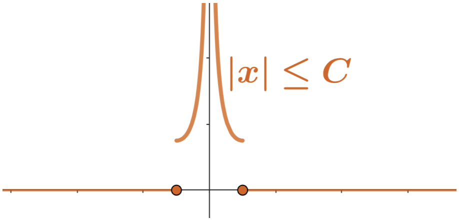
Note that $\widetilde{\mathbb{P}}_{\alpha,T}$ is still centered Gaussian, but is **more confined** than Brownian motion.

But we **do not know** that $\|B_t - B_s\| \leq C$. And we need it for many (t, s) simultaneously...

The function

$$r \mapsto \left(\frac{1}{|r|} + \frac{r^2}{2C^3}\right) \cdot 1_{|r| \leq C}$$

is symmetric quasi-concave on all of $\mathbb{R}$.



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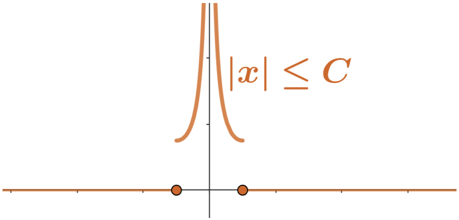

Define the set of paths on $[0, T]$ with locally C-bounded increments:

$$K(T, C) \equiv \{\mathrm{B}_{[0,T]} \; : \; \sup_{|t-s|\le 1} \|\mathrm{B}_t - \mathrm{B}_s\| \le C\}.$$

$\widetilde{\mathbb{P}}_{\alpha,T}$ thus dominates the **truncated** Polaron measure: $\widehat{\mathbb{P}}_{\alpha,T}\big|_{K(T,C)} \preceq \widetilde{\mathbb{P}}_{\alpha,T}$.

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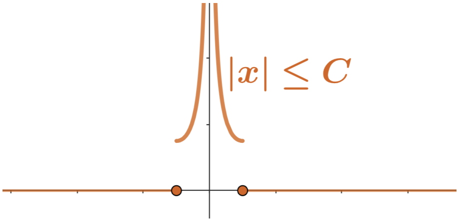

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$\widetilde{\mathbb{P}}_{\alpha,T}$ thus dominates the **truncated** Polaron measure: $\widehat{\mathbb{P}}_{\alpha,T}\big|_{K(T,C)} \preceq \widetilde{\mathbb{P}}_{\alpha,T}$.

Using GCI, one can show the truncation is benign for $C \asymp \sqrt{\log T}$:

$$\left\| \widehat{\mathbb{P}}_{\alpha,T} - \widehat{\mathbb{P}}_{\alpha,T}\big|_{K(T,C)} \right\|_{TV} \le \frac{1}{\alpha^5 T^5}.$$

Where Do We Stand?

We now have a close approximation

$$\widehat{\mathbb{P}}_{\alpha,T}\big|_{K(T,C)} \approx \widehat{\mathbb{P}}_{\alpha,T}$$

which is dominated for $C \asymp \sqrt{\log T}$ via:

$$\widehat{\mathbb{P}}_{\alpha,T}\big|_{K(T,C)} \preceq \widetilde{\mathbb{P}}_{\alpha,T} \propto \exp\left(\alpha \int_0^T \int_0^T \mathbb{1}\{|t-s| \leq 1\} \cdot \frac{-\|B_t - B_s\|^2}{10C^3}\, dt\, ds\right) d\mathbb{P}(B).$$

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Some difficulties:

1. How much more confined is $\widetilde{\mathbb{P}}_{\alpha,T}$ than Brownian motion??
2. We were forced to take $C \asymp \sqrt{\log T}$. (**Serious**)
   - The order of limits is $T \gg \alpha \gg 1$, so $\log T$ is fatal.

Extra Gaussian Confinement, on the Back of an Envelope

The behavior of $\widetilde{\mathbb{P}}_{\alpha,T}$ on $t \in [i, i+1]$ is

$$\exp\left(\int_i^{i+1}\int_i^{i+1} \frac{-\alpha\|\mathrm{B}_t - \mathrm{B}_s\|^2}{10C^3}\,\mathrm{d}t\,\mathrm{d}s\right)\mathrm{d}\mathbb{P}(\mathrm{B}).$$

For small ε, this is roughly

$$\mathbb{P}\left[\int_i^{i+1}\int_i^{i+1} \|B_t - B_s\|^2 \le \varepsilon\right] \approx \mathbb{P}\left[\int_i^{i+1}\int_i^{i+1} \|B_t\|^2 \le \varepsilon\right] \approx e^{-\varepsilon^{-1}}.$$

Indeed, $\mathrm{B}_{[i,i+1]}$ should be small ε^{-1} times for this to hold.

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Indeed, $\mathsf{B}_{[i,i+1]}$ should be small ε^{-1} times for this to hold.

The contribution from value ε is roughly $\exp\left(-\frac{\alpha\varepsilon}{C^3} - \frac{1}{\varepsilon}\right)$. Maximized at $\varepsilon \asymp \sqrt{C^3/\alpha}$.
Rigorous proof: diagonalize in a Fourier basis. In fact with high probability,

$$\sup_{t,s\in[i,i+1]} \|\mathsf{B}_t - \mathsf{B}_s\| \lesssim \sqrt[4]{C^3/\alpha}.$$

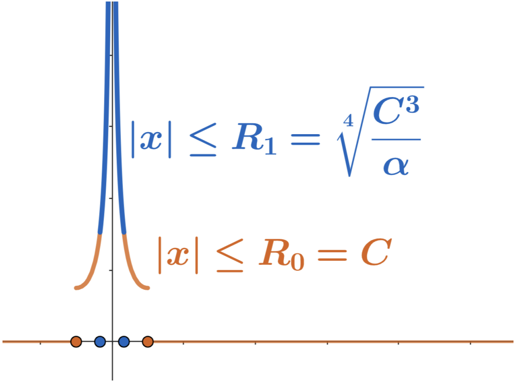
Iterative Improvement

With high probability:

$$\sup_{t,s\in[i,i+1]} \|B_t - B_s\| \lesssim \sqrt[4]{C^3/\alpha}.$$

Recall from before:

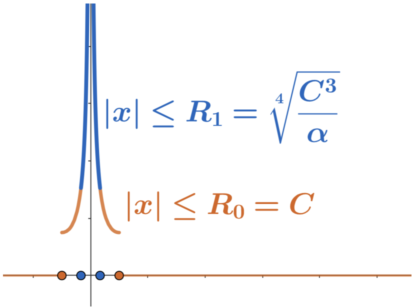
$$V(r) = \frac{1}{r} \text{ is } \textbf{more monotone} \text{ on } \textbf{small distances}.$$

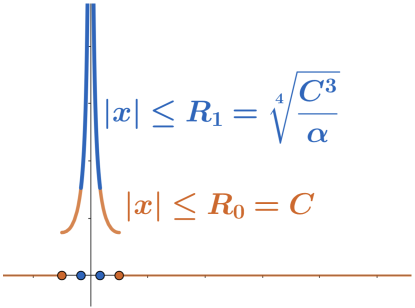


Iterative Improvement: Stronger Confinement Near the Origin

Previously, we used quasi-concavity of

$$r \mapsto \frac{1}{|r|} + \frac{r^2}{2C^3}, \quad |r| \le R_0 \equiv C.$$





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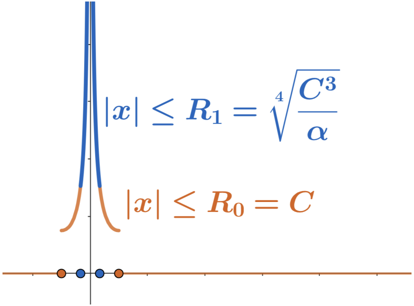

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Iterating, $\sup_{t,s\in[i,i+1]} \|\mathrm{B}_t - \mathrm{B}_s\|$ is bounded by $R_0 \ge R_1 \ge \dots$ with

$$R_{k+1} \approx \sqrt[4]{R_k^3/\alpha}.$$

This stabilizes at the much better $R_* = \widetilde{O}(\alpha^{-1})$. I.e. $\|B_{i+1} - B_i\|^2 \le \widetilde{O}(\alpha^{-2})$.

From $\log T$ to $\log \alpha$ Dependence

The order of limits is $T \gg \alpha \gg 1$, so the $\log T$ factors are a serious problem.

To avoid this, the argument should apply on *most*, but *not all* intervals $[i, i+1]$.

Intuitively, we can take $C \asymp \sqrt{\log(\alpha)}$. The $O(T/\alpha^{10})$ "bad" intervals should contribute total variance $O(T/\alpha^{10})$, which is fine.

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But to use the Gaussian correlation inequality, we to control the full path measure all at once. We cannot decompose

$$[0, T] = \bigcup_{i=0}^{T-1} [i, i+1]$$

and recombine path behaviors arbitrarily. This is a **serious** problem!

From $\log T$ to $\log \alpha$ Dependence: Decomposition of Gaussian Measures

Let $\mu^{\times 2}(2A) = \mu(A)$ be the dilation of μ by a factor of 2.

Lemma

Let $\mu \in \mathcal{P}(\mathcal{X})$ be a centered Gaussian measure, and K a symmetric convex set with $\mu(K) \geq 1-\delta$. Then there exists a decomposition of μ into μ_{good}, μ_{bad} with:

1. $\mu = (1-\delta)\mu_{good} + \delta\mu_{bad}$.
2. $\mu_{good} \preceq \mu$.
3. μ_{good} *is supported inside* $10K$.
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Application with $\delta \leq \alpha^{-10}$ and Brownian motion $\mu_i = \mathbb{P}([i, i+1])$:

- $K = K([i, i+1], 10\sqrt{\log \alpha}) = \left\{ \mathrm{B}_{[i,i+1]} \ : \ \sup_{i \leq s,t \leq i+1} \|\mathrm{B}_t - \mathrm{B}_s\| \leq 10\sqrt{\log \alpha} \right\}$.
- The main argument applies to μ_{good}, via 3.
  - The k-th level of recursion requires μ_{good_k} to be defined.
- Nothing terrible on the rare bad intervals, by 4.

From $\log T$ to $\log \alpha$ Dependence: Decomposition of Gaussian Measures

The lemma gives identical decompositions of Brownian motion on each $[i, i+1]$:

$$\mathbb{P}([i, i+1]) = (1 - \alpha^{-10})\mu_{\mathtt{good}_i} + \alpha^{-10}\mu_{\mathtt{bad}_i}.$$

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Then we can represent the full Wiener measure as a product:

$$\mathbb{P}([0, T]) = \sum_{\gamma \in \{\mathtt{good}, \mathtt{bad}\}^T} w(\gamma) \prod_{i=0}^{T-1} \mu_{\gamma_i},$$

$$w(\gamma) = (1 - \alpha^{-10})^{|\gamma^{-1}(\mathtt{good})|} \alpha^{-10|\gamma^{-1}(\mathtt{bad})|}.$$

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Introducing the Polaron interactions gives a modified decomposition:

$$\widehat{\mathbb{P}}_{\alpha,T} = \sum_{\gamma\in\{\mathtt{good},\mathtt{bad}\}^T} \widehat{w}(\gamma)\widehat{\mathsf{P}}_{\gamma}.$$

Using GCI, the new weight $\widehat{w}(\gamma)$ still concentrates on γ with mostly $\mathtt{good}$ components.

From α^2 to α^4, in One Picture

So far, we got $\|B_{i+1} - B_i\|^2 \le \widetilde{O}(\alpha^{-2})$. This gives $m_{\mathrm{eff}}(\alpha) \gtrsim \alpha^2$, but we want α^4.

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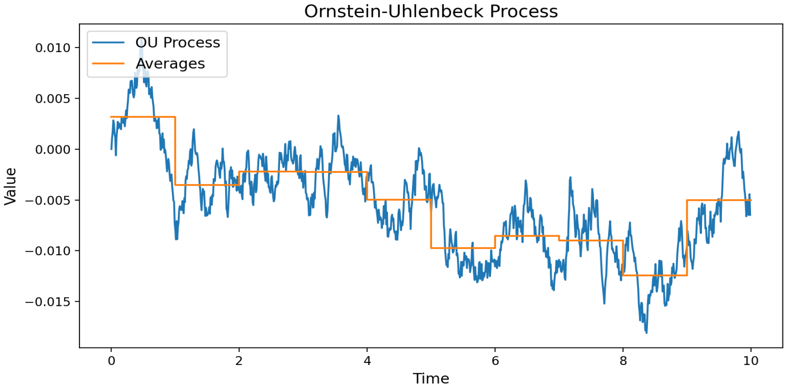
This bound is **optimal** for short-time fluctuations. We must think **long term**.

Heuristically, $\widehat{\mathbb{P}}_{\alpha,T}$ behaves roughly like Ornstein–Uhlenbeck on short time-scales:

$$\mathrm{d}U_t \approx -\alpha U_t + \mathrm{d}B_t.$$



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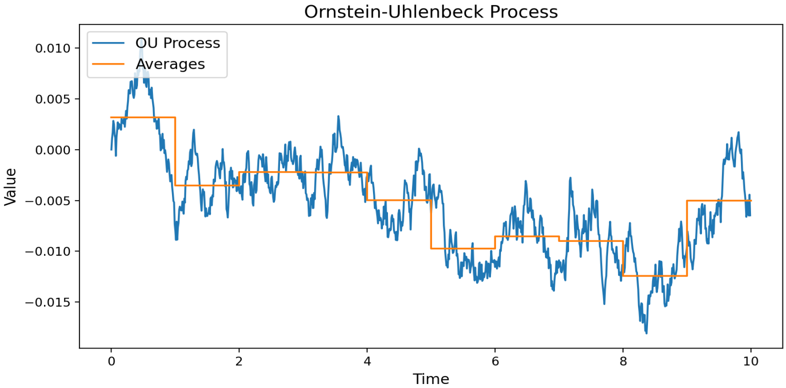

Single-time fluctuations $\|B_{i+1} - B_i\|^2 \asymp \alpha^{-2}$ are dominated by "noise".

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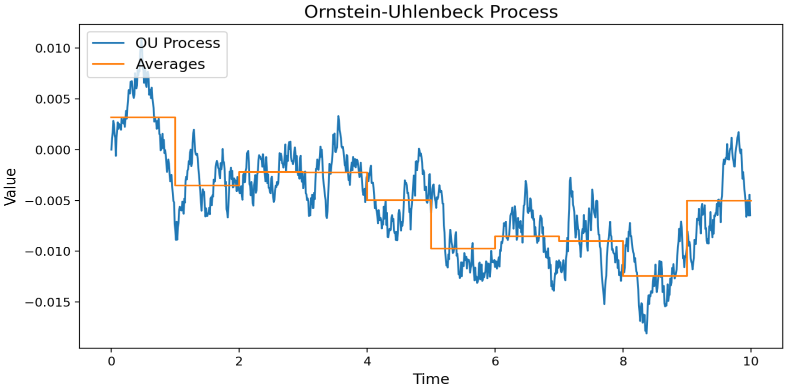

Single-time fluctuations $\|\mathrm{B}_{i+1} - \mathrm{B}_i\|^2 \asymp \alpha^{-2}$ are dominated by "noise".

Interval averages $\overline{B}_{[i,i+1]} = \int_i^{i+1} \mathrm{B}_t \, \mathrm{d}t$ oscillate less: $\|\overline{B}_{[i,i+1]} - \overline{B}_{[i+1,i+2]}\|^2 \asymp \alpha^{-4}$.

- The same holds for $\widehat{\mathbb{P}}_{\alpha,T}$ by another use of GCI.

Conclusion

The *Polaron path measure* $\widehat{\mathbb{P}}_{\alpha,T}$ is a deformation of Brownian motion in $\mathbb{R}^3$:

$$d\widehat{\mathbb{P}}_{\alpha,T}(B) \equiv \frac{1}{Z_{\alpha,T}} \exp\left(\alpha \int_0^T \int_0^T \frac{e^{-|t-s|}}{\|B_t - B_s\|}\, dt\, ds\right) d\mathbb{P}(B).$$

Main result (valid in $\mathbb{R}^d$ for any $d \geq 3$):

$$\lim_{T\to\infty} \mathbb{E}^{\widehat{\mathbb{P}}_{\alpha,T}}\left[\frac{\|B_T\|^2}{T}\right] \leq \frac{(\log\alpha)^6}{c\alpha^4}.$$

Equivalently, a lower bound on the Polaron's effective mass: $m_{\text{eff}}(\alpha) \geq \frac{c\alpha^4}{(\log\alpha)^6}$.

Together with [Brooks-Seiringer 22], this nearly resolves the prediction of [Landau-Pekar 1948] that $m_{\text{eff}}(\alpha) \approx C_* \alpha^4$.

This technique should have applications to other path measures, as we have been discussing with Volker, Steffen and Tobias.