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Statistical Physics with Continuous Symmetries

IV. Quantum Correlation Inequalities

Setting and notation:

- \mathcal{H} a separable \mathbb{C} -Hilbert-space
- $H = H^*$ Hamiltonian, s.t. $\forall \beta > 0$: $e^{-\beta H}$ is trace class
- $A, B, C, \dots \in \mathcal{B}(\mathcal{H})$ operators ("observables")
- The partition function: $Z = Z_\beta := \text{Tr}(e^{-\beta H})$
- Thermal averages: $\langle A \rangle = \langle A \rangle_\beta := Z^{-1} \text{Tr}(e^{-\beta H} A)$
- The Duhamel two-point functions (or, Duhamel correl.)

$$(A, B) = (A, B)_\beta := Z^{-1} \int_0^1 \text{Tr}(e^{-\beta(1-s)H} A^* e^{-\beta s H} B) ds$$

(A, B) is a *scalar product* on $\mathcal{B}(\mathcal{H})$, compatible with the complex structure of $\mathcal{B}(\mathcal{H})$:

$$(A^*, B^*) = (B, A) = \overline{(A, B)}, \quad (A, A) \geq 0$$

The use of moment generating functions: Proposition.

$$\langle A \rangle = \frac{1}{Z} \frac{\partial}{\partial \lambda} \text{Tr}(e^{-\beta H + \lambda A}) \Big|_{\lambda=0}$$

$$(A, B) = \frac{1}{Z} \frac{\partial^2}{\partial \lambda \partial \mu} \text{Tr}(e^{-\beta H + \lambda A^* + \mu B}) \Big|_{\lambda=\mu=0}$$

Proof: Use Lie-Trotter product formula:

$$e^{A+B} = \lim_{n \rightarrow \infty} (e^{A/n} e^{B/n})^n$$

□ HW

And two identities:

$$\begin{aligned}\frac{d}{ds} \text{Tr} \left(e^{-\beta(1-s)H} A^* e^{-\beta s H} B \right) &= \beta \text{Tr} \left(e^{-\beta(1-s)H} [H, A^*] e^{-\beta s H} B \right) \\ &= \beta \text{Tr} \left(e^{-\beta(1-s)H} A^* e^{-\beta s H} [B, H] \right)\end{aligned}$$

$$\frac{d^2}{ds^2} \text{Tr} \left(e^{-\beta(1-s)H} A^* e^{-\beta s H} B \right) = \beta^2 \text{Tr} \left(e^{-\beta(1-s)H} [H, A^*] e^{-\beta s H} [B, H] \right)$$

Proof: Straightforward computation.

□ HW

Bogoliubov's inequality: [N Bogoliubov (1962)]

Let $A \in \mathcal{B}(\mathcal{H})$ be fixed and $k : [0, 1] \rightarrow \mathbb{R}_+$,

$$k(s) := Z^{-1} \text{Tr} \left(e^{-\beta(1-s)H} A^* e^{-\beta s H} A \right)$$

From the *second identity* it follows that $k''(s) \geq 0$ and thus, k is convex. Hence

$$\begin{aligned} \left\langle \frac{AA^* + A^*A}{2} \right\rangle &= \frac{1}{2}(k(0) + k(1)) \\ &\geq \int_0^1 k(s) ds = (A, A) = \sup_{B \neq 0} \frac{|(A, B)|^2}{(B, B)} \\ &\geq \sup_{C : [C, H] \neq 0} \frac{|(A, [C, H])|^2}{([C, H], [C, H])} \end{aligned}$$

From the *first identity*

$$\begin{aligned}
 (A, [C, H]) &= Z^{-1} \int_0^1 \text{Tr} \left(e^{-\beta(1-s)H} A^* e^{-\beta s H} [C, H] \right) \\
 &= Z^{-1} \int_0^1 \frac{1}{\beta} \frac{d}{ds} \text{Tr} \left(e^{-\beta(1-s)H} A^* e^{-\beta s H} C \right) \\
 &= \frac{1}{\beta} \langle [C, A^*] \rangle = \frac{1}{\beta} \langle [A, C^*] \rangle
 \end{aligned}$$

Similarly:

$$([C, H], [C, H]) = \frac{1}{\beta} \langle [C, [C, H]^*] \rangle = \frac{1}{\beta} \langle [[C, H], C^*] \rangle$$

Theorem. [Bogoliubov's inequality] [N Bogoliubov (1962)]

$$\left\langle \frac{AA^* + A^*A}{2} \right\rangle \geq \sup_{C:[C,H]\neq 0} \frac{|\langle [A, C^*] \rangle|^2}{\beta \langle [[C, H], C^*] \rangle} \quad (\text{BOG})$$

Remark: Actually, $s \mapsto k(s)$ is *log-convex* (HW):

$$k''k - (k')^2 \geq 0$$

Hence, the stronger inequality of [G Röpstorff (1976)] follows:

$$\langle A^*A \rangle \geq \langle [A, A^*] \rangle \left(\exp \frac{\beta \langle [C^*, [H, C]] \rangle \langle [A, A^*] \rangle}{|\langle [A, C^*] \rangle|^2} - 1 \right)^{-1}$$

This is very useful in some more complicated cases. However, we'll be content with Bogoliubov's inequality.

Go to the proof of Mermin-Wagner.

Falk-Bruch / Dyson-Lieb-Simon inequality

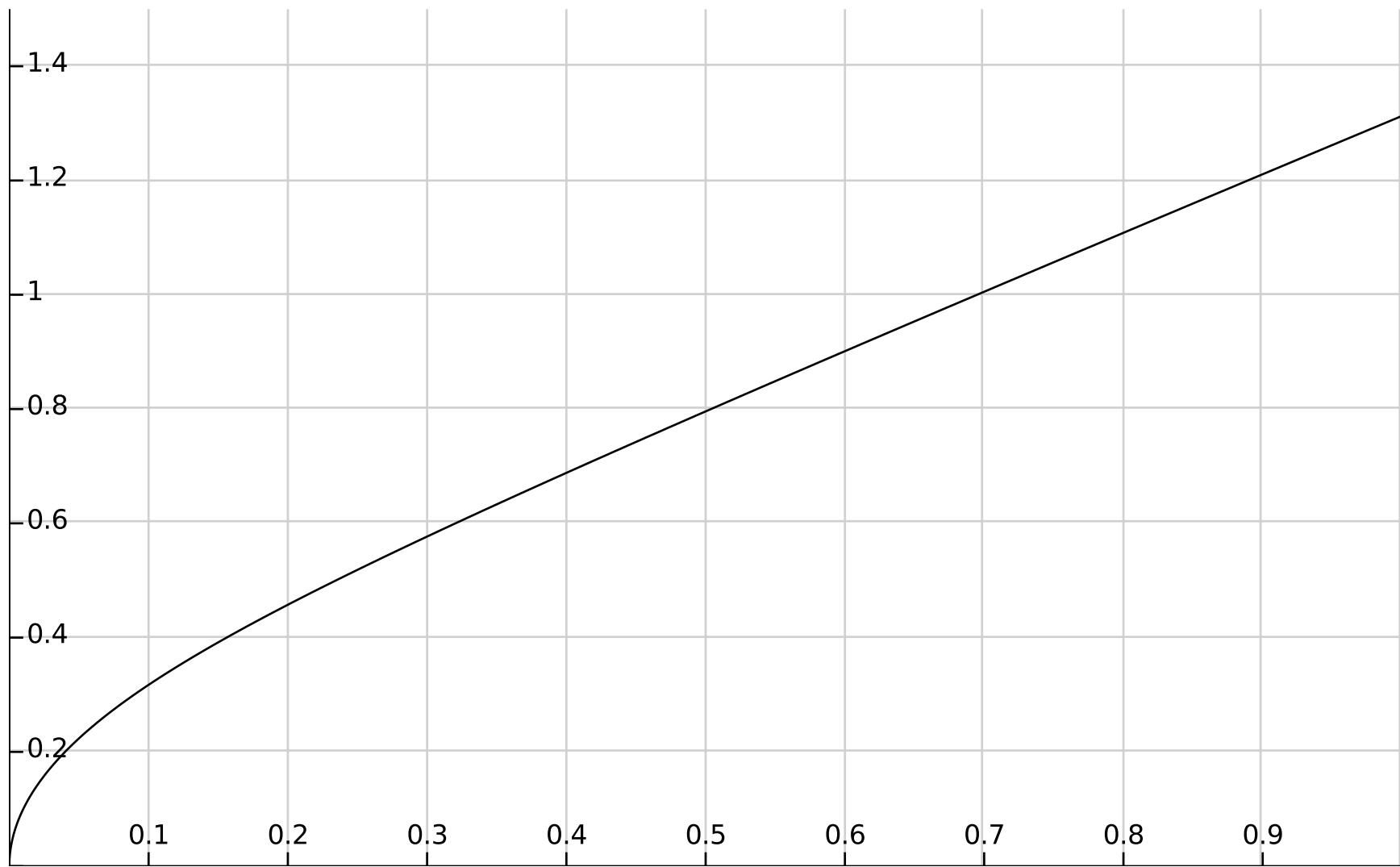
Let $\phi : \mathbb{R}_+ \rightarrow \mathbb{R}_+$,

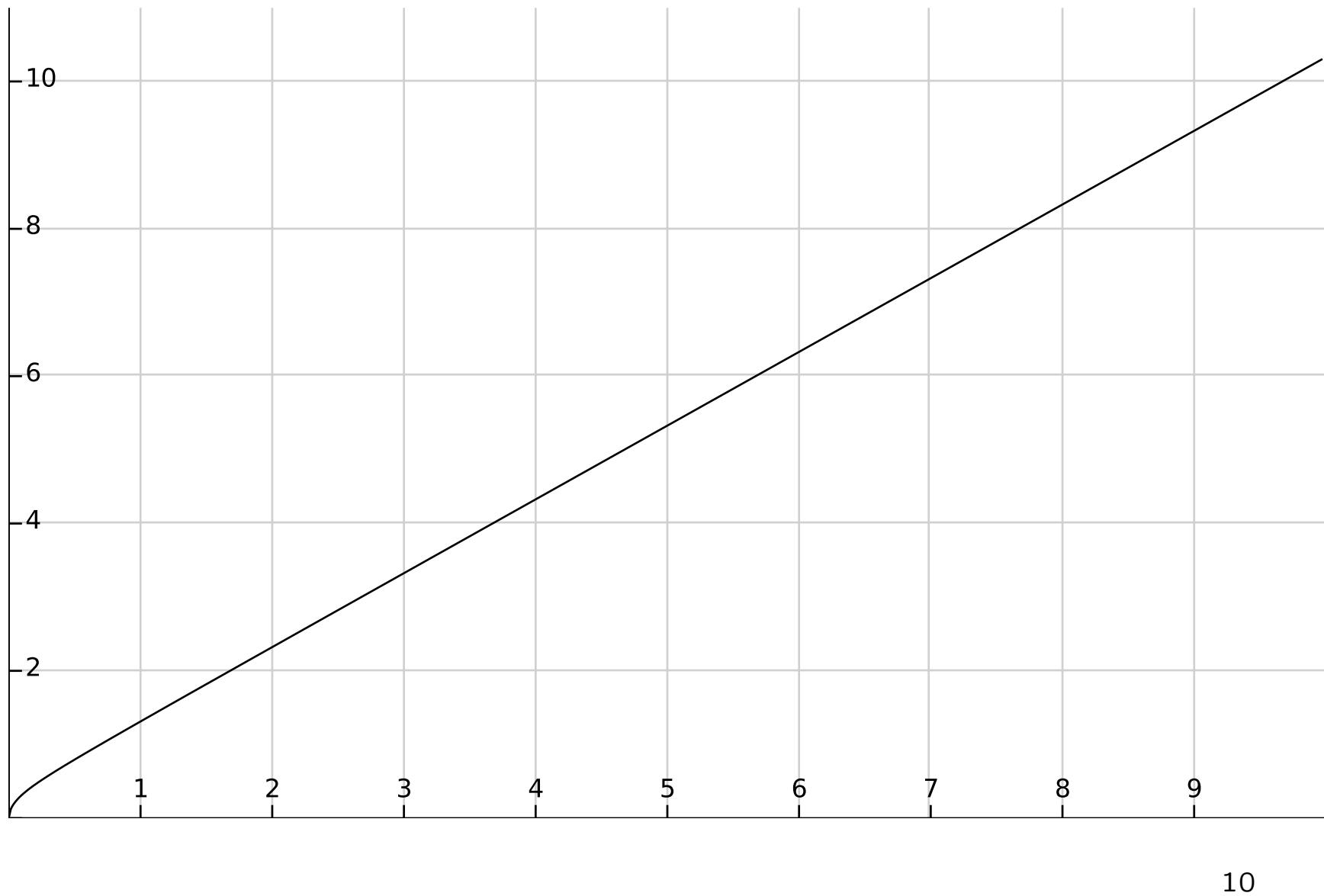
$$\phi(y) = \sqrt{y} \coth \frac{1}{\sqrt{y}}$$

Note (HW):

- Strictly concave: $\phi''(x) < 0$
- Asymptotics as $y \rightarrow 0$: $\phi(y) = \sqrt{y}(1 + \mathcal{O}(e^{-2/\sqrt{y}}))$
- Asymptotics as $y \rightarrow \infty$: $\phi(y) = y + \frac{1}{3} + \mathcal{O}(y^{-1})$

Plots on next pages.





Theorem. [Falk-Bruch inequality] [H Falk, LW Bruch (1969),
 [F Dyson, EH Lieb, B. Simon (1978)]

$$\left\langle \frac{A^*A + AA^*}{2} \right\rangle \leq \frac{\beta \langle [A^*, [H, A]] \rangle}{4} \phi \left(\frac{4(A, A)}{\beta \langle [A^*, [H, A]] \rangle} \right) \quad (\text{FB/DLS})$$

Proof: Recall

$$k(s) = Z^{-1} \text{Tr} \left(e^{-\beta(1-s)H} A^* e^{-\beta s H} A \right)$$

$$\frac{\langle A^*A + AA^* \rangle}{2} = \frac{1}{2}(k(0) + k(1)) \quad =: c$$

$$(A, A) = \int_0^1 k(s) ds \quad =: d$$

$$\beta \langle [A^*, [H, A]] \rangle = k'(1) - k'(0) \quad =: \beta b$$

c for conventional -; *d* for Duhamel -; *b* for Boboliubov correl.;

For simplicity, we assume that the Hamiltonian H has a complete pure point spectrum (this is always the case in finite dimension):

$$H\psi_n = \epsilon_n \psi_n, \quad n \in \mathbb{N}$$

and write

$$(\psi_m, A\psi_n) = A_{m,n}$$

Then

$$k(s) = Z^{-1} \sum_{m,n} |A_{m,n}|^2 e^{-\beta \epsilon_n} e^{\beta(\epsilon_n - \epsilon_m)s} = \int_{\mathbb{R}} e^{st} d\mu(t)$$

where

$$\mu = \sum_{m,n} |A_{m,n}|^2 e^{-\beta \epsilon_n} \delta_{\beta(\epsilon_n - \epsilon_m)}$$

is a positive measure on \mathbb{R} . Thus, $s \mapsto k(s)$ has all the good properties of an *exponential moment generating function*.

Hence,

$$\begin{aligned}
 c &= \frac{1}{2}(k(0) + k(1)) = \int_{\mathbb{R}} \frac{1 + e^t}{2} d\mu(t) \\
 d &= \int_0^1 k(s) ds = \int_{\mathbb{R}} \frac{e^t - 1}{t} d\mu(t) \\
 \beta b &= k'(1) - k'(0) = \int_{\mathbb{R}} t(e^t - 1) d\mu(t)
 \end{aligned}$$

Define the *probability measure* $d\nu$ on \mathbb{R}

$$d\nu(t) := \frac{t(e^t - 1)}{\int_{\mathbb{R}} u(e^u - 1) d\mu(u)} d\mu(t)$$

Note that $t(e^t - 1) = \mathcal{O}(t^2)$ as $t \rightarrow 0$ and thus the integrals below make sense.

Then

$$\frac{4c}{\beta b} = \int_{\mathbb{R}} \frac{2}{t} \coth \frac{t}{2} d\nu(t) \quad \frac{4d}{\beta b} = \int_{\mathbb{R}} \frac{4}{t^2} d\nu(t)$$

and hence

$$\begin{aligned} \phi\left(\frac{4d}{\beta b}\right) &= \phi\left(\int_R \frac{4}{t^2} d\nu(t)\right) \\ &\stackrel{\text{Jensen}}{\geq} \int_R \phi\left(\frac{4}{t^2}\right) d\nu(t) = \int_R \frac{2}{t} \coth \frac{t}{2} d\nu(t) \\ &= \frac{4c}{\beta b} \end{aligned}$$

□ Falk-Bruch

Remark: The inequality is sharp. Saturated by the harmonic oscillator: $[A, A^*] = I$, $H = A^*A$.

Go to the proof of Dyson-Lieb-Simon.