Berezin-Lieb Inequalities and Quantum Stat.-Mech.

Based on joint work with Marek Biskup and Lincoln Chayes

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Abstract:

Berezin and Lieb independently discovered a pair of inequalities that relate traces of quantum observables to expectations of classical random variables.

This is very useful in understanding the behavior of quantum systems on the basis of our understanding of their classical counterparts.

Recently with Lincoln Chayes and Marek Biskup, we obtained related inequalities which are useful in the study of phase transitions.

I will describe this, starting with the original Berezin-Lieb inequalities.

Some general observations

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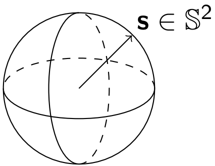

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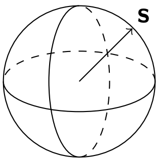

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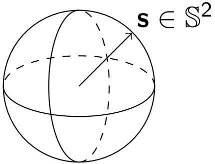

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with an irreducible representation of $\mathrm{SU}(2)$

(which is a double-covering of $\mathrm{SO}(3)$).

Probability measures

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Riesz-Markov theorem : $\mathbf{M}_1(\mathbb{S}^2) \cong$ *states* on $\mathscr{C}(\mathbb{S}^2)$

$$\mathrm{f} \in \mathscr{C}(\mathbb{S}^2) \mapsto \mathsf{E}^{\mu}[\mathrm{f}] = \int_{\mathbb{S}^2} \mu(d\mathbf{s})\, \mathrm{f}(\mathbf{s})\,.$$

- linear functional;
- $\mathsf{E}^{\mu}[\mathrm{f}] \geq 0$ for $\mathrm{f} \geq 0$;
- $\mathsf{E}^{\mu}[1] = 1$.

Noncommutative probability measures

$\mathcal{H}^{(j)} \cong \mathbb{C}^{2j+1}$

$\mathcal{A}^{(j)} = \mathcal{B}(\mathcal{H}^{(j)}) =$ all (bounded) linear operators on $\mathcal{H}^{(j)}$:

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$$F(\beta) = -\frac{1}{\beta} \ln\left(Z(\beta)\right).$$

Expectations = derivatives

Boltzmann Gibbs measure $\mu_\beta \in \mathbf{M}_1(\mathbb{S}^2)$,

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Consider 1-parameter family $\mathrm{H}(\mathbf{s};h) = \mathrm{H}(\mathbf{s}) + h\,\mathrm{f}(\mathbf{s})$.

$$\frac{\partial}{\partial h} F(\beta;h)\Big|_{h=0} \;=\; -\frac{1}{\beta}\frac{\partial}{\partial h}\ln\left(\int_{\mathbb{S}^2} d\mathbf{s}\, e^{-\beta \mathrm{H}(\mathbf{s}) - \beta h \mathrm{f}(\mathbf{s})}\right)\Bigg|_{h=0}$$

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$$= \langle \mathrm{f}\rangle_\beta\,.$$

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Analyze whether $\lim_{j\to\infty} F^{(j)}(\beta) = F^{(\infty)}(\beta)$.

Recovering $\mathbb{S}^2$ in classical case

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- I.i.d. random variables = product measure ⇒ product states
- Average of random variables : is in the symmetric subalgebra.

States and density matrices

$$\mathcal{H}^{(j)} \cong \mathbb{C}^{2j+1}, \quad \mathcal{A}^{(j)} = \mathcal{B}(\mathcal{H}^{(j)}) \cong M_{2j+1}(\mathbb{C})$$

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Pure states : $\rho =$ rank-1 projectors

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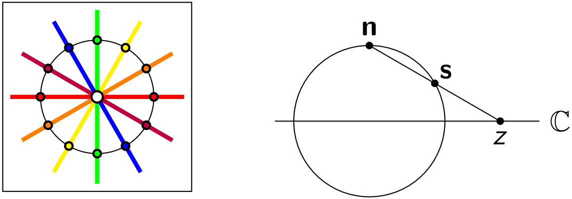

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Explicit calculations for $j = 1/2$

For $\mathbf{s} \in \mathbb{S}^2$, define the projector:

$$\Pi^{(1/2)}(\mathbf{s}) = 1/2(\mathbb{1} + \mathbf{s} \cdot \boldsymbol{\sigma}) = \frac{1}{2} \begin{bmatrix} 1 + s^3 & s^1 - is^2 \\ s^1 + is^2 & 1 - s^3 \end{bmatrix},$$

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Given $x \in \mathrm{SU}(2)$, let $O(x) \in \mathrm{SO}(3)$ be its projection:

$$x\Pi(\mathbf{s})x^* \;=\; \Pi(O(x)\cdot\mathbf{s}).$$

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$$\Pi^{(j)}(\mathbf{s}) := \bigotimes_{i=1}^{2j} \Pi_i^{(1/2)}(\mathbf{s}) .$$

More explicit calculations

$$\mathrm{Tr}\left[\Pi^{(1/2)}(\mathbf{s}_1)\Pi^{(1/2)}(\mathbf{s}_2)\right] = 1-1/4\|\mathbf{s}_1-\mathbf{s}_2\|^2 \quad \text{and} \quad \Pi^{(j)}(\mathbf{s}) := \bigotimes_{i=1}^{2j} \Pi_i^{(1/2)}(\mathbf{s})\,.$$

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Leibniz's law

$$\Rightarrow \qquad \mathbf{S}^{(j)} = \sum_{i=1}^{2j} \mathbb{1}_1 \otimes \cdots \otimes \mathbb{1}_{i-1} \otimes \mathbf{S}_i^{(1/2)} \otimes \mathbb{1}_{i+1} \otimes \cdots \otimes \mathbb{1}_{2j}\,,$$

POV-measure

$$U^{(j)}(x)\Pi^{(j)}(\mathbf{s})U^{(j)}(x)^* = \Pi^{(j)}(O(x)\cdot\mathbf{s})$$

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Define map: $\mathrm{A} \in \mathcal{A}^{(j)} \mapsto \check{\mathrm{A}} \in \mathscr{C}(\mathbb{S}^2)$,

$$\check{\mathrm{A}}(\mathbf{s}) \,=\, \mathrm{Tr}[\mathrm{A}\,\Pi^{(j)}(\mathbf{s})]\,.$$

Surjectivity, not injectivity

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Duffield's Theorem

Suppose $n \in \{1, 2, \dots\}$ and $a_1, \dots, a_n \in \{1, 2, 3\}$.
Then

$$\lim_{j \to \infty} \left[(2j)^{-n} S^{(j),a_1} S^{(j),a_2} \cdots S^{(j),a_n} \right]^{\vee}(\mathbf{s}) = s^{a_1} s^{a_2} \cdots s^{a_n} \, ,$$

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Also, there exist functions $\mathrm{f}^{(j)}$ for $j \in \{0, 1/2, 1, 3/2, 2, \dots\}$ s.t.,

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$$\lim_{j \to \infty} \mathrm{f}^{(j)}(\mathbf{s}) = s^{a_1} s^{a_2} \cdots s^{a_n} \, ,$$

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Digression : weak law of large numbers

Given $\mu \in \mathbf{M}_1(\mathbb{S}^2)$, for each $j \in \{0, 1/2, 1, 3/2, 2, \dots\}$

define quantum state $\omega_\mu^{(j)}$ on $\mathcal{A}^{(j)}$

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Only uses first part of Duffield's theorem.

The Berezin-Lieb inequalities

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Proof: Combine Jensen's inequality with the spectral decomposition of $\hat{\mathrm{f}}^{(j)} \in \mathcal{A}^{(j)}$.

Convergence of free energies

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for Hamiltonians of the form

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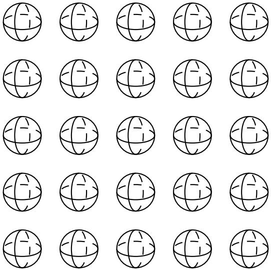
The classical limit for the free energy density:



$\Lambda \subset \mathbb{Z}^d$, finite
Quantum spin at each site $x \in \Lambda$.
Use coherent states on each spin.
The Berezin-Lieb inequalities $\Rightarrow$
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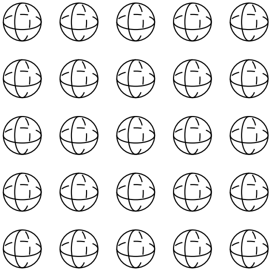

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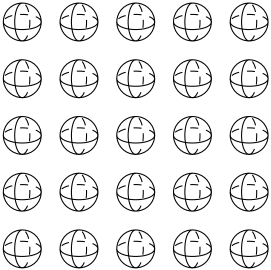

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Q: Does a classical phase transition imply a quantum phase transition?

The classical limit for the free energy density:

By general principles (Gibbs variational principle, subadditivity)

$$f^{(j)}(\beta) = \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|} F_\Lambda^{(j)}(\beta)$$

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E.g.,

$$f^{(j)}(\beta) = \frac{1}{j} \ln\big(\cosh(\beta j h)\big) \longrightarrow |\beta h|\,.$$

Matrix entry bounds

$$\exp\left(\left[\hat{\mathrm{f}}^{(j)}\right]^{\vee}(\mathbf{s})\right) \leq \left[\exp\left(\hat{\mathrm{f}}^{(j)}\right)\right]^{\vee}(\mathbf{s}) \leq \exp\left(\mathrm{f}(\mathbf{s}) + O\left(\beta|\Lambda|/\sqrt{j}\right)\right)$$

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ψ-Theorem:
For quantum spin systems which are "reflection-positive", for which a phase-transition occurs in the classical limit, via a Chessboard-estimate-Peierls-type argument, the quantum spin system has a similar phase transition when $j = O(\beta^2)$.