Quantum Spin Systems at Positive Temperature

joint work with Marek Biskup and Lincoln Chayes

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If *one can prove that* a classical spin system has a phase transition, then can one deduce the same for the quantum model *for large enough values of spin*?

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Ours is not the first result of this kind . . . notably, see Frohlich and Lieb (1978).

Part I: Quantum Spin Systems and Coherent States

Brief review of quantum spins

The single-site Hilbert space for a quantum spin is $\mathcal{H}^{(s)} \cong \mathbb{C}^{2s+1} = \text{Span}\{|m\rangle \; : \; m = s, s-1, \dots, -s\}$: $s \in \{\frac{1}{2}, 1, \frac{3}{2}, 2, \dots\}$ is the "spin".

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Spin matrices:

$$S^z|m\rangle\ =\ m|m\rangle\,, \quad S^{\pm}|m\rangle\ =\ \sqrt{s(s+1) - m(m\pm 1)}\,|m\pm 1\rangle\,,$$
$$S^x\ =\ \frac{1}{2}(S^+ + S^-)\,, \quad S^y = \frac{1}{2i}(S^+ - S^-)\,.$$

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This forms a representation of $\mathfrak{su}(2) = \mathrm{Lie}(\mathrm{SU}(2))$.

Coherent State Vectors

Let $\mathbb{S}^2$ denote the sphere.
The coherent state vector in direction $\omega \in \mathbb{S}^2$ is

$$|\omega\rangle \;=\; \sum_{m=-s}^{s} \sqrt{\binom{2s}{s+m}}\,[\cos(\theta/2)]^{s+m}\,[\sin(\theta/2)]^{s-m}\,e^{i(s-m)\phi}\,|m\rangle\,,$$

where $\theta \in [0, \pi]$ is azimuthal angle, $\phi \in [0, 2\pi)$ is polar angle.

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Given $\mathbf{r} \in \mathbb{R}^3$,

$$e^{i\mathbf{r}\cdot\mathbf{S}} P_\omega e^{-i\mathbf{r}\cdot\mathbf{S}} = P_{\omega'} , \text{ where } \omega' = e^{\mathbf{r}\cdot\mathbf{L}}\omega ,$$

$$L^x = \begin{bmatrix} 0 & & \\ & 0 & -1 \\ & 1 & 0 \end{bmatrix} , \ L^y = \begin{bmatrix} 0 & & 1 \\ & 0 & \\ -1 & & 0 \end{bmatrix} , \ L^z = \begin{bmatrix} 0 & -1 & \\ 1 & 0 & \\ & & 0 \end{bmatrix}$$

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A specific example Hamiltonian: the Heisenberg ferromagnet,

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- $\mathbf{S}_\alpha$, $\mathbf{S}_{\alpha'}$: spin "vector-matrix": $\mathbf{S}_\alpha = (S_\alpha^x, S_\alpha^y, S_\alpha^z)$.
- S_α^x, S_α^y, S_α^z: the spin matrices on $\mathcal{H}_\alpha^{(s)}$, tensored with $\mathbb{1}$.
- We scale each spin matrix by s^{-1} to facilitate classical limit.

Part II: Berezin-Lieb Inequalities and Matrix-Entry Bounds

First Berezin-Lieb Inequality

Given $\boldsymbol{\omega} = (\omega_\alpha : \alpha \in \mathbb{Z}_L^d) \in (\mathbb{S}^2)^{\mathbb{Z}_L^d} =: \Omega_L$, define

$$|\boldsymbol{\omega}\rangle = \bigotimes_{\alpha \in \mathbb{Z}_L^d} [|\omega_\alpha\rangle]_\alpha \quad \text{and} \quad P_{\boldsymbol{\omega}} = |\boldsymbol{\omega}\rangle\langle\boldsymbol{\omega}|\,.$$

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$$\langle A \rangle_{\boldsymbol{\omega}} = \mathrm{Tr}(P_{\boldsymbol{\omega}} A) = \langle \boldsymbol{\omega} | A | \boldsymbol{\omega} \rangle \, .$$

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Lieb proved the lower bound on the partition function,

$$\frac{\mathrm{Tr}[\exp(-\beta H_L^{(s)})]}{\dim(\mathcal{H}_L^{(s)})} \geq \int_{\Omega_L} \exp\left(-\beta\langle H_L^{(s)}\rangle_{\boldsymbol{\omega}}\right) \frac{d\boldsymbol{\omega}}{|\Omega_L|}\,.$$

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The proof uses the "resolution of the identity":

$$\mathbb{1}_{\mathcal{H}_L^{(s)}} = \frac{\dim(\mathcal{H}_L^{(s)})}{|\Omega_L|} \int_{\Omega_L} d\boldsymbol{\omega}\, P_{\boldsymbol{\omega}}\,.$$

Second Berezin-Lieb Inequality

Given operator A on $\mathcal{H}_L^{(s)}$, a (nice) function $\omega \mapsto [A]_\omega$ is called an "upper symbol" if

$$A = \frac{\dim(\mathcal{H}_L^{(s)})}{\Omega_L} \int_{\Omega_L} d\omega\, [A]_\omega\, P_\omega\,.$$

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Classical Limit of Pressure

Easy to see

$$\lim_{s\to\infty}\langle H_L^{(s)}\rangle_{\omega} = H_L^{(\infty)}(\omega) = -\sum_{\langle\alpha,\alpha'\rangle\subset\mathbb{Z}_L^d}\omega_\alpha\cdot\omega_{\alpha'}\,.$$

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Thus Lieb proved the classical limit for the thermodynamic pressure

$$\lim_{s\to\infty} \lim_{L\to\infty} \frac{1}{L^d} \ln \frac{\mathrm{Tr}[e^{-\beta H_L^{(s)}}]}{\dim(\mathcal{H}_L^{(s)})} = \lim_{L\to\infty} \frac{1}{L^d} \ln \int_{\Omega_L} e^{-\beta H_L^{(\infty)}(\omega)} \frac{d\omega}{|\Omega_L|} .$$

This result holds for any reasonable QSS Hamiltonian.

Bounds for "Matrix Entries"

Theorem 1. *Given a constant $c > 0$, there exists a constant $C < \infty$ such that*

$$e^{-\beta\langle H_L^{(s)}\rangle_\omega} \leq \langle e^{-\beta H_L^{(s)}}\rangle_{\boldsymbol{\omega}} \leq e^{-\beta[H_L^{(s)}]+\beta C L^d/s},$$

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For any operator A on $\mathcal{H}_L^{(s)}$,

$$\mathrm{Tr}[Ae^{-\beta H_L^{(s)}}] = \frac{\dim(\mathcal{H}_L^{(s)})}{|\Omega_L|}\int_{\Omega_L}[A]_\omega\langle e^{-\beta H_L^{(s)}}\rangle_\omega\, d\omega\,.$$

Bounds on Gibbs States Expectations

Gibbs state, at inverse-temperature β:

$$\langle A \rangle_{\beta,L}^{(s)} = \frac{\mathrm{Tr}[A e^{-\beta H_L^{(s)}}]}{\mathrm{Tr}[e^{-\beta H_L^{(s)}}]}\,.$$

By Theorem 1,

$$\langle A \rangle_{\beta,L}^{(s)} \le e^{\beta C L^d / s} \frac{\int_{\Omega_L} [A]_\omega e^{-\beta [H_L^{(s)}]_\omega}\, d\omega}{\int_{\Omega_L} e^{-\beta \langle H_L^{(s)} \rangle_\omega}\, d\omega}\,.$$

Comparison to Classical Limit

For each measurable $E \subset \Omega_L$, can define

$$\hat{\chi}_E^{(s)} = \frac{\dim(\mathcal{H}_L^{(s)})}{|\Omega_L|} \int_E d\omega \, P_\omega \, .$$

Can use this to define measure $\mu_{\beta,L}^{(s)}$ on Ω_L, $\mu_{\beta,L}^{(s)}(E) = \langle \hat{\chi}^{(s)} \rangle_{\beta,L}^{(s)}$. Have

$$\mu_{\beta,L}^{(s)}(E) \leq e^{\beta C L^d / s} \frac{\int_E e^{-\beta [H_L^{(s)}]_\omega} \, d\omega}{\int_{\Omega_L} e^{-\beta \langle H_L^{(s)} \rangle_\omega} \, d\omega} \, .$$

Compare to the Gibbs measure for the classical Hamiltonian

$$\mu_{\beta,L}^{(\infty)}(E) = \frac{\int_E e^{-\beta H_L^{(\infty)}(\omega)} \, d\omega}{\int_{\Omega_L} e^{-\beta H_L^{(\infty)}(\omega)} \, d\omega} \, .$$

Part III: Reflection Positivity and Chessboard Estimates

Basic Definitions

Suppose L is even.
Let $\Lambda_L = \mathbb{Z}_L^d$, suppose $\exists \Lambda_L^+, \Lambda_L^- \subset \Lambda_L$ with $\Lambda_L = \Lambda_L^+ \sqcup \Lambda_L^-$, and suppose $\exists$ bijection $\theta : \Lambda_L^+ \xrightarrow{\cong} \Lambda_L^-$.

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There are natural choices of Λ_L^+, Λ_L^-, θ: "pairs-of-planes".

A quantum Hamiltonian is reflection positive if $(\cdot, \cdot)_\phi$ is positive semidefinite for every pair-of-planes when $\phi(\cdot) = \langle \cdot \rangle_{\beta,L}^{(s)}$.

(1) The anisotropic Heisenberg antiferromagnet:

$$H = + \sum_{\langle \alpha, \alpha' \rangle} s^{-2} (J_1 S^x_\alpha S^x_{\alpha'} + J_2 S^y_\alpha S^y_{\alpha'} + S^z_\alpha S^z_{\alpha'}) \tag{1}$$

where $0 \leq J_1, J_2 < 1$.

(2) The non-linear XY-model:

$$H = - \sum_{\langle \alpha, \alpha' \rangle} \mathscr{P}\Big(s^{-2} (S^x_\alpha S^x_{\alpha'} + S^y_\alpha S^y_{\alpha'}) \Big) \tag{2}$$

where $\mathscr{P}(x) = \mathscr{P}_1(x^2) \pm x \mathscr{P}_2(x^2)$ for two polynomials $\mathscr{P}_1, \mathscr{P}_2$ (of sufficiently high degree) with positive coefficients.

(3) The orbital compass model on $\mathbb{Z}^2$:

$$H = \sum_{\langle \alpha, \alpha' \rangle} \begin{cases} s^{-2}\, S^x_\alpha S^x_{\alpha'}, & \text{if } \alpha' = \alpha \pm \hat{e}_x, \\ s^{-2}\, S^y_\alpha S^y_{\alpha'}, & \text{if } \alpha' = \alpha \pm \hat{e}_y. \end{cases} \tag{3}$$

Chessboard Estimates

Let ℓ be an integer such that 2ℓ divides L.
Then tile $\Lambda_L = \mathbb{Z}_L^d$ by copies of $[1, \ell]^d$.
Label the tiles by $\mathbf{t} \in \mathbb{Z}_{L/\ell}^d$: shifted by $\ell\mathbf{t}$.

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Let $\mathfrak{A}_\ell^{(s)}$ be the operators localized in a given fixed tile, and given any other tile $\mathbf{t}$, let $\tau_{\mathbf{t}}^{(s)} : \mathfrak{A}_\ell^{(s)} \to \mathfrak{A}^{(s)}$ be the isomorphism that
(i) moves along a "path of reflections" in edges of tiles, and
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(i) moves along a "path of reflections" in edges of tiles, and
(ii) complex-conjugates if the path has odd length.

Let $\Delta : \mathfrak{A}_\ell^{(s)} \to \mathfrak{A}^{(s)}$ be the product

$$\Delta(A) = \prod_{\mathbf{t} \in \mathbb{Z}_{L/\ell}^d} \tau_{\mathbf{t}}^{(s)}(A) \,.$$

Theorem. (Abstract Chessboard Estimate) *If the Hamiltonian is r.p., then for any collection of operators* $\left(A_{\mathbf{t}} \in \mathfrak{A}_{\ell}^{(s)} \,:\, \mathbf{t} \in \mathbb{Z}_{L/\ell}^{d}\right)$,

$$\left|\left\langle \prod_{\mathbf{t}\in\mathbb{Z}_{L/\ell}^{d}} \tau_{\mathbf{t}}^{(s)}(A_{\mathbf{t}}) \right\rangle_{\beta,L}^{(s)}\right| \leq \prod_{\mathbf{t}\in\mathbb{Z}_{L/\ell}^{d}} \left(\left\langle \Delta(A_{\mathbf{t}}) \right\rangle_{\beta,L}^{(s)}\right)^{\frac{1}{L^d}} .$$

Given an event $E \subset \Omega_\ell^{(s)} = (\mathbb{S}^2)^{[1,\ell]^d}$, and $\mathbf{t} \in \mathbb{Z}^d_{L/\ell}$, let $\hat{\tau}_{\mathbf{t}}(E)$ be the cylinder event in $\Omega_L^{(s)}$ such that

$$\tau_{\mathbf{t}}^{(s)}\big(\hat{\chi}_E^{(s)}\big) \,=\, \hat{\chi}^{(s)}_{\hat{\tau}_{\mathbf{t}}(E)}\,.$$

Let

$$\hat{\Delta}(E) \,=\, \bigcap_{\mathbf{t}\in\mathbb{Z}^n_{L/\ell}} \hat{\tau}_{\mathbf{t}}(E)\,.$$

Corollary. *For any* $\mathbf{t}_1, \dots, \mathbf{t}_n$ *disjoint, and* $E_1, \dots, E_n \subset \Omega_\ell$,

$$\mu^{(s)}_{\beta,L}\Big(\bigcap_{k=1}^n \hat{\tau}_{\mathbf{t}_k}(E_k)\Big) \leq\, e^{-\beta n C/s} \prod_{k=1}^n \left[\frac{\int_{\Delta(E_k)} e^{-\beta[H_L^{(s)}]_\omega}\, d\omega}{\int_{\Omega_L} e^{-\beta\langle H_L^{(s)}\rangle_\omega}\, d\omega}\right]^{1/L^d} .$$