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QUANTUM SPIN SYSTEMS AT POSITIVE TEMPERATURE

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ABSTRACT. We develop a novel approach to phase transitions in quantum spin models based on a relation to the corresponding classical spin systems. Explicitly, we show that whenever chessboard estimates can be used to prove a phase transition in the classical model, the corresponding quantum model will have a similar phase transition, provided the inverse temperature β and the magnitude of the quantum spins $\mathcal{S}$ satisfy $\beta \ll \sqrt{\mathcal{S}}$. From the quantum system we require that it is reflection positive and that it has a meaningful classical limit; the core technical estimate may be described as an extension of the Berezin-Lieb inequalities down to the level of matrix elements. The general theory is further applied to prove phase transitions in various quantum spin systems with $\mathcal{S} \gg 1$. The most notable examples are the quantum orbital-compass model on $\mathbb{Z}^2$ and the quantum 120-degree model on $\mathbb{Z}^3$ which are shown to exhibit symmetry breaking at low-temperatures despite the infinite degeneracy of their (classical) ground state.

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(S. S. is presenting the poster, and is now at the University of Rochester.)

1. Introduction

Two views on quantum mechanics and classical mechanics:

(1) If you start with classical mechanics, then you may be able to quantize to obtain quantum deformations. The choice of how to quantize sometimes involves choices.
(2) If you start with quantum mechanics, then you may be able to take the classical limit. E.g., by sending Planck's constant to 0.

We take the second perspective. The reciprocal of the spin plays the role of Planck's constant, so $s \to \infty$ is the classical limit.

Question: What does the classical limit tell us about quantum spin systems?

This is a natural question because it is often easier to understand the classical limit than the quantum spin system, itself. Just one example is provided by the Heisenberg ferromagnet. The classical model has a proven phase transition in $d \geq 3$ [25], but the method of proof, while applicable to the quantum antiferromagnet [19], is inapplicable to the quantum ferromagnet [44]. (For more on this example, see the open problem "LONG RANGE ORDER FOR THE QUANTUM HEISENBERG MODEL" on the IAMP webpage.)

Let us specialize our previous question:

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

This question is still too general, so the answer is, almost certainly, "no." But by specifying particular families of models, the answer may become, "yes," and it may provide a method for proving phase transitions in quantum models.

MAIN RESULT, IN WORDS

We consider quantum spin systems such that:

(i) they are reflection positive;
(ii) their classical limits can be proved to have phase transitions, using generalized chessboard estimates to facilitate a Peierls-type argument;
(iii) the spin dimension s is large enough, specifically $s^{-2} = O(T)$.

For such systems we can prove a phase transition, specifically, phase coexistence.

Our result follows in the tradition of Frohlich and Lieb's proof of a phase transition for the anisotropic Heisenberg antiferromagnet [24]. But our proof is different, in that we use coherent states.

2. Coherent States

The Hilbert space for a single spin $\mathcal{H} \cong \mathbb{C}^{2s+1}$ has standard basis $\{|m\rangle : m = s, s-1, \dots, -s\}$ where $S^z|m\rangle = m|m\rangle$ and

$$S^{\pm}|m\rangle = \sqrt{s(s+1) - m(m \pm 1)}\, |m \pm 1\rangle .$$

There is a more symmetric family of vectors called coherent state vectors. For each point on the sphere $\omega \in \mathbb{S}^2$, the c.s. vector in direction $\omega = (\theta, \phi)$ is

$$|\omega\rangle = \sum_{m=-s}^{s} \left[\binom{2s}{s+m} \right]^{1/2} \cos^{s+m}(\theta/2) \sin^{s-m}(\theta/2) e^{i(s-m)\phi}\, |m\rangle .$$

Of course this basis is highly dependent. One can easily estimate inner-product between two c.s. vectors satisfies $|\langle\omega|\omega'\rangle|^2 \leq e^{-s\|\omega-\omega'\|^2/2}$.

It is even better to look at the coherent state projectors

$$P_\omega^{(s)} := |\omega\rangle\langle\omega| .$$

(We explicitly incluce s, which is helpful later.) For one thing, $P_\omega^{(s)}$ is the projector onto the eigenspace of the operator

$$\omega \cdot \boldsymbol{S} = \omega_x S^x + \omega_y S^y + \omega_z S^z ,$$

corresponding to the eigenvalue s, which is the maximum possible. In this sense, the c.s. vectors are the "closest to classical". Also,

$$e^{i\boldsymbol{r}\cdot\boldsymbol{S}}(\omega \cdot \boldsymbol{S})e^{-i\boldsymbol{r}\cdot\boldsymbol{S}} = \left(e^{\boldsymbol{r}\cdot\boldsymbol{L}}\omega\right) \cdot \boldsymbol{S} ,$$

where L^x, L^y and L^z are the generators for rotations about the three axes. Therefore, the family $\{P_\omega^{(s)} : \omega \in \mathbb{S}^2\}$ forms an orbit of the conjugation representation of $\mathrm{SU}(2)$.

One of the most important properties of coherent projections is the "resolution of the identity"

$$\mathbb{1} = \frac{\dim(\mathcal{H})}{|\mathbb{S}^2|} \int_{\mathbb{S}^2} d\omega\, P_\omega^{(s)} .$$

Lieb used these coherent states to prove that one could commute the thermodynamic and classical limit when calculating pressure for a quantum spin system.

3. Berezin-Lieb Inequalities

Consider a sequences of "lattices": $\Lambda_N = [1,N]^d$ with periodic boundary conditions. Consider a Hamiltonian such as

$$H_N^{(s)} = \sum_{<\alpha,\alpha'>\in\Lambda_N} h_{\alpha,\alpha'}(s^{-1}\boldsymbol{S}_\alpha, s^{-1}\boldsymbol{S}_{\alpha'})\,.$$

Here, the restriction $<\alpha,\alpha'>$ means that the pair of sites are nearest-neighbors, but any finite range interaction is also okay. It is assumed that $h_{\alpha,\alpha'}(\boldsymbol{S}_\alpha, \boldsymbol{S}_{\alpha'})$ is a (possibly noncommutative) polynomial in the spin variables for reasons we mention below. Let us also assume it is periodic with respect to the shifts $(\alpha,\alpha') \mapsto (\alpha+e_i, \alpha'+e_i)$, for $i=1,\dots,d$.

The Hamiltonian acts on the tensor product Hilbert space $\mathcal{H}_N \cong \bigotimes_{\alpha\in\Lambda_N}[\mathbb{C}^{2s+1}]_\alpha$. The spin matrix-vector is $\boldsymbol{S}_\alpha = (S_\alpha^x, S_\alpha^y, S_\alpha^z)$. It acts at site α, and is tensored with $\mathbb{1}$, elsewhere.

One uses the spin matrices, rescaled by s^{-1}, so that the $s\to\infty$ limit of the Hamiltonian will exist. The classical configuration space is $\Omega_N = [\mathbb{S}^2]^{\Lambda_N}$. Given $\boldsymbol{\omega} = (\omega_\alpha)_{\alpha\in\Lambda_N}$,

$$H_N^{(\infty)}(\boldsymbol{\omega}) = \sum_{<\alpha,\alpha'>\in\Lambda_N} h_{\alpha,\alpha'}(\omega_\alpha, \omega_{\alpha'})\,.$$

In [34], Lieb proved

$$\lim_{s\to\infty}\lim_{N\to\infty}\frac{1}{|\Lambda_N|}\ln\left(\frac{\mathrm{Tr}\ e^{-\beta H_N^{(s)}}}{\dim(\mathcal{H}_N^{(s)})}\right) = \lim_{N\to\infty}\frac{1}{|\Lambda_N|}\ln\int_{\Omega_N} e^{-\beta H_N^{(\infty)}(\boldsymbol{\omega})}\,\frac{d\boldsymbol{\omega}}{|\Omega_N|}\,.$$

Let $Z_{\beta,N}^{(s)} = \mathrm{Tr}[e^{-\beta H_N^{(s)}}]$ and $Z_{\beta,N}^{(\infty)} = \int_{\Omega_N} e^{-\beta H_N^{(\infty)}(\boldsymbol{\omega})}\,d\boldsymbol{\omega}$ be the quantum and classical partition functions.

Given $\boldsymbol{\omega}\in\Omega_N$, and an operator A on $\mathcal{H}_N^{(s)}$, one defines the "lower symbol"

$$\langle A\rangle_{\boldsymbol{\omega}} = \mathrm{Tr}\left(A\bigotimes_{\alpha\in\Lambda_N}[P_{\omega_\alpha}^{(s)}]_\alpha\right)\,.$$

Any real or complex function $\boldsymbol{\omega}\in\Omega_N\mapsto[A]_{\boldsymbol{\omega}}$ is called an "upper symbol" for A if

$$A = \frac{\dim(\mathcal{H}_N^{(s)})}{|\Omega_N|}\int_{\Omega_N} d\boldsymbol{\omega}\,[A]_{\boldsymbol{\omega}}\bigotimes_{\alpha\in\Lambda_N}[P_{\omega_\alpha}^{(s)}]_\alpha\,.$$

There are always infinitely many such functions for each operator A. The upper and lower symbols are named because they allow upper and lower bounds on the quantum partition function:

$$e^{-\beta\langle H_N^{(s)}\rangle_{\boldsymbol{\omega}}}\,\frac{d\boldsymbol{\omega}}{|\Omega_N|} \le \frac{\mathrm{Tr}\ e^{-\beta H_N^{(s)}}}{\dim(\mathcal{H}_N^{(s)})} \le \int_{\Omega_N} e^{-\beta[H_N^{(s)}]_{\boldsymbol{\omega}}}\,\frac{d\boldsymbol{\omega}}{|\Omega_N|}\,.$$

Lieb proved these bounds. (Consult [42] for a better proof of the upper bound than in [34], which is also due to Lieb). They were also known to Berezin, though his interest was quite different [4]. Both the lower symbols and properly-chosen upper symbols converge to the classical Hamiltonian, as $s\to\infty$. But this most recent result was proved by Lieb only for the Heisenberg model. It was proved by Duffield for general Hamiltonians [16].

4. Bounds on "Matrix Entries"

It is natural to ask whether the quantum (finite-volume) Gibbs states, themselves converge to the classical Gibbs-state. To compare the two, define

$$\hat{\chi}_E^{(s)} = \frac{\dim(\mathcal{H}_N^{(s)})}{|\Omega_N|} \int_E d\boldsymbol{\omega} \bigotimes_{\alpha \in \Lambda_N} [P_{\omega_\alpha}^{(s)}]_\alpha \, .$$

for each measurable set $E \subset \Omega_N$. Then one can define a probability measure on Ω_N, based on the quantum Gibbs state

$$\mu_{\beta,N}^{(s)}(E) = \left(Z_{\beta,N}^{(s)}\right)^{-1} \mathrm{Tr}\left(\hat{\chi}_E^{(s)} \, e^{-\beta H_N^{(s)}}\right) .$$

Of course, the classical Gibbs measure is $\mu_{\beta,N}^{(\infty)}(E) = \left(Z_{\beta,N}^{(s)}\right)^{-1} \int_E e^{-\beta H_N^{(\infty)}(\boldsymbol{\omega})}$. It is useful to know the lower symbol of the Gibbs weight, because

$$\frac{d\mu_{\beta,N}^{(s)}}{d\boldsymbol{\omega}} = \frac{\langle e^{-\beta H_N^{(s)}} \rangle_{\boldsymbol{\omega}}}{\int_{\Omega_N} \langle e^{-\beta H_N^{(s)}} \rangle_{\boldsymbol{\omega}} \, d\boldsymbol{\omega}} \, .$$

The key technical result we proved is about this.

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

$$e^{-\beta \langle H_N^{(s)} \rangle_{\boldsymbol{\omega}}} \leq \langle e^{-\beta H_N^{(s)}} \rangle_{\boldsymbol{\omega}} \leq e^{-\beta [H_N^{(s)}]_{\boldsymbol{\omega}} + \beta C |\Lambda_N| / s} ,$$

for all β, s such that $s > c\beta^2$.

Of course, the lower bound in the theorem is one of Lieb's original bounds, but the upper bound is new. Using this, one obtains

$$\mu_{\beta,N}^{(s)}(E) \leq e^{\beta C |\Lambda_N|/s} \frac{\int_E e^{-\beta [H_N^{(s)}]_{\boldsymbol{\omega}}} \, d\boldsymbol{\omega}}{\int_{\Omega_N} e^{-\beta \langle H_N^{(s)} \rangle_{\boldsymbol{\omega}}} \, d\boldsymbol{\omega}} \, .$$

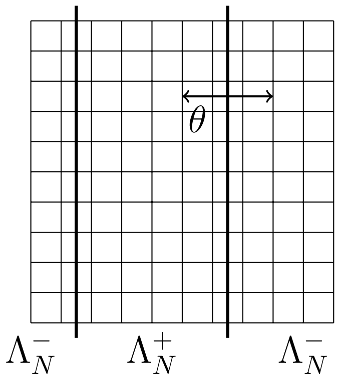
One can phrase this, as if in the context of large deviations, as

$$\frac{1}{|\Lambda_N|} \ln\left(\mu_{\beta,N}^{(s)}(E)\right) \leq \frac{\beta C}{s} + \frac{1}{|\Lambda_N|} \ln\left(\frac{\int_E e^{-\beta [H_N^{(s)}]_{\boldsymbol{\omega}}} \, d\boldsymbol{\omega}}{\int_{\Omega_N} e^{-\beta \langle H_N^{(s)} \rangle_{\boldsymbol{\omega}}} \, d\boldsymbol{\omega}}\right) .$$

In this case, $\beta C/s$ is just an $O(1)$ correction, and in fact it is $O(1/s)$ as $s \to \infty$.

Unfortunately, for the purposes of proving a phase transition using a Peierls-type argument, one needs estimates on events such as bad spin configurations on a contour of length $O(|\partial \Lambda_N|)$, whose probabilities do not have large-deviation type exponential decay in $|\Lambda_N|$. The way to overcome this problem is to use chessboard estimates.

5. Chessboard Estimates



A pair of planes on Λ_N is a pair of hyperplanes orthogonal to one of the coordinate directions, positioned on the dual graph, with spacing equal to half the lattice length. These decompose the lattice into Λ_N^+ and Λ_N^-, with a reflection θ interchanging the two. This is reflection in either of the planes, which is the same for both. Denoting the operators on $\mathcal{H}_N^{(s)}$ as $\mathfrak{A}$, this induces a decomposition $\mathfrak{A} = \mathfrak{A}_+ \otimes \mathfrak{A}_-$, with an isomorphism $\vartheta : \mathfrak{A}_+ \to \mathfrak{A}_-$.

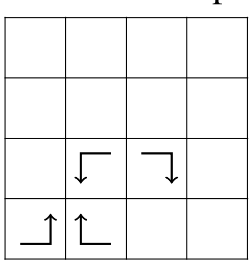
Given an operator, $A \in \mathfrak{A}_+$, let $\overline{A}$ be the complex conjugation, not conjugate transpose. Then there is a bilinear form on $\mathfrak{A}_+$ defined from the Gibbs state. Namely

$$(A, B) \mapsto \frac{\mathrm{Tr}\left(A \otimes \overline{\theta(B)}\, e^{-\beta H_N^{(s)}}\right)}{\mathrm{Tr}\ e^{-\beta H_N^{(s)}}}\,.$$

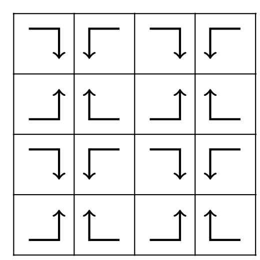
The Hamiltonian H_N is called "reflection positive" if this bilinear form is positive semidefinite for each choice of pair-of-planes. All the Hamiltonians listed in Section 0 are reflection positive, although to make this so, one must first perform certain unitary transformations.

References for reflection positivity and chessboard estimates are [25, 19, 24, 22, 23]

Using the Cauchy-Schwarz inequality and translation invariance, one can prove the following useful fact. Consider any n such that N/n is even. One can consider the small block of sidelength n and tile Λ_N by it. Let $\mathfrak{A}_n$ be the set of operators localized just in the block, and for each tiling translation $\boldsymbol{t} \in n \cdot (\mathbb{Z}/(N/n)\mathbb{Z})^d$, let $\tau_{\boldsymbol{t}} : \mathfrak{A}_n \to \mathfrak{A}$ be the homomorphism which embeds an operator $A \in \mathfrak{A}_n$ in $\mathfrak{A}$ by translating by $\boldsymbol{t}$ **through a sequence of reflections**. Actually, let us also define $\hat{\tau}_{\boldsymbol{t}}$ to be an real homomorphism, but not a complex one, which also complex conjugates if $\boldsymbol{t}$ is on the odd sublattice.



This is depicted in the figure to the left where the crooked arrow stands for some operator or one of its reflection localized on a tile. Given an operator $A \in \mathfrak{A}_n$, let $\mathcal{D}(A)$ be the complete dissemination in Λ_N: $\mathcal{D}(A) = \prod_{\boldsymbol{t}} \hat{\tau}_{\boldsymbol{t}}(A)$. See right figure.



The chessboard estimates say the following. Suppose that $A_1, \dots, A_k$ are a sequence of operators in $\mathfrak{A}_n$ and $\boldsymbol{t}_1, \dots, \boldsymbol{t}_k$ are a sequence of disjoint tiles. Then

$$\left|\left\langle \prod_{i=1}^{k} \hat{\tau}_{\boldsymbol{t}_1}(A_i)\right\rangle_{\beta,N}^{(s)}\right| \le \prod_{i=1}^{k}\left[\langle \mathcal{D}(A_i)\rangle_{\beta,N}^{(s)}\right]^{n^d/N^d}\,.$$

Combining this with the bound from our theorem is useful, because each $\mathcal{D}(A_i)$ is an operator with macroscopically many terms. Therefore, one does fully expect to have large-deviation type of values for the expectation, namely exponential in the volume (or more precisely in N^d/n^d). Moreover, this is set-up perfectly to apply to the "chessboard-Peierls" argument.

(A page from our paper)

To showcase our approach, we will prove phase transitions in the following five quantum systems (defined by their respective formal Hamiltonians):

(1) The anisotropic Heisenberg antiferromagnet:

$$H = + \sum_{\langle \boldsymbol{r},\boldsymbol{r}'\rangle} \mathcal{S}^{-2}\big(J_1 S^x_{\boldsymbol{r}} S^x_{\boldsymbol{r}'} + J_2 S^y_{\boldsymbol{r}} S^y_{\boldsymbol{r}'} + S^z_{\boldsymbol{r}} S^z_{\boldsymbol{r}'}\big) \tag{0.1}$$

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

(2) The non-linear XY-model:

$$H = - \sum_{\langle \boldsymbol{r},\boldsymbol{r}'\rangle} \mathcal{P}\biggl(\frac{S^x_{\boldsymbol{r}} S^x_{\boldsymbol{r}'} + S^y_{\boldsymbol{r}} S^y_{\boldsymbol{r}'}}{\mathcal{S}^2}\biggr) \tag{0.2}$$

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

(3) The non-linear nematic model:

$$H = - \sum_{\langle \boldsymbol{r},\boldsymbol{r}'\rangle} \mathcal{P}\big(\mathcal{S}^{-2}(\boldsymbol{S}_{\boldsymbol{r}} \cdot \boldsymbol{S}_{\boldsymbol{r}'})^2\big) \tag{0.3}$$

where $\mathcal{P}$ is a "large" polynomial with positive coefficients and $\boldsymbol{S}_{\boldsymbol{r}} \cdot \boldsymbol{S}_{\boldsymbol{r}'} = S^x_{\boldsymbol{r}} S^x_{\boldsymbol{r}'} + S^y_{\boldsymbol{r}} S^y_{\boldsymbol{r}'} + S^z_{\boldsymbol{r}} S^z_{\boldsymbol{r}'}$.

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

$$H = \sum_{\langle \boldsymbol{r},\boldsymbol{r}'\rangle} \begin{cases} \mathcal{S}^{-2}\, S^x_{\boldsymbol{r}} S^x_{\boldsymbol{r}'}, & \text{if } \boldsymbol{r}' = \boldsymbol{r} \pm \hat{\mathrm{e}}_x, \\ \mathcal{S}^{-2}\, S^y_{\boldsymbol{r}} S^y_{\boldsymbol{r}'}, & \text{if } \boldsymbol{r}' = \boldsymbol{r} \pm \hat{\mathrm{e}}_y. \end{cases} \tag{0.4}$$

(5) The 120-degree model on $\mathbb{Z}^3$:

$$H = \sum_{\langle \boldsymbol{r},\boldsymbol{r}'\rangle} \mathcal{S}^{-2}\, T^j_{\boldsymbol{r}} T^j_{\boldsymbol{r}'} \quad \text{if} \quad \boldsymbol{r}' = \boldsymbol{r} \pm \hat{\mathrm{e}}_j \tag{0.5}$$

where

$$T^j_{\boldsymbol{r}} = \begin{cases} S^x_{\boldsymbol{r}}, & \text{if } j = 1, \\ -\frac{1}{2} S^x_{\boldsymbol{r}} + \frac{\sqrt{3}}{2} S^y_{\boldsymbol{r}}, & \text{if } j = 2, \\ -\frac{1}{2} S^x_{\boldsymbol{r}} - \frac{\sqrt{3}}{2} S^y_{\boldsymbol{r}}, & \text{if } j = 3. \end{cases} \tag{0.6}$$

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