Validity of spin wave theory for the quantum Heisenberg model

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Outline

1. Introduction: continuous symmetry breaking and spin waves
2. Main results: free energy at low temperatures
3. Sketch of the proof: upper and lower bounds

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Spontaneous symmetry breaking

General question: rigorous understanding of the phenomenon of **spontaneous breaking** of a **continuous symmetry**.

Easier case: **abelian continuous symmetry**.

Several rigorous results based on:

- reflection positivity,
- vortex loop representation
- cluster and spin-wave expansions,

by Fröhlich-Simon-Spencer, Dyson-Lieb-Simon, Bricmont-Fontaine-
-Lebowitz-Lieb-Spencer, Fröhlich-Spencer, Kennedy-King, ...

Spontaneous symmetry breaking

Harder case: **non-abelian symmetry**.

Few rigorous results on:

- classical Heisenberg (Fröhlich-Simon-Spencer by RP)
- quantum Heisenberg *antiferromagnet* (Dyson-Lieb-Simon by RP)
- classical N-vector models (Balaban by RG)

Notably absent: quantum Heisenberg *ferromagnet*

Quantum Heisenberg ferromagnet

The simplest quantum model for the spontaneous symmetry breaking of a continuous symmetry:

$$H_\Lambda := \sum_{\langle x,y\rangle \subset \Lambda} (S^2 - \vec{S}_x \cdot \vec{S}_y)$$

where:

- Λ is a cubic subset of $\mathbb{Z}^3$ (possibly with periodic b.c.)
- $\vec{S}_x = (S_x^1, S_x^2, S_x^3)$ and S_x^i are the generators of a $(2S+1)$-dim representation of $SU(2)$, with $S = \frac{1}{2}, 1, \frac{3}{2}, \ldots$:

$$[S_x^i, S_y^j] = i\epsilon_{ijk} S_x^k \delta_{x,y}$$

- The energy is normalized s.t. $\inf \mathrm{spec}(H_\Lambda) = 0$.

Ground states

One special ground state is

$$|\Omega\rangle := \otimes_{x\in\Lambda}|S_x^3 = -S\rangle$$

All the other ground states have the form

$$(S_T^+)^n|\Omega\rangle, \qquad n = 1, \ldots, 2S|\Lambda|$$

where $S_T^+ = \sum_{x\in\Lambda} S_x^+$ and $S_x^+ = S_x^1 + iS_x^2$.

Excited states: spin waves

A special class of excited states (**spin waves**) is obtained by raising a spin in a coherent way:

$$|1_k\rangle := \frac{1}{\sqrt{2S|\Lambda|}} \sum_{x\in\Lambda} e^{ikx} S_x^+ |\Omega\rangle \equiv \frac{1}{\sqrt{2S}} \hat{S}_k^+ |\Omega\rangle$$

where $k \in \frac{2\pi}{L}\mathbb{Z}^3$. They satisfy

$$H_\Lambda |1_k\rangle = S\epsilon(k)|1_k\rangle$$

where $\epsilon(k) = 2\sum_{i=1}^3 (1 - \cos k_i)$.

Excited states: spin waves

More excited states?

They can be looked for *in the vicinity* of

$$|\{n_k\}\rangle = \prod_k (2S)^{-n_k/2} \frac{(\hat{S}_k^+)^{n_k}}{\sqrt{n_k!}} |\Omega\rangle$$

If $N = \sum_k n_k > 1$, these are not eigenstates.

They are neither normalized nor orthogonal.

However, H_Λ is almost diagonal on $|\{n_k\}\rangle$ in the low-energy (long-wavelength) sector.

Expectation:

low temperatures $\Rightarrow$
$\Rightarrow$ low density of spin waves $\Rightarrow$
$\Rightarrow$ negligible interactions among spin waves.

The linear theory obtained by neglecting spin wave interactions is the **spin wave approximation**, in very good agreement with experiment.

Spin waves

In 3D, it predicts

$$f(\beta) \simeq \frac{1}{\beta}\int \frac{d^3k}{(2\pi)^3}\log(1 - e^{-\beta S\epsilon(k)})$$
$$m(\beta) \simeq S - \int \frac{d^3k}{(2\pi)^3}\frac{1}{e^{\beta S\epsilon(k)} - 1}$$

Spin waves

In 3D, it predicts

$$f(\beta) \underset{\beta\to\infty}{\simeq} \beta^{-5/2} S^{-3/2} \int \frac{d^3k}{(2\pi)^3} \log(1 - e^{-k^2})$$

$$m(\beta) \underset{\beta\to\infty}{\simeq} S - \beta^{-3/2} S^{-3/2} \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{k^2} - 1}$$

How does one obtain these formulas?

Holstein-Primakoff representation

A convenient representation:

$$S_x^+ = \sqrt{2S}\, a_x^+ \sqrt{1 - \frac{a_x^+ a_x}{2S}}\ , \quad S_x^3 = a_x^+ a_x - S,$$

where $[a_x, a_y^+] = \delta_{x,y}$ are **bosonic operators**.

Hard-core constraint: $n_x = a_x^+ a_x \leq 2S$.

Holstein-Primakoff representation

In the bosonic language

$$H_\Lambda = S \sum_{\langle x,y \rangle} \Bigg(-a_x^+ \sqrt{1 - \frac{n_x}{2S}} \sqrt{1 - \frac{n_y}{2S}} a_y$$

$$-a_y^+ \sqrt{1 - \frac{n_y}{2S}} \sqrt{1 - \frac{n_x}{2S}} a_x + n_x + n_y - \frac{1}{S} n_x n_y \Bigg)$$

$$\equiv S \sum_{\langle x,y \rangle} (a_x^+ - a_y^+)(a_x - a_y) - K \equiv T - K$$

The spin wave approximation consists in neglecting K and the on-site hard-core constraint.

Previous results

$$H_\Lambda = S \sum_{\langle x,y \rangle} (a_x^+ - a_y^+)(a_x - a_y) - K$$

For large S, the interaction K is of relative size $O(1/S)$ as compared to the hopping term.

Easier case: $S \to \infty$ with βS constant (CG 2012)

[The classical limit is $S \to \infty$ with βS^2 constant (Lieb 1973).

See also Conlon-Solovej (1990-1991).]

Harder case: fixed S, say $S = 1/2$. So far, not even a sharp upper bound on the free energy was known. Rigorous upper bounds, off by a constant, were given by Conlon-Solovej and Toth in the early 90s.

Outline

Main theorem

Main Result [Correggi-Giuliani-S 2013]:

Theorem (Free energy at low temperature)

For any $S \geq 1/2$,

$$\lim_{\beta \to \infty} f(S, \beta) \beta^{5/2} S^{3/2} = \int_{\mathbb{R}^3} \log\left(1 - e^{-k^2}\right) \frac{d^3 k}{(2\pi)^3}\,.$$

The proof comes with explicit bounds on the remainder:

Relative errors:
- $O((\beta S)^{-3/8})$ (upper bound)
- $O((\beta S)^{-1/40+\epsilon})$ (lower bound)

Outline

1. Introduction: continuous symmetry breaking and spin waves
2. Main results: free energy at low temperatures
3. Sketch of the proof: upper and lower bounds

$S = 1/2$

We sketch the proof for $S = 1/2$ only.

In this case the Hamiltonian takes the form:

$$H_\Lambda = \frac{1}{2} \sum_{\langle x,y \rangle} \left[(a_x^+ - a_y^+)(a_x - a_y) - 2 n_x n_y \right] \equiv T - K$$

(projected onto $n_x \leq 1$ for all x) or, equivalently

$$H_\Lambda = \frac{1}{2} \sum_{\langle x,y \rangle} \left(a_x^+(1-n_y) - a_y^+(1-n_x) \right) \left(a_x(1-n_y) - a_y(1-n_x) \right)$$

Upper bound

We localize in Dirichlet boxes B of side ℓ:

$$f(\beta,\Lambda) \le \left(1+\ell^{-1}\right)^{-3} f^D(\beta,B)$$

In each box, we use the Gibbs variational principle:

$$f^D(\beta,B) = \frac{1}{\ell^3}\inf_{\Gamma}\left[\mathrm{Tr}\, H_B^D\Gamma + \frac{1}{\beta}\mathrm{Tr}\,\Gamma\ln\Gamma\right]$$

For an upper bound we use as trial state

$$\Gamma_0 = \frac{Pe^{-\beta T^D}P}{\mathrm{Tr}(Pe^{-\beta T^D}P)},$$

where $P = \prod_x P_x$ and $P_{\mathbf{x}}$ enforces $n_x \le 1$.

Upper bound

To bound the effect of the projector, we use

$$1 - P \leq \sum_x (1 - P_x) \leq \frac{1}{2} \sum_x n_x(n_x - 1)$$

Therefore, $\langle 1 - P \rangle$ can be bounded via Wick's rule: using $\langle a_x a_x^+ \rangle \simeq (\mathrm{const.})\beta^{-3/2}$ we find

$$\frac{\mathrm{Tr} e^{-\beta T^D}(1 - P)}{\mathrm{Tr} e^{-\beta T^D}} \leq (\mathrm{const.})\ell^3 \beta^{-3}$$

Optimizing, we find $\ell \propto \beta^{7/8}$, which implies

$$f(\beta) \leq C_0 \beta^{-5/2} \left(1 - O(\beta^{-3/8})\right).$$

Lower bound. Main steps

Proof of the lower bound: three main steps.

1. localization and preliminary lower bound
2. restriction of the trace to the low energy sector
3. estimate of the interaction on the low energy sector

Lower bound. Step 1.

We localize the system into boxes B of side ℓ:

$$f(\beta, \Lambda) \geq f(\beta, B).$$

Key ingredient for a preliminary lower bound:

Lemma (1)

$$H_B \geq c\ell^{-2}(\frac{1}{2}\ell^3 - S_T)$$

where $\vec{S}_T = \sum_{x \in B} \vec{S}_x$ *and* $|\vec{S}_T|^2 = S_T(S_T + 1)$.

Proof of Lemma 1

Proof.

$$\left(\frac{1}{4} - \vec{S}_x \cdot \vec{S}_y\right) + \left(\frac{1}{4} - \vec{S}_y \cdot \vec{S}_z\right) \geq \frac{1}{2}\left(\frac{1}{4} - \vec{S}_x \cdot \vec{S}_z\right)$$

and hence

$$\sum_{i=1}^{n} \left(\frac{1}{4} - \vec{S}_{x_{i-1}} \cdot \vec{S}_{x_i}\right) \geq \frac{1}{2n}\left(\frac{1}{4} - \vec{S}_{x_0} \cdot \vec{S}_{x_n}\right)$$

for distinct sites $x_0, \ldots, x_n$. Apply this to any pair $(x, y) \in B \times B$, connecting it via a path that stays as close as possible to the straight line connecting the two. Then sum over all x and y. □

Lower bound. Step 1.

Since H_B commutes with $\vec{S}_T$,

$$\mathrm{Tr}(e^{-\beta H_B}) = \sum_{S_T=0}^{\ell^3/2} (2S_T + 1)\mathrm{Tr}_{S_T^3=-S_T}(e^{-\beta H_B})$$

By Lemma 1, the r.h.s. is bounded from above by

$$(\ell^3{+}1) \sum_{N=0}^{\ell^3/2} \binom{\ell^3}{N} e^{-c\beta\ell^{-2}N} \leq (\ell^3{+}1) \left(1 + e^{-c\beta\ell^{-2}}\right)^{\ell^3},$$

where $N = \frac{1}{2}\ell^3 + S_T^3 = \frac{1}{2}\ell^3 - S_T$.

Lower bound. Steps 1 and 2.

Optimizing over ℓ we find

$$f(\beta,\Lambda) \geq -(\mathrm{const.})\beta^{-5/2}(\log\beta)^{5/2}.$$

We can now cut off the "high" energies:

$$\mathrm{Tr} P_{H_B \geq E_0} e^{-\beta H_B} \leq e^{-\beta E_0/2} e^{-\frac{\beta}{2}\ell^3 f(\beta/2,B)} \leq 1\,,$$

if $E_0 \simeq \ell^3 \beta^{-5/2}(\log\beta)^{\frac{5}{2}}$.

We are left with the trace on $H_B \leq E_0$, which we compute on the sector $S_T^3 = -S_T$.

Note: Lemma 1 $\Rightarrow$ apriori bound on the particle number:

$$N = \frac{1}{2}\ell^3 + S_T^3 = \frac{1}{2}\ell^3 - S_T \leq c\ell^2 E_0$$

Lower bound. Step 3.

If $\rho_E(x, y)$ is the two-particle density matrix,

$$\langle E|K|E\rangle = \sum_{\langle x,y\rangle} \langle E|n_x n_y|E\rangle \leq 3\ell^3 ||\rho_E||_\infty$$

Lemma (2)

For all $E > 0$

$$\|\rho_E\|_\infty \leq (\mathrm{const.}) E^3 \|\rho_E\|_1$$

Now: $\ell = \beta^{1/2+\epsilon} \Rightarrow E_0 \simeq \ell^{-2+O(\epsilon)} \Rightarrow \|\rho_E\|_\infty \leq \ell^{-6+O(\epsilon)}$

$$\Rightarrow \frac{1}{\ell^3}\langle E|K|E\rangle \leq \ell^{-6+O(\epsilon)} = \beta^{-3+O(\epsilon)}, \quad \text{as desired.}$$

Lower bound. Step 3: Proof of Lemma 2.

Key observation: the eigenvalue equation implies

$$-\tilde{\Delta}\rho_E(x,y) \leq 4E\rho_E(x,y),$$

where $\tilde{\Delta}$ is the Neumann Laplacian on

$$B^2 \setminus \{(x,x) : x \in B\}.$$

Remarkable: the many-body problem has been reduced to a 2-body problem!!

Lower bound. Step 3: Proof of Lemma 2.

We extend ρ on $\mathbb{Z}^6$ by Neumann reflections and find

$$-\Delta \rho_E(z) \leq 4E\rho_E(z) + 2\rho_E(z)\chi_1^R(z)$$

where $\chi_1^R(z_1, z_2)$ is equal to 1 if z_1 is at distance 1 from one of the images of z_2, and 0 otherwise.

Therefore,

$$\rho_E(z) \leq (1 - E/3)^{-1} \Big(\langle \rho_E \rangle_z + \frac{1}{6} \|\rho_E\|_\infty \chi_1^R(z) \Big)$$

Lower bound. Step 3: Proof of Lemma 2.

Iterating,

$$\rho_E(z) \le \left(1-\frac{E}{3}\right)^{-n}\left((P_n*\rho_E)(z)+\frac{1}{6}\|\rho_E\|_\infty \sum_{j=0}^{n-1} P_j*\chi_1^R(z)\right)$$

where $P_n(z,z')$ is the probability that a SSRW on $\mathbb{Z}^6$ starting at z ends up at z' in n steps. For large n:

$$P_n(z,z') \simeq \left(\frac{3}{\pi n}\right)^3 e^{-3|z-z'|^2/n} \; .$$

Moreover, if G is the Green function on $\mathbb{Z}^6$,

$$\sum_{j=0}^{n-1} P_j(z,z') \le \sum_{j=0}^{\infty} P_j(z,z') = 12G(z-z')$$

Lower bound. Step 3: Proof of Lemma 2.

Let us now pretend for simplicity that χ_1^R is equal to χ_1. In this simplified case we find:

$$\rho(z) \leq \frac{1}{(1-\frac{E}{3})^n}\left(\frac{27}{\pi^3 n^3}\sum_{w\in\mathbb{Z}^6} e^{-\frac{3}{n}|z-w|^2}\rho(w)+2\|\rho\|_\infty G*\chi_1(z)\right)$$

Picking $n \sim E^{-1}$ we get:

$$\rho(z) \leq (\text{const.})E^3\|\rho\|_1 + (1+\delta)\times 2\times 0.258\times\|\rho\|_\infty$$

where we used the fact that

$$(G*\chi_1)(z_1,z_2) \leq \frac{1}{2}\int \frac{\sum_{i=1}^3 \cos p_i}{\sum_{i=1}^3(1-\cos p_i)}\frac{d^3p}{(2\pi)^3} = 0.258$$

Summary

- Using the Holstein-Primakoff representation of the 3D quantum Heisenberg ferromagnet, we prove the correctness of the spin wave approximation to the free energy at the lowest non trivial order in a low temperature expansion, with explicit estimates on the remainder.
- The proof is based on upper and lower bounds. In both cases we localize the system in boxes of side $\ell = \beta^{1/2+\epsilon}$.

Summary

- The upper bound is based on a trial density matrix that is the natural one, i.e., the Gibbs state associated with the quadratic part of the Hamiltonian projected onto the subspace satisfying the local hard-core constraint.
- The lower bound is based on a preliminary rough bound, off by a log. This uses an estimate on the excitation spectrum

$$H_B \geq (\text{const.})\ell^{-2}(S_{max} - S_T)$$

Summary

- The preliminary rough bound is used to cut off the energies higher than $\ell^3\beta^{-5/2}(\log\beta)^{5/2}$. In the low energy sector we pass to the bosonic representation.
- In order to bound the interaction energy in the low energy sector, we use a new functional inequality, which allows us to reduce to a 2-body problem. The latter is studied by random walk techniques on a modified graph.

Thank you!