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Spin-Wave Theory of the Ferromagnetic Quantum Heisenberg Model

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1 — INTRODUCTION

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

nearest neighbour pairs in a cube of side-length L in $\mathbb{Z}^3$.

Hilbert space: on $\bigotimes_{x\in\Lambda_L} \mathbb{C}^{2S+1}$;

spin operators: $\vec{S}_x = \begin{pmatrix} S_x^1 \\ S_x^2 \\ S_x^3 \end{pmatrix}$ a spin-S operator (where $S \in \{\frac{1}{2}, 1, \frac{3}{2}, 2 \dots\}$)

$$[S_x^i, S_y^j] = \delta_{x,y}\, i \sum_{k=1}^{3} \varepsilon_{ijk} S_x^k$$

$$(\vec{S}_x)^2 = (S_x^1)^2 + (S_x^2)^2 + (S_x^3)^2 = S(S+1)\mathbb{1}.$$

We are interested in the t.dyn. quantities:

- the free energy in the t.dyn. limit
- (the magnetization — not in this talk.)

HEURISTIC SPIN-WAVE THEORY

ground state: w.l.o.g

$$|gs\rangle = \bigotimes_{x\in\Lambda_L} |-S\rangle_x , \qquad \text{where} \qquad S^3_x |-S\rangle_x = -S\,|-S\rangle_x .$$

Raising op. of 3-component of spin: $S^+_x := S^1_x + i S^2_x$.

Bloch 1930: What are the lowest energy excitations?

⇝ Coherently distributed excitation: SPIN WAVE/MAGNON

$$S^+_k := \frac{1}{\sqrt{|\Lambda_L|}} \sum_{x\in\Lambda_L} e^{ik\cdot x} S^+_x , \qquad \left(\text{momentum } k\in \tfrac{2\pi}{L}\mathbb{Z}^3 \text{ p.b.c.}\right)$$

$$|k\rangle = \frac{1}{\sqrt{2S}} S^+_k |gs\rangle$$

These are eigenvectors of H_{Λ_e}!

$$H_{\Lambda_L}|k\rangle = S\,\mathcal{E}(k)\,|k\rangle, \qquad \mathcal{E}(k) = 2\sum_{i=1}^{3} (1-\cos k_i)$$

spin-wave disp. relation.
(lattice laplacian in Fourier space)

Now try Multi-spin-wave states: $S^+_{k_1} S^+_{k_2}|gs\rangle$

These states have problems:

- not eigenstates
- not orthogonal

Intuitive reason:

Can not be behave like indep. particle modes, obviously, since S^+_x can be applied at most S times!

Nevertheless, a very successful theory is obtained by treating spin-waves as independent bosonic modes of energy $S\mathcal{E}(k)$.

⇝ Predictions:

free energy: $f(S,\beta) =$ free energy of non-interacting bosons with disp. rel. $S\mathcal{E}(k)$ $\displaystyle = \frac{1}{\beta}\int_{[-\pi,\pi]^3}\frac{d^3k}{(2\pi)^3}\log\left(1-e^{-\beta S\mathcal{E}(k)}\right)$

$\mathcal{E}(k)\simeq k^2$ + scale out β^S

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

magnetization: $$m(S,\beta) = S - \underbrace{\int\frac{d^3k}{(2\pi)^3}\frac{1}{e^{\beta S\mathcal{E}(k)}-1}}_{\text{"number of excited spin waves"}} \sim S - \beta^{-3/2}S^{-3/2}\int\frac{d^3k}{(2\pi)^3}\frac{1}{e^{k^2}-1}.$$

SYSTEMATIC SPIN-WAVE THEORY

to avoid problems with the "spin-wave creation operator" S_k^+, transform into true bosonic operators:

Holstein-Primakoff representation:

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

($a_x^\dagger, a_x$ satisfy usual bosonic CCR.)

Valid on the subspace of bosonic Fock space where

$$n_x \le 2S \quad \forall x\in\Lambda_L.$$

④ Thus:

- $$H_{\Lambda_L} = S \sum_{\langle x,y\rangle \subset \Lambda_L} \Big(-a_x^\dagger \sqrt{1-\frac{n_x}{2S}}\sqrt{1-\frac{n_y}{2S}}\, a_y - a_y^\dagger \sqrt{1-\frac{n_y}{2S}}\sqrt{1-\frac{n_x}{2S}}\, a_x + n_x + n_y - \frac{1}{S} n_x n_y \Big).$$

- The zero-temperature ground state maps on vacuum in Fock space:
  $|gs\rangle \longmapsto \Omega$

For low temp. or large S: $\frac{n_x}{2S} \ll 1$, expand $\sqrt{1-\frac{n_x}{2S}}$:

$$
\begin{aligned}
H_{\Lambda_L} = S\Big[& \sum_{\langle x,y\rangle \subset \Lambda_L} \left(-a_x^\dagger a_y - a_y^\dagger a_x + n_x + n_y \right) && \Big\} =: T \quad \text{2nd quant of lattice Laplacian} \\
+ & \sum_{\langle x,y\rangle} \frac{1}{S}\, \text{"}a^\dagger a^\dagger a\, a\text{"} && \Big\} =: I \quad \text{quartic interaction} \\
+ & \sum_{\langle x,y\rangle} \frac{1}{S^2} (\cdots) \Big] && \Big\} =: R \quad \text{remainder}
\end{aligned}
$$

Laplacian diagonalized by Fourier transform:

$$T = \sum_{k\in\Lambda^*} a_k^\dagger a_k\, \varepsilon(k), \qquad \varepsilon(k) = \sum_{i=1}^{3} 2(1-\cos k_i).$$

Spin-wave theory:

$$H_{\Lambda_L} \simeq S\,T. \longrightarrow \text{system of non-interacting bosons.}$$

<u>Consistent?</u>

Bose-Einstein distribution

$$\left\langle \frac{n_x}{2S} \right\rangle = \frac{1}{2S} \operatorname{tr}\, n_x \frac{e^{-\beta S T}}{Z} \sim \frac{1}{S} (\beta S)^{-3/2},$$

Expansion believable if S large or β large.

Scaling regimes (→ Lieb '73, Conlon-Solovej '90)

$$\boxed{\begin{matrix} S = \text{const} \\ \beta \to \infty \end{matrix}}$$

low-temp. limit

(most difficult)

- Conlon-Solovej, Toth '90: non-sharp bounds
- Correggi-Giuliani-Seiringer '13: free energy

$$\boxed{\begin{matrix} S \to \infty \\ \beta S = \text{const.} \end{matrix}}$$

"intermediate limit"

- Conlon-Solovej '90 (for ext. mgn. field $\neq 0$)
- Correggi-Giuliani '12: free energy

↑ WE STUDY THIS REGIME!

- quantum (spin waves as bosons)
- much easier than low.temp. limit:
  - $\langle n_x \rangle \sim$ const.
  - explicit expansion in $\frac{1}{S}$.

$$\boxed{\begin{matrix} S \to \infty \\ \beta S^2 = \text{const} \end{matrix}}$$

classical limit:

- Lieb '73: → class. Heisenberg
- Conlon-Solovej '90-'91

<u>All these papers prove:</u>

<u>Leading</u> order is given by <u>non-interacting</u> bosons.

<u>Here</u> : <u>corrections due to the interaction?</u>

$I \rightsquigarrow$ correction.

$R \rightsquigarrow$ to be estimated.

2 - RESULT

$$f(S,\beta) = \lim_{\Lambda_L\to\infty} f(S,\beta,\Lambda_L), \quad f(S,\beta,\Lambda_L) = -\frac{1}{\beta L^d} \log \operatorname{tr} e^{-\beta H_{\Lambda_L}} .$$

THEOREM (arXiv: 1604.02548)

Let $d=2,3$.

Let $\beta S =: \tilde\beta$ fixed and suff. large, then for $S\to\infty$:

$$\frac{f(S,\beta)}{S} \leq \frac{1}{\tilde\beta}\int_{[-\pi,\pi]^d} \frac{d^dk}{(2\pi)^d} \log\left(1-e^{-\tilde\beta\varepsilon(k)}\right) - \frac{1}{S}\cdot\frac{1}{4d}\left(\int_{[-\pi,\pi]^d}\frac{d^dk}{(2\pi)^d}\,\frac{\varepsilon(k)}{e^{\tilde\beta\varepsilon(k)}-1}\right)^2$$

LEADING: free spin waves
($\rightsquigarrow$ Correggi - Giuliani '12)

new: FIRST ORDER

$$+\frac{1}{S^2}(\text{error}), \quad |\text{error}| \leq \begin{cases} C\tilde\beta^{-3} & (d=3) \\ C\tilde\beta^{-2}(\log S\tilde\beta)^3 & (d=2) \end{cases}$$

REMARKS:

- it holds for $d=2$!
  (Even though we know from Mermin-Wagner theorem that there is no ferromagnetic phase in 2d.)

- hints at peculiar temp. dependence if we extrapolate from our limit ($\tilde\beta$ fix, $S\to\infty$) to low temp. limit (S fix, $\beta\to\infty$):

  $\rightsquigarrow$ c.f. landmark papers of spin-wave theory in physics:
  (2 papers by Dyson)

DYSON 1956: $(d=3)$

$$\frac{f(S,\beta)}{S} = \frac{1}{\tilde{\beta}} \int_{[-\pi,\pi]^3} \frac{d^3k}{(2\pi)^3} \log\left(1 - e^{-\tilde{\beta}\varepsilon(k)}\right) \qquad \sim \underline{\underline{\tilde{\beta}^{-5/2}}}$$

big gap!

$$- \underline{\underline{\tilde{\beta}}}^{-5} \left[\underbrace{\frac{1}{S} \frac{3}{128(2\pi)^3} \zeta(5/2)}_{= \text{ our first order term!}} + \mathcal{O}(S^{-2}) \right]$$

$$+ \mathcal{O}(\tilde{\beta}^{-5.5})$$

No $\tilde{\beta}^{-3}$, $\tilde{\beta}^{-2.75}$ ... why? Before Dyson all these exponents (and others) where around!

Subtle cancellation expected / required.

→ See Section 4 for an analysis in 2nd order formal perturbation theory.

SKETCH OF PROOF

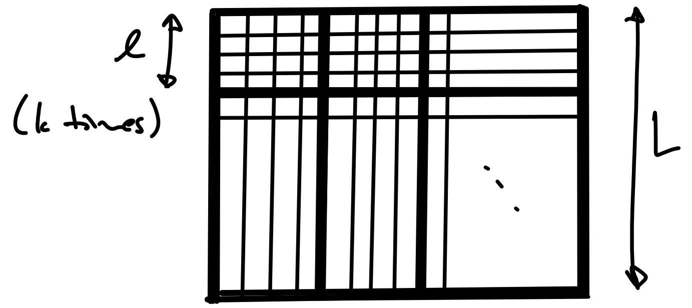
Standard tool to get an upper bound on the free energy:

Gibbs' variational principle:

$$f(S,\beta,\Lambda_L) \le \frac{1}{|\Lambda_L|}\operatorname{tr} H_{\Lambda_L}\Gamma + \frac{1}{\beta|\Lambda_L|}\operatorname{tr}\Gamma\log\Gamma \qquad \forall\,\Gamma\ge 0,\ \operatorname{tr}\Gamma = 1.$$

(states)

1) Apply once: break up into decoupled Dirichlet boxes Λ_ℓ.
(to deal with the tdyn. limit)



$$f(S,\beta,\Lambda_L) \le \frac{1}{(1+\ell^{-1})^d} f^{\text{Dirichlet}}(S,\beta,\Lambda_\ell)$$

For k → ∞ we get bound on the thermodynamic limit as intended.

2) Estimate f on Λ_ℓ with trial state:

recall $H_{\Lambda_\ell} = S\Big[\underbrace{T}_{\text{quadratic}} + \underset{\frac{1}{S}(a^\#)^4}{\underset{\shortparallel}{I}} + \underset{O(1/S^2)}{\underset{\shortparallel}{R}}\Big]$

$\downarrow$

trial state:

$$\Gamma^D := \frac{P\, e^{-\tilde\beta T} P}{\operatorname{tr} P e^{-\tilde\beta T}}, \qquad P = \prod_{x\in\Lambda_\ell} \mathbb{1}(n_x \le 2S).$$

Evaluating:

$$f^{\text{Dirichlet}}(S,\beta,\Lambda_\ell) \le \frac{1}{\ell^d}\operatorname{tr} H\Gamma^D + \frac{1}{\beta\ell^d}\operatorname{tr}\Gamma^D\log\Gamma^D$$

$$= \frac{1}{\ell^d} \operatorname{tr} S(\cancel{T} + I + R) \frac{P e^{-\tilde\beta T} P}{\operatorname{tr} P e^{-\tilde\beta T}}$$

} from the expect. of Hamiltonian

$$\leq - \cancel{\tilde\beta \operatorname{tr} P e^{-\tilde\beta T}} T$$

[CG12]

$$+ \frac{1}{\beta \ell^d} \operatorname{tr} \frac{P e^{-\tilde\beta T} P \log (P e^{-\tilde\beta T} P)}{\operatorname{tr} P e^{-\tilde\beta T}}$$

$$- \frac{1}{\beta \ell^d} \log \operatorname{tr} P e^{-\tilde\beta T}$$

} from entropy

3) get rid of P_S : $\Gamma^{qf} := \dfrac{e^{-\tilde\beta T}}{\operatorname{tr} e^{-\tilde\beta T}}$ ← Quasifree, nice b.c. we can use Wick then!

Dyson: "kinematical interaction"

$$f(S,\Lambda,\Lambda_e) \leq \underbrace{\frac{S}{\ell^d} \langle I \rangle_{qf}} + \underbrace{\frac{S}{\ell^d} \langle R \rangle_{qf}}_{\leq C S^{-2} \tilde\beta^{-3}.} - \underbrace{\frac{1}{\beta \ell^d} \log \operatorname{tr} e^{-\tilde\beta T}}_{\text{leading order (free Bose gas)}} + \mathcal{O}(\underbrace{\langle 1 - P \rangle_{qf}})$$

Can not be improved with the quasifree trial state! (see Sec. 4)

explicit calc. (tedious due to Dirichlet b.c.):

$$= \text{first order correction} + \mathcal{O}\left(\frac{1}{S\ell} (\log \ell)\right)$$

error due to replacing sums by integrals

in 2D

PROP.: $\langle 1 - P \rangle_{qf} \leq e \ell^3 (2S+1) \Big(\underbrace{\frac{\pi^{3/2}}{8} \zeta(3/2) \cdot \tilde\beta^{-3/2}}_{< 1 \text{ for } \tilde\beta \text{ large enough}} \Big)^{2S}$ (in $d=2$ with log)

$\Longrightarrow$ exp. decay in $S \to \infty$.

cf. S^{-2}: can completely forget $\langle 1 - P \rangle_{qf}$.

Proof: recall $P = \prod_{x\in\Lambda_\ell} \mathbb{1}(u_x \le 2S)$.

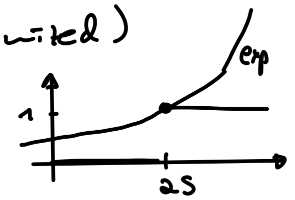
$$\langle P\rangle_{qf} = \mathbb{P}(\forall x\in\Lambda_\ell : u_x \le 2S).$$

$$\langle 1-P\rangle_{qf} = \mathbb{P}(\exists x\in\Lambda_\ell : u_x > 2S) \le \sum_{x\in\Lambda_\ell} \mathbb{P}(u_x > 2S)$$

$$= \sum_{x\in\Lambda_\ell} \langle \mathbb{1}(u_x > 2S)\rangle_{qf}$$

parameter λ (to be optimized)

$$\langle \mathbb{1}(u_x > 2S)\rangle_{qf} \le \langle e^{\lambda(u_x - 2S)}\rangle_{qf}$$



Wick + optimizing

$$\le (2S+1)\, e\, \langle u_x\rangle_{qf}^{2S}.$$

Direct calc. in Fourier space:

$$\langle u_x\rangle_{qf} \le \begin{cases} \frac{\pi^{3/2}}{8}\zeta(3/2)\,\tilde\beta^{-3/2} & (d=3) \\ 4\pi\,\tilde\beta^{-1}\log(\ell) & (d=2). \end{cases}$$

// c.f. also [CG12]

■

All terms in (*) have been estimated.

Now optimize ℓ between:

- $\frac{1}{\ell}$ for approximating sums by integrals and for boundary errors from Dirichlet conditions in calculating $\langle I\rangle_{qf}$.
- $\frac{1}{S^2}$ from estimate of $\langle R\rangle_{qf}$.

Resulting choice: $\ell = \tilde\beta^{d} S^2$.

■

4 – PERTURBATION THEORY & TEMP. DEP. OF INTERACTION CORRECTIONS

recall: $H = S(\underbrace{T}_{\mathcal{O}(1)} + \underbrace{I}_{\mathcal{O}(\frac{1}{S})} + R)$, $R = \underbrace{\mathcal{Y}}_{\mathcal{O}(\frac{1}{S^2})} + \underbrace{\tilde{R}}_{\mathcal{O}(\frac{1}{S^3})}$

In the quasifree Gibbs state: $\frac{1}{\ell^d}\langle \mathcal{Y}\rangle_{qf} \sim \tilde{\beta}^{-3}$.

We can only improve if we use a different trial state!

2nd order perturbation theory:

$$\frac{f(S,\beta,\Lambda_\ell)}{S} = \underbrace{-\frac{1}{\tilde{\beta}\ell^3}\log \operatorname{tr} e^{-\tilde{\beta}T}}_{\text{leading}} + \underbrace{\frac{1}{\ell^3}\langle I + \overset{1/S^2}{\mathcal{Y}}\rangle_{qf}}_{\text{first order}}$$

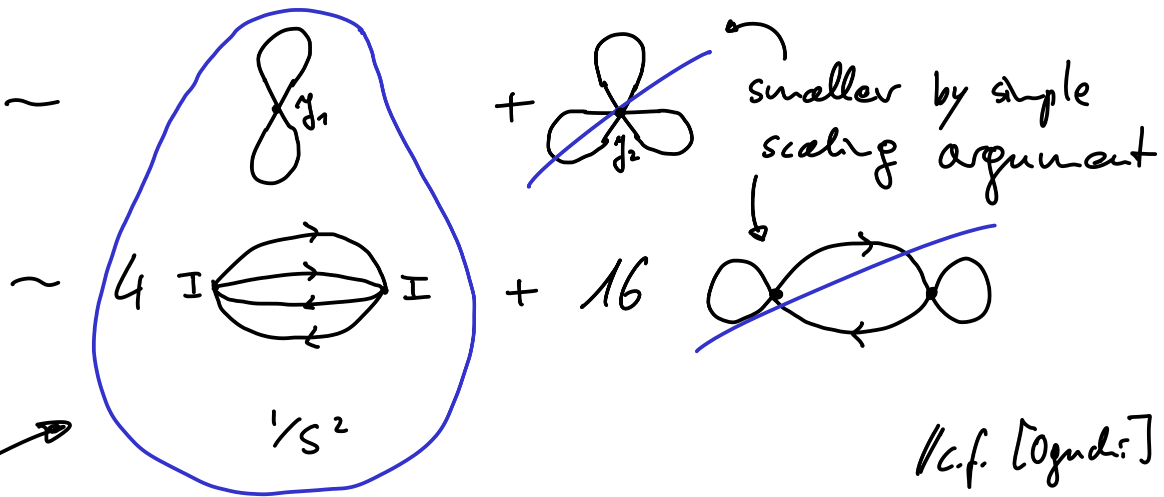
$$(**) \qquad -\frac{1}{\tilde{\beta}\ell^3}\int_0^{\tilde{\beta}} ds \int_0^s ds' \Big[\langle \underbrace{e^{sT} I e^{-sT}}_{1/S}\, \underbrace{e^{s'T} I e^{-s'T}}_{1/S} \rangle_{qf} - \langle I \rangle_{qf}^2 \Big]$$

$$+ \mathcal{O}(S^{-3})$$

Repres. by connected diagrams:

$\frac{1}{\ell^3}\langle \mathcal{Y}\rangle \sim$

$(**) \sim$



// c.f. [Ogudi]

Individually $\sim \tilde{\beta}^{-3}$. But: cancel up to a remainder of order $\tilde{\beta}^{-5}$!