Phys 726 - Lecture 15

* Long-range magnetic order may exist in the ground state of a spin system governed by a Heisenberg model Hamiltonian

$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j = 2 \sum_{i<j} J(\vec{R}_i - \vec{R}_j)\, \vec{S}_i \cdot \vec{S}_j$$

→ the operators $\vec{S}_j = \frac{3}{4} \hat{n}_j (2 - \hat{n}_j)$ represent the spin angular momentum of a localized electron with quenched charge fluctuations ($\hat{n}_j \approx 1$)

→ here we're considering spin $S = 1/2$, but in real magnetic systems the spin value may be a higher one that represents some combination of spin and orbital angular momentum

→ In a translationally invariant system, the natural ordering vector is the pair $\pm \vec{Q}$ that minimizes $J(\vec{q}) = \sum_{R} e^{i\vec{q}\cdot\vec{R}} J(\vec{R}) = J(-\vec{q})$

→ We derived an approximate (relaxed unit vector constraint on classical spins) solution

$$\vec{S}_j = \frac{1}{\sqrt{N}} \sum_{q} S_{\vec{q}}\, e^{i\vec{q}\cdot\vec{R}_j}$$

$$= \frac{1}{\sqrt{N}} \Big(\underbrace{S_{\vec{Q}}}_{\frac{\sqrt{N}}{2}(\vec{e}_x + i\vec{e}_y)}\, e^{i\vec{Q}\cdot\vec{R}_j} + \underbrace{S_{-\vec{Q}}}_{\frac{\sqrt{N}}{2}(\vec{e}_x - i\vec{e}_y)}\, e^{-i\vec{Q}\cdot\vec{R}_j} \Big)$$

$$= \vec{e}_x \cos \vec{Q}\cdot\vec{R}_j - \vec{e}_y \sin \vec{Q}\cdot\vec{R}_j$$

→ This implies a <u>correlation function</u>

$$\vec{S}_j\cdot\vec{S}_{j'} = \left(\vec{e}_x \cos\vec{Q}\cdot\vec{R}_j - \vec{e}_y \sin\vec{Q}\cdot\vec{R}_j\right)$$
$$\cdot \left(\vec{e}_x \cos\vec{Q}\cdot\vec{R}_{j'} - \vec{e}_y \sin\vec{Q}\cdot\vec{R}_{j'}\right)$$

$$= (\cos\vec{Q}\cdot\vec{R}_j)(\cos\vec{Q}\cdot\vec{R}_{j'}) + (\sin\vec{Q}\cdot\vec{R}_j)(\sin\vec{Q}\cdot\vec{R}_{j'})$$

$$= \cos[\vec{Q}\cdot(\vec{R}_j - \vec{R}_{j'})]$$

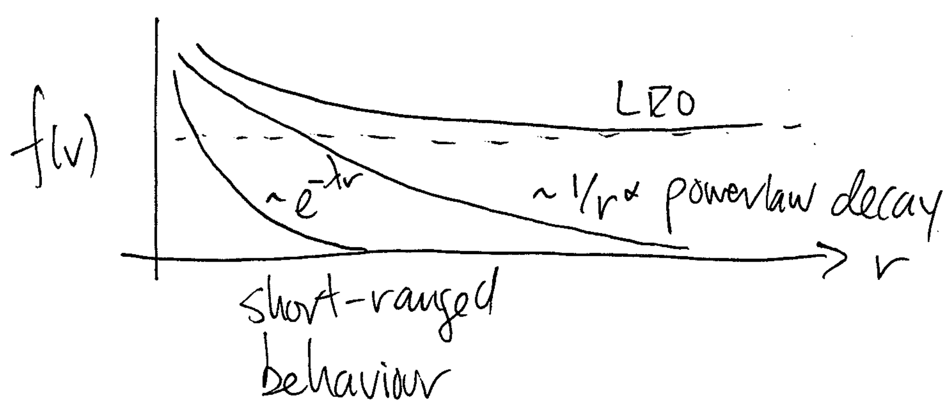
→ In the quantum case,

$$C(\vec{R}_i - \vec{R}_j) = \langle \vec{S}_i \cdot \vec{S}_j \rangle$$

ground state expectation value

Onsite, $C(0) = \langle S_i^2 \rangle = S(S+1) = \frac{3}{4}$.

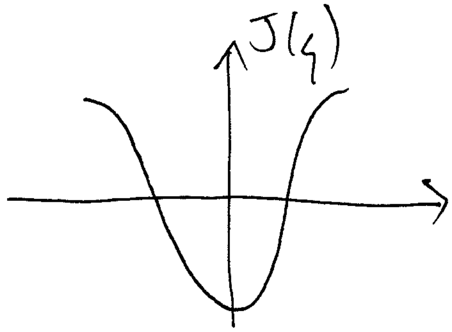
At long separations, $C(\vec{r}) \sim (\cos \vec{Q}\cdot\vec{r}) f(r)$, where $f(r)$ is a monotonically decreasing function. We say that the system has long range order if $\lim_{r\to\infty} f(r) \neq 0$.



→ the particular behavior depends on whether quantum fluctuations are weak or strong; in the latter case, they may wipe out the classical order

Ferromagnetic ground state

* The simplest spin configuration arises when $J(\vec{q})$ has its minimum at $\vec{q}=0$



→ the ground state corresponds to all spins aligned, either

$$|\psi\rangle = |\uparrow\uparrow\uparrow\uparrow\cdots\rangle$$

$$\text{or } |\psi\rangle = |\downarrow\downarrow\downarrow\downarrow\cdots\rangle$$

→ the state is immune to quantum fluctuations, since

$$\vec{S}_i\cdot\vec{S}_j = \frac{1}{2}\left(S_i^+S_j^- + S_i^-S_j^+\right) + S_i^zS_j^z$$

acting on $|\psi\rangle$ leaves the state unchanged:

$$\vec{S}_i\cdot\vec{S}_j|\psi\rangle = \frac{1}{2}\left(\overbrace{S_i^+S_j^-}^{\text{forbidden}} + \underbrace{S_i^-S_j^+}_{\text{forbidden}}\right)|\uparrow\uparrow\uparrow\cdots\uparrow_i\cdots\uparrow_j\cdots\rangle$$

$$+ S_i^zS_j^z|\uparrow\uparrow\uparrow\cdots\uparrow_i\cdots\uparrow_j\cdots\rangle = \frac{1}{4}|\psi\rangle$$

→ in other words, $|\psi\rangle$ is an eigenstate

$$\hat{H}|\psi\rangle = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j |\psi\rangle = \sum_{ij} J_{ij} S_i^z S_j^z |\psi\rangle$$

$$= \sum_{ij} \frac{1}{4} J_{ij} |\psi\rangle$$

with ground state energy

$$\frac{1}{4} \sum_{ij} J_{ij} = \frac{1}{4} \sum_{\vec{R}\vec{R}'} J(\vec{R}-\vec{R}') = \frac{1}{4} N_{sites} \sum_{\vec{R}} J(\vec{R})$$

$$= \frac{1}{4} N_{sites} J(\vec{q}=0)$$

in the FM case, the J_{ij} values must be predominantly negative

* Excited states will involve some deviation from perfect FM alignment

→ Consider $|\tilde{\psi}_i\rangle = S_i^- |\uparrow\uparrow\uparrow \cdots\rangle$

$$= |\uparrow\uparrow \cdots \uparrow \downarrow_i \uparrow\uparrow \cdots\rangle$$

one spin flipped in position i

→ but $|\tilde{\psi}_i\rangle$ isn't an eigenstate, since $\hat{H}$ won't leave the state invariant:

raises

$$\text{e.g. } \vec{S}_i \cdot \vec{S}_j |\psi_i'\rangle = \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)|\uparrow \cdots \uparrow \downarrow_i \uparrow \cdots \uparrow_j \cdots\rangle$$

lowers

$$+ S_i^z S_j^z |\uparrow \cdots \uparrow \downarrow_i \uparrow \cdots \uparrow_j \cdots\rangle$$

$$= \frac{1}{2}|\uparrow \cdots \uparrow \uparrow_i \uparrow \cdots \uparrow \downarrow_j \uparrow \cdots\rangle$$

$$- \frac{1}{4}|\uparrow \cdots \uparrow \downarrow_i \uparrow \cdots \uparrow_j \cdots\rangle$$

which have a substantial amplitude for moving the flipped spin from i to j

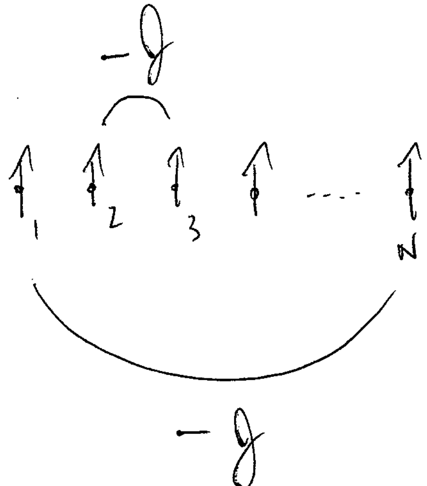
→ this is similar to hopping in tight-binding models: we expect eigenstates that are delocalized across the system

$$\text{e.g. } |\tilde{\psi}_{q=0}\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} S_i^- |\uparrow_1 \uparrow_2 \uparrow_3 \cdots \uparrow_N\rangle$$

EXAMPLE: Ferromagnetic quantum Heisenberg model on the linear chain
(1D, spin $S=1/2$, nearest neighbour interactions only)

$$\hat{H} = \sum_{ij} J_{ij}\, \vec{S}_i \cdot \vec{S}_j = 2\sum_{i<j} J_{ij}\, \vec{S}_i \cdot \vec{S}_j \equiv -\mathcal{J} \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

$J_{i,i+1} = J_{i+1,i} = -\mathcal{J} < 0$



nearest-neighbour coupling favours spin alignment

periodic boundary conditions

→ Let $\hat{T}$ be an operator that translates the system by one lattice spacing. Then

$$\hat{T} \sum_i \vec{S}_i \cdot \vec{S}_{i+1} = \sum_i \vec{S}_{i+1} \cdot \vec{S}_{i+2}\, \hat{T} = \underbrace{\sum_i \vec{S}_i \cdot \vec{S}_{i+1}\, \hat{T}}_{\text{relabelling}}$$

or $[\hat{T}, \hat{H}] = 0$

* We expect the energy eigenstates to also be states of translational symmetry

→ trivially true for the FM ground state

$$\hat{T}|\psi\rangle = \hat{T}|\uparrow_1 \uparrow_2 \cdots \uparrow_N\rangle = |\uparrow_1 \uparrow_2 \cdots \uparrow_N\rangle$$

→ excited states $|\tilde{\psi}\rangle$ and $\hat{T}|\tilde{\psi}\rangle$ represent the same physical state and can thus differ by at most a phase

→ N applications of $\hat{T}$ maps the system onto itself, so

$$\hat{T}^N|\tilde{\psi}\rangle = |\tilde{\psi}\rangle$$

→ eigenvalues of the translation operator are N^{th} roots of unity

$$e^{2\pi i n/N} \quad \text{for } n = 1, 2, \ldots N$$

$$\text{or } n = -\frac{N}{2}+1, \ldots, 0, 1, \ldots, \frac{N}{2}$$

which just defines a set of wave vectors

$$\{q\} = \left\{ \frac{2\pi n}{Na} : n = -\frac{N}{2}+1, \cdots, 0, 1, \cdots \frac{N}{2} \right\} = \left\{ \frac{2\pi n}{L} \right\}$$

lattice spacing a

chain length $L = Na$

with $-\frac{\pi}{a} < q \leq \frac{\pi}{a}$ defining the BZ.

→ A family of single-spin-flip excitations:

$$|\tilde{\psi}_q\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{iqja} S_j^- |\uparrow_1 \uparrow_2 \cdots \uparrow_N\rangle$$

→ Let's treat these as candidate eigenstates and check that

$$\hat{H} |\tilde{\psi}_q\rangle = (E_0 + \hbar\omega_q) |\tilde{\psi}_q\rangle$$

ground state energy

$\hat{H}|\psi\rangle = E_0 |\psi\rangle$

"spin-wave" dispersion

$$\hat{H}|\hat{\psi}_q\rangle = -J\sum_{l=1}^{N}\vec{S}_l\cdot\vec{S}_{l+1}\frac{1}{\sqrt{N}}\sum_j e^{iqja}|\uparrow\cdots\uparrow\downarrow_j\uparrow\cdots\uparrow\rangle$$

$$= -\frac{1}{\sqrt{N}}J\sum_{j,l}e^{iqja}\left\{\frac{1}{2}\left(S_l^+S_{l+1}^- + S_l^-S_{l+1}^+\right) + \underbrace{S_l^zS_{l+1}^z}\right\}|\uparrow\cdots\downarrow_j\cdots\uparrow\rangle$$

gives $+\frac{1}{4}$ for every aligned n.n. pair but $-\frac{1}{4}$ when $l=j$ or $l+1=j$

$\Rightarrow$ diagonal contribution

$$-\frac{J}{4}(N-2) + \frac{J}{4}\cdot 2$$

$$= -\frac{J}{4}N + \frac{J}{2} + \frac{J}{2}$$

$$= E_0 + J$$

EXERCISE:

1. Work out what happens with the off-diagonal part
2. Determine the dispersion relation $\hbar\omega_q$
3. If the spin-wave excitations are bosonic, explain how they are thermally occupied