Phys 726 - Lecture 14

Long-range magnetic order

* We've seem that electronic models on a lattice subject to strong Coulomb repulsion can lead to Heisenberg models in the low-energy regime
  - → charge degrees of freedom are quenched
  - → localized electrons behave as a pure angular momentum
  - → interactions described by an effective model of the spin degrees of freedom
  - → exchange coupling $J_{ij} = J(\vec{R}_i, \vec{R}_j)$ acting between spins labelled i and j at atomic positions $\vec{R}_i$ and $\vec{R}_j$ in the crystal

* Most general Heisenberg model

$$H = \sum_{ij} \vec{S}_i \cdot \overleftrightarrow{J}_{ij} \cdot \vec{S}_j$$

spin-S degree of freedom

$$= \sum_{ij} \left\{ J_{ij}^{\perp} \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right) + J_{ij}^{\parallel} S_i^z S_j^z \right\}$$

accounts for anisotropy in the exchange

→ we'll consider only the spin-rotation-invariant version

→ we'll also assume that the exchange couplings in a crystalline environment are translationally invariant

$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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

* Ground state of the Heisenberg model is difficult to determine

→ complicated quantum many-body problem

→ no "free theory" as there is for noninteracting fermions and bosons

→ some exact results for the linear chain (Bethe-Hulthén) and theorems on the absence of order in 1D and 2D (Mermin-Wagner-Hohenberg)

→ Let's start with a huge simplification: treat $\vec{S}_i$ as <u>classical</u> unit vectors living in a 3D lattice (finite sized, having N sites, a trivial basis, and hence N unit cells)

→ Construct a Fourier transformed variable

$$\vec{S}_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_j \vec{S}_j e^{-i\vec{q}\cdot\vec{R}_j}$$

where $\vec{q}$ is a wave vector in the BZ.

Recall that $\{\vec{R}\} = \{ n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 : n_1, n_2, n_3 \in \mathbb{Z}\}$ describes the Bravais lattice. $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are primitive lattice vectors. The reciprocal lattice

$\{\vec{G}\} = \{ n_1\vec{g}_1 + n_2\vec{g}_2 + n_3\vec{g}_3 : n_1, n_2, n_3 \in \mathbb{Z} \}$

is defined in terms of

$$\vec{g}_1 = \frac{2\pi\,(\vec{a}_2 + \vec{a}_3)}{\vec{a}_1 \cdot (\vec{a}_2 + \vec{a}_3)} \quad \text{and cyclic permutations.}$$

$\vec{q} = q_1\vec{b}_1 + q_2\vec{b}_2 + q_3\vec{b}_3$ are N independent wave vectors that live in the BZ (the Wigner-Seitz cell in reciprocal space)

e.g. $q_i = \dfrac{n_i}{N_i}$ $\quad i = 1,2,3$; $n_i \in \mathbb{Z}$

and $N_i \sim N^{1/3}$ counting the number of unit cells in each direction

→ Further relations

$$\vec{S}_q^* = \left(\frac{1}{\sqrt{N}} \sum_j \vec{S}_j e^{-i\vec{q}\cdot\vec{R}_j}\right)^*$$

$$= \left(\frac{1}{\sqrt{N}} \sum_j \vec{S}_j e^{+i\vec{q}\cdot\vec{R}_j}\right) = \vec{S}_{-q}$$

$$\frac{1}{N} \sum_j e^{i\vec{q}\cdot\vec{R}_j} = \delta_{q,0}$$

$$\frac{1}{N} \sum_q e^{i\vec{q}\cdot(R_j - R_{j'})} = \delta_{jj'}$$

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

→ Plug into the Heisenberg model

$$H = \sum_{jj'} J_{jj'} \vec{S}_j \cdot \vec{S}_{j'}$$

$$= \sum_{jj'} J_{jj'} \frac{1}{\sqrt{N}} \sum_q S_{\vec{q}}\, e^{i\vec{q}\cdot\vec{R}_j} \cdot \frac{1}{\sqrt{N}} \sum_{\vec{q}'} S_{\vec{q}'}\, e^{i\vec{q}'\cdot\vec{R}_{j'}}$$

$$= \frac{1}{N} \sum_{\vec{q}\vec{q}'} \sum_{jj'} e^{i\vec{q}\cdot\vec{R}_j} J_{jj'} e^{i\vec{q}'\cdot\vec{R}_{j'}} \vec{S}_{\vec{q}} \cdot \vec{S}_{\vec{q}'}$$

$$= \frac{1}{N} \sum_{\vec{q}\vec{q}'} \sum_{\vec{R}\vec{R}'} e^{i\vec{q}\cdot\vec{R}} J(\vec{R}-\vec{R}') e^{i\vec{q}'\cdot\vec{R}'} \vec{S}_{\vec{q}} \cdot \vec{S}_{\vec{q}'}$$

$$= \frac{1}{N} \sum_{\vec{q}\vec{q}'} \sum_{\vec{R}\vec{R}'} e^{i\vec{q}\cdot(\vec{R}+\vec{R}')} J(\vec{R}) e^{i\vec{q}'\cdot\vec{R}'} \vec{S}_{\vec{q}} \cdot \vec{S}_{\vec{q}'}$$

$$= \frac{1}{N} \sum_{\vec{q}\vec{q}'} \sum_{R} J(\vec{R}) e^{i\vec{q}\cdot\vec{R}} \underbrace{\left(\sum_{R'} e^{i(\vec{q}+\vec{q}')\cdot\vec{R}'} \right)}_{N\delta_{\vec{q}+\vec{q}',\vec{0}}} \vec{S}_{\vec{q}} \cdot \vec{S}_{\vec{q}'}$$

$$= \sum_{\vec{q}} \Big(\underbrace{\sum_{R} J(\vec{R}) e^{i\vec{q}\cdot\vec{R}}}_{\text{real-valued}} \Big) \underbrace{\vec{S}_{\vec{q}} \cdot \vec{S}_{-\vec{q}}}_{\sim |S_{\vec{q}}|^2}$$

$$J(\vec{q}) = \sum_{R} J(\vec{R}) e^{iq\cdot R} = J(-\vec{q}) = J(\vec{q})^*$$

→ Total energy is equal to a weighted sum over the square of the Fourier component in each mode

→ for the ground state, we expect the spin amplitude to accumulate in the modes where $J(\vec{q})$ is most negative

Energy minimization

* Minimization must be carried out subject to the constraint that each spin is a unit vector

i.e.
$$S_j^2 = \vec{S}_j \cdot \vec{S}_j = \frac{1}{\sqrt{N}} \sum_{q} e^{i\vec{q}\cdot\vec{R}_j} \vec{S}_{\vec{q}} \cdot \frac{1}{\sqrt{N}} \sum_{\vec{q}'} e^{i\vec{q}'\cdot\vec{R}_j} \vec{S}_{\vec{q}'}$$

$$= \frac{1}{N} \sum_{\vec{q}\vec{q}'} e^{i(\vec{q}+\vec{q}')\cdot\vec{R}_j} \vec{S}_{\vec{q}} \cdot \vec{S}_{\vec{q}'}$$

$$= \frac{1}{N} \sum_{\vec{q}\vec{q}'} e^{i(\vec{q}-\vec{q}')\cdot\vec{R}_j} \vec{S}_{\vec{q}} \cdot \vec{S}_{-\vec{q}'}$$

for <u>each</u> of $j = 1, 2, \ldots, N$ (N constraint equations that must be enforced)

→ exact approach is to introduce Lagrange multipliers

$$\tilde{H} = \sum_{\vec{q}} J(q) \vec{S}_q \cdot \vec{S}_{-q} - \sum_{j=1}^{N} \lambda_j \left(\frac{1}{N} \sum_{\vec{q}\vec{q}'} e^{i(\vec{q}-\vec{q}')\cdot\vec{R}_j} \vec{S}_{\vec{q}} \cdot \vec{S}_{-\vec{q}} - 1 \right)$$

and enforce $\frac{\partial \hat{H}}{\partial \vec{S}_{\vec{q}}} = 0$, $\frac{\partial \hat{H}}{\partial \lambda_1} = 0, \ldots, \frac{\partial \hat{H}}{\partial \lambda_N} = 0$

→ Simple alternative is to "relax" the constraint and treat it on average

$S_j^2 = 1$ for each of $j = 1, \ldots, N$ $\Longrightarrow$ $\overline{S}^2 = \frac{1}{N} \sum_j S_j^2 = 1$

i.e. $$N\overline{S}^2 = \sum_j S_j^2 = \sum_j \underbrace{\left(\frac{1}{N} \sum_{\vec{q}\vec{q}'} e^{i(\vec{q}-\vec{q}')\cdot\vec{R}_j} \right)}_{\delta_{\vec{q},\vec{q}'}} \vec{S}_{\vec{q}} \cdot \vec{S}_{-\vec{q}}$$

$$= \sum_q \vec{S}_{\vec{q}} \cdot \vec{S}_{-\vec{q}} = 1$$

There are two possibilities:

(i) $J(\vec{q})$ has its minimum at $\vec{q}=0$ (Ferromagnetism)

or (ii) $J(\vec{q})$ has two co-equal minima at $\vec{q}=+\vec{Q}$ and $\vec{q}=-\vec{Q}$

→ Let's treat the second case.

The solution to $N\bar{S}^2 = \sum_{q} \vec{S}_q \cdot \vec{S}_{-q} = \sum_{q} |S_q|^2$ is the one in which $\vec{S}_{\vec{Q}}$ and $\vec{S}_{-\vec{Q}}$ survive and all other $S_{\vec{q}}$ vanish.

Hence, the onsite constraints look like

$$S_j^2 = \vec{S}_j \cdot \vec{S}_j = \frac{1}{N} \sum_{\vec{q}\vec{q}'} e^{i(\vec{q}-\vec{q}')\cdot\vec{R}_j} \vec{S}_{\vec{q}} \cdot \vec{S}_{-\vec{q}}$$

$$= \frac{1}{N}\left(2\vec{S}_{\vec{Q}} \cdot \vec{S}_{-\vec{Q}} + \vec{S}_{\vec{Q}} \cdot \vec{S}_{\vec{Q}}\, e^{2i\vec{Q}\cdot\vec{R}_j} + \vec{S}_{-\vec{Q}} \cdot \vec{S}_{-\vec{Q}}\, e^{-2i\vec{Q}\cdot\vec{R}_j} \right) = 1$$

(constant, independent of site j)

Remove the j dependent by requiring

$$\vec{S}_{\vec{Q}} \cdot \vec{S}_{\vec{Q}} = \vec{S}_{-\vec{Q}} \cdot \vec{S}_{-\vec{Q}} = 0$$

and $\vec{S}_{\vec{Q}} \cdot \vec{S}_{-\vec{Q}} = |S_{\vec{Q}}|^2 \neq 0$

→ Use a decomposition into real and imaginary parts

$$S_{\vec{Q}} = R_{\vec{Q}} + i I_{\vec{Q}}$$

$$S_{-\vec{Q}} = S_{\vec{Q}}^{*} = R_{\vec{Q}} - i I_{\vec{Q}}$$

to obtain

$$\vec{S}_{\vec{Q}} \cdot \vec{S}_{-\vec{Q}} = R_{\vec{Q}}^2 + I_{\vec{Q}}^2 > 0$$

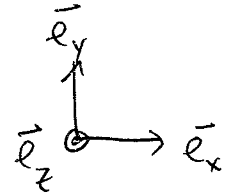
$$\vec{S}_{\vec{Q}} \cdot \vec{S}_{\vec{Q}} = R_{\vec{Q}}^2 - I_{\vec{Q}}^2 + 2i R_{\vec{Q}} \cdot I_{\vec{Q}} = 0$$

→ Satisfied by $\vec{R}_{\vec{Q}} = \vec{I}_{\vec{Q}}$ and $\vec{R}_{\vec{Q}} \cdot \vec{I}_{\vec{Q}} = 0$

in which case

$$S_j^2 = \frac{1}{N} \left(2 \cdot 2 R_{\vec{Q}}^2 + 0 + 0 \right) = 1$$

Then we're free to choose



$$\left.\begin{aligned} \vec{R}_{\vec{Q}} &= \tfrac{1}{2}\sqrt{N}\,\vec{e}_x \\ \vec{I}_{\vec{Q}} &= \tfrac{1}{2}\sqrt{N}\,\vec{e}_y \end{aligned}\right\} \qquad \begin{aligned} &R_{\vec{Q}}^2 = I_{\vec{Q}}^2 = \frac{N}{4} \\ &\vec{R}_{\vec{Q}} \cdot \vec{I}_{\vec{Q}} \sim \vec{e}_x \cdot \vec{e}_y = 0 \end{aligned}$$

So that

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

$$= \frac{1}{\sqrt{N}} \left(S_{\vec{Q}}\, e^{i\vec{Q}\cdot R_j} + S_{-\vec{Q}}\, e^{-i\vec{Q}\cdot R_j} \right)$$

$$= \frac{1}{\sqrt{N}} \cdot \frac{\sqrt{N}}{2} \left((\vec{e}_x + i\vec{e}_y)\, e^{i\vec{Q}\cdot R_j} + (\vec{e}_x - i\vec{e}_y)\, e^{-i\vec{Q}\cdot R_j} \right)$$

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

→ resulting <u>helical</u> spin structure accounts for ferromagnetism ($\vec{Q}=0$), antiferromagetism ($\vec{Q}$ on the edge of the BZ), and other ordering patterns that don't share the periodicity of the lattice