Lecture IV: Quantum Magnetism

▷ References:

D. C. Mattis, *Theory of Magnetism*, Springer

A. Auerbach, *Interacting electrons and quantum magnetism*, Springer

▷ We have seen that residual interactions in magnetic insulators can lead to an exchange Hamiltonian for local moments:

$$\hat{H} = J \sum_{\langle mn \rangle} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n$$

Sign of J depends on material parameters:

Coulomb interaction favours ferromagnetism $J < 0$ (cf. Hund's rule) and superexchange processes favour antiferromagnetism $J > 0$

What are the low-energy collective excitations of the magnetic system?

▷ Classical ground states:

Ferromagnet: all spins aligned along a given direction

Antiferromagnet: (where possible) all neighbouring spins antiparallel

▷ Quantum ground states:

Ferromagnet: as classical

Antiferromagnet: spin exchange interaction (viz. $S_m^+ S_n^-$) $\rightsquigarrow$ zero point fluctuations

▷ *Formation of magnetically ordered state breaks continuous spin rotation symmetry. So should, by Goldstone's theorem, be accompanied by low-energy collective excitations — spin waves. How can we explore excitation spectrum?*

▷ Elementary excitations?

For large spin S, helpful to switch to a representation in which deviations of spin from g.s. are presented as bosons:

$$\begin{array}{ll}
|S^z = S\rangle & |n = 0\rangle \\
|S^z = S-1\rangle & |n = 1\rangle \\
|S^z = S-2\rangle & |n = 2\rangle \\
\cdots & \cdots \\
|S^z = -S\rangle & |n = 2S\rangle
\end{array}$$

i.e. n ("hardcore") bosons per site

Mapping useful when spin excitation involves $n \ll 2S$

▷ Mapping of operators: $\hat{S}^z$, $\hat{S}^{\pm} = \hat{S}^x \pm i\hat{S}^y$?

with $\hbar = 1$, operators obey spin algebra

$$[\hat{S}^+, \hat{S}^-] = 2\hat{S}^z, \qquad [\hat{S}^z, \hat{S}^{\pm}] = \pm\hat{S}^{\pm}$$

cf. bosons: $[a, a^\dagger] = 1, \qquad n = a^\dagger a$

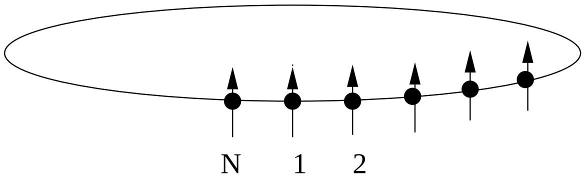
According to mapping, $\hat{S}^z = S - a^\dagger a$; therefore, to first approximation in $S \gg 1$,

$$\hat{S}^- \simeq (2S)^{1/2} a^\dagger, \qquad \hat{S}^+ \simeq (2S)^{1/2} a$$

In fact, exact equivalence provided by Holstein-Primakoff transformation

$$\hat{S}^- = (2S)^{1/2} a^\dagger \left(1 - \frac{a^\dagger a}{2S}\right)^{1/2}, \qquad \hat{S}^+ = (\hat{S}^-)^\dagger, \qquad \hat{S}^z = S - a^\dagger a$$

▷ Ferromagnetic Heisenberg spin S chain



Quantum ground state: all spins aligned along, say, z-direction,

$\hat{S}^z_i|\text{g.s.}\rangle = S|\text{g.s.}\rangle$ for all i

In 'spin-wave' approximation

$$\begin{aligned}
\hat{H} &= -J\sum_{m=1}^{N}\left\{\hat{S}^z_m\hat{S}^z_{m+1} + \frac{1}{2}(\hat{S}^+_m\hat{S}^-_{m+1} + \hat{S}^-_m\hat{S}^+_{m+1})\right\} \\
&= -J\sum_m\left\{S^2 - S(a^\dagger_m a_m - a^\dagger_{m+1}a_{m+1}) + S(a_m a^\dagger_{m+1} + a^\dagger_m a_{m+1}) + O(S^0)\right\} \\
&= -J\sum_m\left\{S^2 - 2S a^\dagger_m a_m + S\left(a^\dagger_m a_{m+1} + \text{h.c.}\right) + O(S^0)\right\}
\end{aligned}$$

p.b.c. $\hat{S}_{m+N} = \hat{S}_m$ and $a_{m+N} = a_m$

Hamiltionian bilinear in bose operators; diagonalised by discrete Fourier transform,

$$a_k = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{ikn} a_n, \qquad a_n = \frac{1}{\sqrt{N}}\sum_k^{\text{B.Z.}} e^{-ikn} a_k, \qquad [a_k, a^\dagger_{k'}] = \delta_{kk'}$$

noting $\sum_n e^{i(k-k')n} = N\delta_{kk'}$

$$\hat{H} = -JNS^2 + \sum_k^{\text{B.Z.}} \omega_k a^\dagger_k a_k + O(S^0), \qquad \omega_k = 2JS(1-\cos k) = 4JS\sin^2(k/2)$$

cf. free-particle spectrum

Higher order corrections $\rightsquigarrow$ spin-wave interactions

How does this compare to the AF spin system?

▷ Antiferromagnet Heisenberg spin S chain

$$\hat{H} = J \sum_m \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_{m+1}$$

Classical g.s. no longer an eigenstate — nevertheless, classical Néel state serves a reference for spin-wave expansion

Convenient to implement canonical transformation in which spins on one sublattice, say B, are rotated through 180^o about the x-axis,

$$\text{i.e.} \qquad \hat{S}^x_B \mapsto \hat{S}^x_B, \qquad \hat{S}^y_B \mapsto -\hat{S}^y_B, \qquad \hat{S}^z_B \mapsto -\hat{S}^z_B$$

$$\hat{H} = -J \sum_m \left[\hat{S}^z_m \hat{S}^z_{m+1} - \frac{1}{2}(\hat{S}^+_m \hat{S}^+_{m+1} + \hat{S}^-_m \hat{S}^-_{m+1}) \right]$$

applying spin wave expansion: $S^-_m \simeq (2S)^{1/2} a^\dagger_m$, etc.

$$\hat{H} = -NJS^2 + JS \sum_m \left[2a^\dagger_m a_m + a_m a_{m+1} + a^\dagger_m a^\dagger_{m+1} \right] + O(S^0)$$

$\rightsquigarrow$ processes that do not conserve particle number!

Fourier representation: $a_m = N^{-1/2} \sum_k e^{-ikm} a_k$, etc.

$$\hat{H} = -NJS(S+1) + JS \sum_k \left(a^\dagger_k \quad a_{-k} \right) \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} a_k \\ a^\dagger_{-k} \end{pmatrix} + O(S^0)$$

where $\gamma_k = \cos k$.

Bogoliubov transformation: (cf. Lorentz boost)

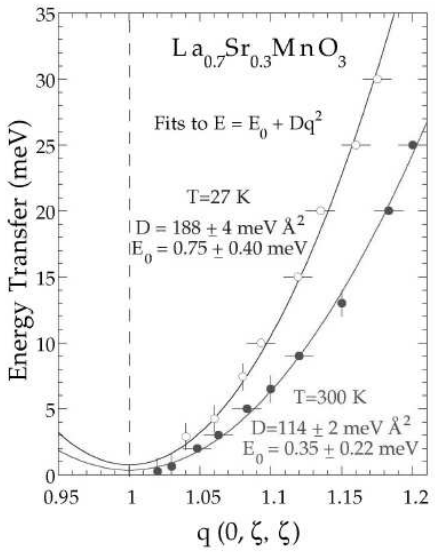
$$\begin{pmatrix} \alpha_k \\ \alpha^\dagger_{-k} \end{pmatrix} = \begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} a_k \\ a^\dagger_{-k} \end{pmatrix}$$

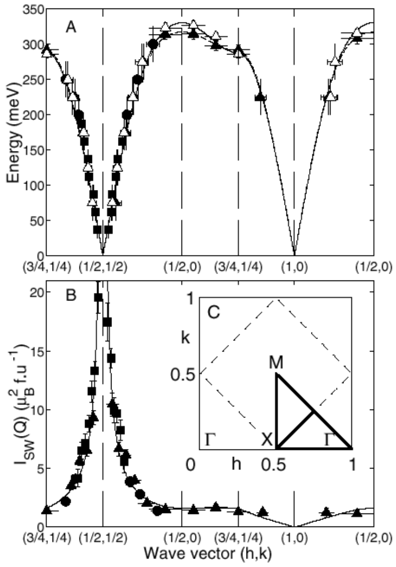
preserves commutation relations, N.B. metric $g = \sigma_z$

off-diagonal terms removed by setting $\cosh(2\theta_k) = (1-\gamma_k^2)^{1/2} = |\sin k|$

$$\hat{H} = -NJS^2 + 2JS \sum_k |\sin k| \left[\alpha^\dagger_k \alpha_k + \frac{1}{2} \right] + O(S^0)$$

$\rightsquigarrow$ linear (i.e. relativistic) excitation spectrum





▷ Magnetisation and sublattice magnetisation

Ferromagnet:

$$\langle \frac{1}{N}\sum_i \hat{S}_i^z \rangle = S - \langle \frac{1}{N}\sum_i a_i^\dagger a_i \rangle = S - \langle \frac{1}{N}\sum_k a_k^\dagger a_k \rangle$$
$$= S - \int \frac{d\mathbf{k}}{(2\pi)^d}\frac{1}{e^{\beta\omega_k}-1} \sim \frac{k_{\rm B}T}{J}\int k^{d-1}dk\frac{1}{k^2}$$

divergent for $T \neq 0$ in $d \leq 2$, i.e. no long-range order

Antiferromagnet:(sublattice magnetisation)

At $T = 0$, do quantum zero-point fluctuations destroy long-range order?

$$\langle g.s.|\frac{1}{N}\sum_i \hat{S}_i^z|\text{g.s.}\rangle = S - \langle \text{g.s.}|\frac{1}{N}\sum_k a_k^\dagger a_k|\text{g.s.}\rangle = S - \frac{1}{N}\sum_k \left[(1-\gamma_k^2)^{-1/2} - 1\right]$$

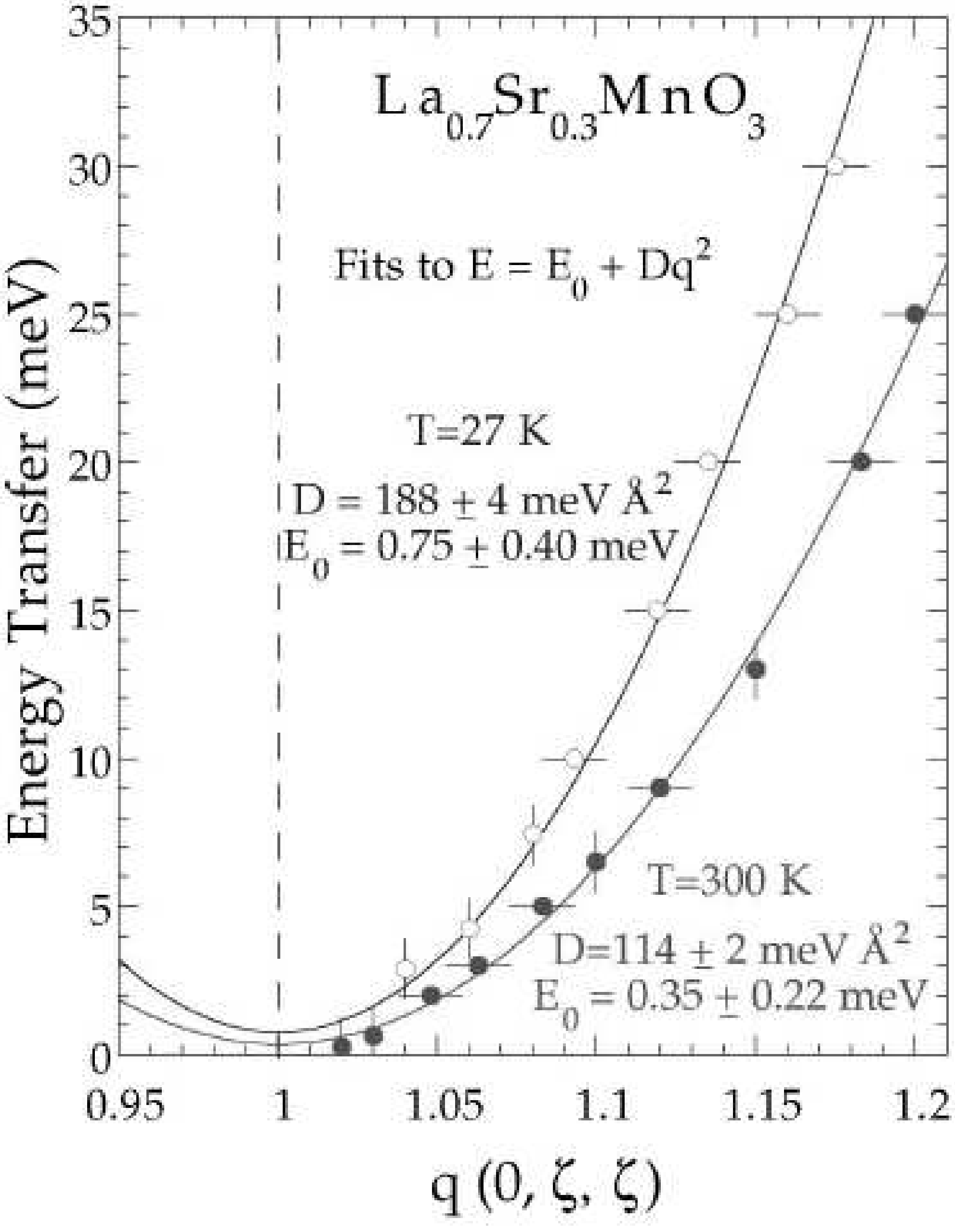
diverges only in $d = 1$!

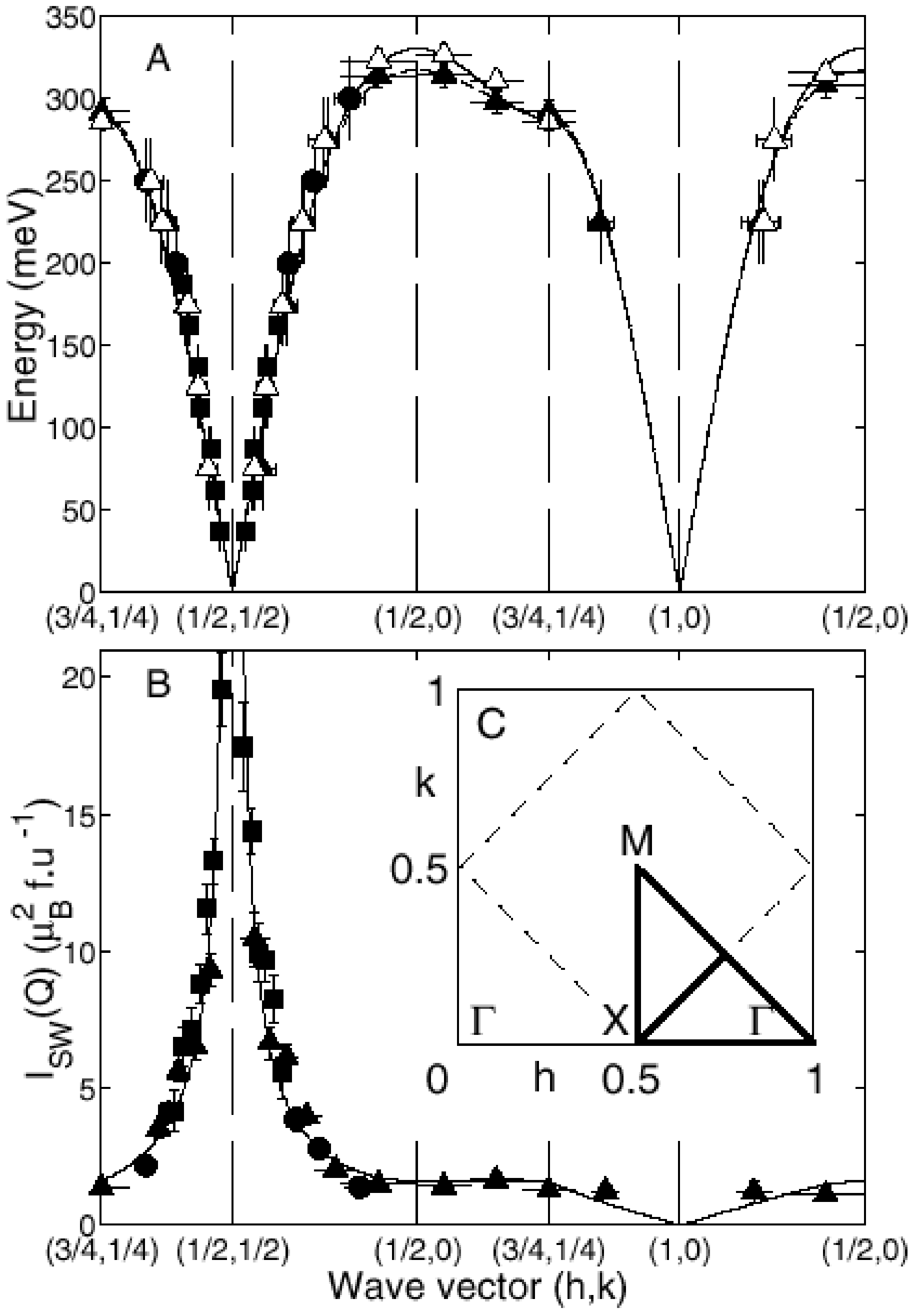
▷ Frustration

AF exchange interaction on bipartite lattice ⇝ Néel ordering
which, in $d > 1$ survives zero-point fluctuations

However, suppose that lattice is not bipartite (or spin interactions long-ranged)
⇝ frustration of Néel order, e.g. triangular lattice

Can zero-point fluctuations lead to spin liquid phase...?


La0.7Sr0.3MnO3
Fits to E = E0 + Dq2
T=27 K
D = 188 ± 4 meV Å2
E0 = 0.75 ± 0.40 meV
T=300 K
D=114 ± 2 meV Å2
E0 = 0.35 ± 0.22 meV
Energy Transfer (meV)
q (0, ζ, ζ)
0
5
10
15
20
25
30
35
0.95
1
1.05
1.1
1.15
1.2



R. Coldea *et al.*, Spin Waves and Electronic Interactions in La_2CuO_4, 2001