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Quantum Theory of Condensed Matter I

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Sheet 5

Antiferromagnetic Heisenberg Model [26P]

A spin S Heisenberg model on an arbitrary periodic D-dimensional lattice (coordination number z) is given by

$$H = J \sum_{\langle mn \rangle} \mathbf{S}_m \cdot \mathbf{S}_n, \qquad J > 0, \quad \mathbf{S}_\alpha^2 \left| m_\alpha \right\rangle = S(S+1) \left| m_\alpha \right\rangle, \tag{1}$$

where $\langle . \rangle$ denotes the summation over nearest neighbors only, and m_α the magnetic quantum number at site α. In a system where $S \gg 1$ holds quantum fluctuations of the spin become less important (proof this statement by considering Heisenberg's uncertainty relation for $|\langle [S_i, S_j] \rangle|$). The ground state under this condition (Néel state, $|\mathrm{Ne}\rangle$) is a staggered spin configuration, i.e., all neighboring spins are antiparallel. However, the true ground state exhibits zero-point fluctuations so that the antiparallel configuration will only serve as a reference state from which we start our analysis.

(a)(6P) First, we try to find the upper and lower bound for the ground state of a system with L sites.

- Calculate the upper bound by evaluating $\langle \mathrm{Ne}|H|\mathrm{Ne}\rangle$. Why can't $|\mathrm{Ne}\rangle$ be the ground state?
- For the lower bound, examine the interaction of $\mathbf{S}_i$ with its z neighbors $\mathbf{S}_m$, $H_i = \mathbf{S}_i \cdot \sum_m \mathbf{S}_m$. Rewrite H_i such that one can maximize $(\sum_m \mathbf{S}_m)^2$ and minimize the remaining term. Why can't this minimum be reached by the true ground state?

(b)(10P) Show that the antiferromagnon spectrum, by neglecting magnon-magnon interaction, is given by

$$\omega(\mathbf{k}) = JzS\sqrt{1-\gamma_{\mathbf{k}}^2}, \text{ with } \gamma_{\mathbf{k}} = \frac{1}{z}\sum_{\boldsymbol{\delta}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}}. \tag{2}$$

To accomplish this you can apply the following steps: Define two kinds of Holstein-Primakoff bosons (explain choice!):
On sublattice A

$$S_{A\mathbf{j}}^+ = \sqrt{2S}\left(1 - \frac{a_{\mathbf{j}}^\dagger a_{\mathbf{j}}}{2S}\right)^{1/2} a_{\mathbf{j}}, \qquad S_{A\mathbf{j}}^- = \sqrt{2S} a_{\mathbf{j}}^\dagger \left(1 - \frac{a_{\mathbf{j}}^\dagger a_{\mathbf{j}}}{2S}\right)^{1/2}, \tag{3}$$

on sublattice B

$$S_{B\mathbf{l}}^- = \sqrt{2S}\left(1 - \frac{b_{\mathbf{l}}^\dagger b_{\mathbf{l}}}{2S}\right)^{1/2} b_{\mathbf{l}}, \qquad S_{B\mathbf{l}}^+ = \sqrt{2S} b_{\mathbf{l}}^\dagger \left(1 - \frac{b_{\mathbf{l}}^\dagger b_{\mathbf{l}}}{2S}\right)^{1/2}, \tag{4}$$

where $[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0$ and $[a_i, a_j^\dagger] = \delta_{ij}$, accordingly for the operators of sublattice B. Thus, our ansatz for each sublattice is equivalent to the case of ferromagnetic coupling.
Express the model Hamiltonian using this transformation and expand it assuming

$$\langle a_{\mathbf{j}}^\dagger a_{\mathbf{j}} \rangle / S \ll 1. \tag{5}$$

Neglect terms which are not bilinear in the magnon operators, i.e., neglect magnon-magnon interactions. Apply a Fourier transformation, $a_{\mathbf{j}} \stackrel{\text{FT}}{\to} c_{\mathbf{k}}, b_{\mathbf{j}} \stackrel{\text{FT}}{\to} d_{\mathbf{k}}$, $(a_{\mathbf{j}}^\dagger \stackrel{\text{FT}}{\to} c_{\mathbf{k}}^\dagger, b_{\mathbf{j}}^\dagger \stackrel{\text{FT}}{\to} d_{\mathbf{k}}^\dagger)$. (Assume the reduced Brillouin zone to contain $L/2$ $\mathbf{k}$-vectors.) Show that this leads to

$$H_0 = JzS \sum_{\mathbf{k}} (\gamma_{\mathbf{k}}(c_{\mathbf{k}} d_{-\mathbf{k}} + d_{\mathbf{k}}^\dagger c_{-\mathbf{k}}^\dagger) + (c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + d_{\mathbf{k}}^\dagger d_{\mathbf{k}})). \tag{6}$$

Rewrite H_0 in a symmetrized form consisting of two parts $(2/(zJS))H_0 = \sum_{\mathbf{k}} H_{\mathbf{k}}^{(1)} + \sum_{\mathbf{k}} H_{\mathbf{k}}^{(2)}$ with $H_{\mathbf{k}}^{(1)}$ containing operators of sublattice A only with $(\mathbf{k})$ index and operators of sublattice B only with $(-\mathbf{k})$ index and accordingly for $H^{(2)}$. Show that the *Bogoliubov transformation*,

$$\alpha_{\mathbf{k}} = u_{\mathbf{k}} c_{\mathbf{k}} - v_{\mathbf{k}} d_{-\mathbf{k}}^\dagger, \qquad \alpha_{\mathbf{k}}^\dagger = u_{\mathbf{k}} c_{\mathbf{k}}^\dagger - v_{\mathbf{k}} d_{-\mathbf{k}} \tag{7}$$

brings $H_{\mathbf{k}}^{(1)}$ to diagonal form. Why is the condition $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$ necessary? Apply a corresponding procedure to $H_{\mathbf{k}}^{(2)}$ with new operators $\beta_{\mathbf{k}}$, $\beta_{\mathbf{k}}^\dagger$ and express, finally, H_0 in this new basis.

(c)(4P) What is the long-wavelength limit of the spectrum? Connect this finding with the Goldstone theorem[1].

(d)(6P) Calculate the staggered magnetization density

$$m = \frac{1}{L} \left\langle \sum_{\mathbf{i}\in A} S_{\mathbf{i}}^z - \sum_{\mathbf{j}\in B} S_{\mathbf{j}}^z \right\rangle . \tag{8}$$

Show that for the one-dimensional Heisenberg model quantum fluctuations destroy the antiferromagnetic long-range order for any finite spin S. *Hint:* Express the sum over $\mathbf{k}$ as an integral. What is the effect in $D = 3$ for a simple cubic lattice?

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[1] When a continuous symmetry is spontaneously broken, a massless boson appears (gapless in relation to the vacuum).