Leo Radzihovsky

PHYS 7450: Advanced Solid State Physics

Homework Set 4

Issued February 26, 2015
Due March 12, 2015

Reading Assignment: My lecture notes 4 on Magnetism in Insulators, X-G Wen textbook, J. Solyom, Solids I, Ch. 14, 15.

1. Curie paramagnetism

   Consider a single quantum spin $\mathbf{J}$ in an external magnetic field B.

   (a) Compute the (i) free energy, F (ii) magnetization, $M = \frac{g_L \mu_B}{\hbar}\langle \mathbf{J} \rangle = -\partial F/\partial B$ (iii) Curie magnetic susceptibility $\partial M/\partial B$ at $B \to 0$.

   (b) Show that $\chi_C(T)$ exhibits the characteristic $1/T$ divergence at low T.

   (c) Show that at low T and high B that M saturates and find the saturation value.

   (d) Using classical statistical mechanics and treating $\mathbf{J}$ as a classical vector with a continuous orientation over 4π steradians, repeat above computation and show that in the large J limit the quantum results reduce to this classical analysis.

2. Classical ferromagnetic Ising model mean-field theory

   Compute the magnetization, M, transition temperature T_c and the susceptibility χ within mean-field analysis, showing that they exhibit a PM-FM phase transition.

3. Heisenberg antiferromagnet (AFM)

   (a) Verify that Holstein-Primakoff representation of spin operators satisfies the spin commutation algebra

   (b) Considering Neél as the approximate AFM ground state for $J < 0$, use Holstein-Primakoff bosonic representation for A and B sublattices of the Neél state to derive Bogoluibov-like Hamiltonian ($\mathbf{r}, \mathbf{r}'$ are nearest neighbors on a cubic lattice)

$$H_{AFM} \approx 2NzJS^2 - 2JS \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \left(a^\dagger_{\mathbf{r}} a_{\mathbf{r}} + b^\dagger_{\mathbf{r}'} b_{\mathbf{r}'} + a_{\mathbf{r}} b_{\mathbf{r}'} + b^\dagger_{\mathbf{r}'} a^\dagger_{\mathbf{r}} \right). \tag{1}$$

(c) Diagonalize this Hamiltonian on a 3d cubic lattice using Bogoluibov transformation

$$\alpha_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} b^\dagger_{-\mathbf{k}}, \beta_{\mathbf{k}} = u_{\mathbf{k}} b_{-\mathbf{k}} - v_{\mathbf{k}} a^\dagger_{\mathbf{k}},$$

obtaining

$$H = E_0 + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} \left[\alpha^\dagger_{\mathbf{k}}\alpha_{\mathbf{k}} + \beta^\dagger_{\mathbf{k}}\beta_{\mathbf{k}}\right],$$

and find:

i. the ground state energy E_0 that includes the mean-field energy of the Neél state and the zero-point quantum fluctuations,

ii. the coherence factors $u_{\mathbf{k}}, v_{\mathbf{k}}$,

iii. the spectrum $\hbar\omega_{\mathbf{k}}$, showing that at small k it is linear in k; what is the speed of magnon sound c_{afm}?

iv. the $T = 0$ expectation value of spin projection $\langle AFM|S^z_i|AFM\rangle$ that is reduced from its fully polarized $\pm S$ value (in the Neél state that is not the ground state), by $\frac{2}{N}\sum_{\mathbf{k}}\langle AFM|a^\dagger_{\mathbf{k}}a_{\mathbf{k}}|AFM\rangle$ (note the analogy with the condensate depletion by interactions in the Bogoluibov theory of weakly interacting superfluid),

v. and generalize the last calculation to finite T.

Hint:

- You will need to introduce a_i and b_i Holstein-Primakoff, with appropriate changes from the standard definition for the B sublattice (e.g., relative minus sign between the A and B sublattice for S^z_i, creation operator replaced by annihilation operator) to account for the Néel state of alternating spin between A and B sublattices, $S^z_i = S(-1)^i$, i.e., $|-S\rangle$, $|+S\rangle$ on the A and B sublattices, respectively.
- Note that in the Neél state the period is doubled as A and B sublattices are not the same. Thus there are $N/2$ unit cells in the crystal with N sites.
- At finite T the population of the Holstein-Primakoff bosons is given by the corresponding Bose factors.

4. Another very useful representation of spin operators is via Schwingers bosons (the so-called spinor representation of spin),

$$z^\dagger = (z^\dagger_1, z^\dagger_2),$$

with

$$\mathbf{S} = \frac{1}{2} z^\dagger \boldsymbol{\sigma} z = \frac{1}{2} z^\dagger_\alpha \boldsymbol{\sigma}_{\alpha\beta} z_\beta, \quad (2)$$

$$S_z = \frac{1}{2}(z^\dagger_1 z_1 - z^\dagger_2 z_2),\ S^+ = z^\dagger_1 z_2,\ S^- = z^\dagger_2 z_1. \quad (3)$$

Use above definitions and Pauli matrix $\boldsymbol{\sigma}$ algebra to show that,

(a) SU(2) transformation $U = e^{i\frac{\theta}{2}\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}}$ of a Schwingers bosons, $z_\alpha \to U_{\alpha\beta} z_\beta$ corresponds to a SO(3) rotation $\mathbf{R}$ of the spin $\mathbf{S} \to \mathbf{RS}$ by angle θ about axis $\hat{n}$.

Hint: It is sufficient to demonstrate above for a specific, simple axis of rotation $\hat{n}$, e.g., $\hat{n} = \hat{z}$, $\hat{n} = \hat{x}$, $\hat{n} = \hat{y}$,

(b) $\mathbf{S}^2 = S(S+1)$, when bosons satisfy the constraint $S = \frac{1}{2} z^\dagger z = \frac{1}{2}(z_1^\dagger z_1 + z_2^\dagger z_2)$

Hint:

It is useful to take advantage of the following identity of Pauli matrices:

$$\boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{\sigma}_{\gamma\beta} = -\delta_{\alpha\beta}\delta_{\gamma\delta} + 2\delta_{\alpha\delta}\delta_{\beta\gamma}$$

(How do you prove this?)

(c) components of $\mathbf{S}$ satisfy spin algebra commutation relations,

$$[S_i^z, S_i^\pm] = \pm S_i^\pm, \ [S_i^+, S_i^-] = 2S_i^z.$$

5. One-dimensional transverse-field quantum Ising model via Jordan-Wigner transformation

Consider a 1d spin-1/2 transverse-field Ising model (TFIM)

$$H_{TFIM} = -J \sum_{\langle i,j \rangle} S_i^x S_j^x - h \sum_i S_i^z,$$

with nearest neighbors exchange J. This model can be solved exactly by mapping it onto 2d classical Ising model or equivalently using Jordan-Wigner (spinless) fermion representation

$$S_i^+ = c_i^\dagger e^{i\pi \sum_{j<i} c_j^\dagger c_j}, \quad S_i^- = e^{-i\pi \sum_{j<i} c_j^\dagger c_j} c_i, \quad S_i^z = c_i^\dagger c_i - \frac{1}{2} = \frac{1}{2}(c_i^\dagger c_i - c_i c_i^\dagger), \quad (4)$$

where $c_i, c_i^\dagger$ satisfy usual fermion anticommutation algebra

$$\{c_i, c_j^\dagger\} = \delta_{ij}, \ \{c_i, c_j\} = 0, \ \{c_i^\dagger, c_j^\dagger\} = 0.$$

This representation allows one to map the TFIM onto free, spinless fermions Hamiltonian when expressed in terms of $c_i, c_i^\dagger$.

(a) By carefully taking into account the Jordan-Wigner "string" (exponential factor above), demonstrate that above spin representation indeed satisfies spin-1/2 algebra on the same site, and with spins simply commuting on distinct sites.

(b) Use above representation to write the TFIM in terms of the fermions, showing that it is indeed given by a quadratic fermionic Bogoluibov-like Hamiltonian,

$$H_{TFIM} = -\frac{1}{4} J \sum_i (c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}) - \frac{1}{2} h \sum_i (c_i^\dagger c_i - c_i c_i^\dagger).$$

(c) Diagonalize this Hamiltonian, such that in terms of true quasi-particles $\gamma_{\mathbf{k}}$, the Hamiltonian is

$$H_{TFIM} = \sum_{\mathbf{k}} E_{\mathbf{k}} \gamma_{\mathbf{k}}^{\dagger} \gamma_{\mathbf{k}} + E_0,$$

and thereby find the spectrum of excitations, E_k, identify its gap (minimium excitation energy), and the ground state energy E_0.

Hints:

- It is crucial to observe that for spin S_i^{α} at site i, the "string" has a number operator that counts the total number of fermions to the left of, but not including site i.
- Think about the (anti)commutation relation between the string operator at j and the fermion operator at i.
- Since the fermion number operator at site i can only be $0, 1$, one can rewrite the string operator acting on these two states in a simple form that is easy to to manipulate.
- Since this is a fermionic Bogoluibov Hamiltonian, to retain fermionic nature (anticommutation relations) of the transformed quasi-particles, the transformation coherence factors must satisfy $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$, or equivalently the transformation U is unitary (rather than the pseudo-unitary for the bosons), written in terms of $\sin \theta_{\mathbf{k}}, \cos \theta_{\mathbf{k}}$; actually it is just orthogonal 2×2 rotation.