PC4902: Elements of QMBT, Pt 2 Problems 5

Key: **E**asy; **M**oderate; **D**ifficult; **O**ptional

1. [EM] For a one-dimensional Heisenberg antiferromagnet of (an even number) N spins with $S \gg 1$, the Hamiltonian may be approximated by the quadratic expression

$$\hat{H} = JS \sum_j \left(\hat{a}_j^\dagger \hat{a}_{j+1}^\dagger + \hat{a}_j \hat{a}_{j+1} + 2\hat{a}_j^\dagger \hat{a}_j \right) - NJS^2,$$

where $\{\hat{a}_j^\dagger, \hat{a}_j\}$ are the Holstein-Primakoff Bose operators and the sum includes the sites of both sub-lattices. In the lecture we considered a Bose operator that creates a running wave; in one dimension this would be

$$\hat{b}_k^\dagger = \frac{1}{\sqrt{N}} \sum_j e^{ikja} \hat{a}_j^\dagger \,,$$

where a is the lattice spacing and $k = 2\pi \times [\text{integer}]/Na$ is the wave vector appropriate to periodic boundary conditions. Show that in terms of these new operators, the Hamiltonian can be written as

$$\hat{H} = JS \sum_k \left(\cos ka \{ \hat{b}_k^\dagger \hat{b}_{-k}^\dagger + \hat{b}_k \hat{b}_{-k} \} + 2\hat{b}_k^\dagger \hat{b}_k \right) - NJS^2.$$

Use this form for the Hamiltonian to obtain the commutators of $\hat{H}$ with $\hat{b}_k^\dagger$ and $\hat{b}_{-k}$:

$$\begin{aligned} \left[\hat{H}, \hat{b}_k^\dagger \right] &= 2JS \left(\hat{b}_k^\dagger + \cos ka \, \hat{b}_{-k} \right) \\ \left[\hat{H}, \hat{b}_{-k} \right] &= -2JS \left(\hat{b}_{-k} + \cos ka \, \hat{b}_k^\dagger \right). \end{aligned}$$

Make the Bogoliubov transformation $\hat{\beta}_k^\dagger = u_k \hat{b}_k^\dagger + v_k \hat{b}_{-k}$ to help solve the equation of motion for the excitation creation operator $\hat{\beta}_k^\dagger$, and so obtain the excitation spectrum

$$\epsilon_k = 2JS \left| \sin ka \right| .$$

[OD] If you have plenty of time, solve for the coefficients u_k and v_k that appear in the Bogoliubov transformation, and hence show that

$$\hat{H} = \sum_k \epsilon_k \left\{ \hat{\beta}_k^\dagger \hat{\beta}_k + \tfrac{1}{2} \right\} - NJS(S+1).$$

You can then integrate the zero-point energy of the magnons to obtain the spin-wave approximation to the ground state energy

$$E_0 = -NJS \left(S + 1 - \frac{2}{\pi} \right).$$

Even for $S = \frac{1}{2}$ (the worst possible case) this is quite a good approximation to the exact result, $E_0 = -NJ\left(\ln 2 - \frac{1}{4} \right)$. The agreement may well be fortuitous here: to find out, we would need to analyse higher-order terms in the expansion in powers of $1/S$.

2. [EM] Show to your own satisfaction that the Jordan–Wigner transformation from spin-$\frac{1}{2}$ operators to fermions,

$$\hat{S}^z_j \to \hat{c}^\dagger_j \hat{c}_j - \tfrac{1}{2}\,, \quad \hat{S}^+_j \to \hat{c}^\dagger_j\, e^{i\pi\hat{\Sigma}_j}, \quad \hat{S}^-_j \to \hat{c}_j\, e^{i\pi\hat{\Sigma}_j},$$

where

$$\hat{\Sigma}_j = \sum_{i<j} \hat{c}^\dagger_i \hat{c}_i\,,$$

correctly reproduces the commutation relations of the spin components. Note that we have written $e^{i\pi}$ instead of the (-1) used in lectures.

In a one-dimensional chain of N spins $S = \frac{1}{2}$ with anisotropic interactions, the Hamiltonian operator takes the form

$$\hat{H} = \sum_j \left\{ J_X \hat{S}^x_j \hat{S}^x_{j+1} + J_Y \hat{S}^y_j \hat{S}^y_{j+1} \right\},$$

where J_X and J_Y are constants. Use the Jordan–Wigner transformation to show that the Hamiltonian may be re-written as

$$\hat{H} = \sum_j \left\{ -t\big(\hat{c}^\dagger_j \hat{c}_{j+1} + \hat{c}^\dagger_{j+1}\hat{c}_j\big) + \Delta\big(\hat{c}^\dagger_j \hat{c}^\dagger_{j+1} + \hat{c}_{j+1}\hat{c}_j\big)\right\}, \qquad (1)$$

where $t = -\frac{1}{4}(J_X + J_Y)$ and $\Delta = \frac{1}{4}(J_X - J_Y)$; it will save some work if you express the Hamiltonian in terms of $\hat{S}^+_j$ and $\hat{S}^-_j$ *before* making the transformation to fermions.

[OD] The fermion excitation spectrum can be found by the equation-of-motion method. The Hamiltonian (1) is similar in structure to the lowest-order Bose approximation to the antiferromagnetic Heisenberg Hamiltonian, which suggests a similar method of solution. We define a creation operator for a running wave,

$$\hat{d}^\dagger_k = \frac{1}{\sqrt{N}} \sum_j e^{ikja}\hat{c}^\dagger_j\,,$$

and evaluate the commutators of $\hat{d}^\dagger_k$ and $\hat{d}_{-k}$ with $\hat{H}$. The equation of motion for an excitation can be solved using Bogoliubov combinations of the form

$$\begin{pmatrix} \hat{f}^\dagger_k \\ \hat{f}_{-k} \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ -v^*_k & u^*_k \end{pmatrix} \begin{pmatrix} \hat{d}^\dagger_k \\ \hat{d}_{-k} \end{pmatrix}, \quad \text{for } k > 0 \text{ only},$$

where $|u_k|^2 + |v_k|^2 = 1$, if the transformation is to preserve the anti-commutation relations. Also note the sign difference (compared with the Bose case) that appears in transformation itself: this is needed to ensure that $\hat{f}^\dagger_k$ and $\hat{f}^\dagger_{-k}$ anticommute.

The spectrum should come out to be

$$\epsilon_k = \tfrac{1}{2}\big(J_X^2 + J_Y^2 + 2J_X J_Y \cos[2ka]\big)^{1/2}.$$

Does the result make sense for the special cases $J_X = J_Y$ (the isotropic XY model) and $J_Y = 0$ (the Ising model)?