Physics 848: Problem Set 3

Due Thursday, October 27 at 11:59 PM

Note: each problem is worth 10 points unless otherwise stated.

1. Consider the *anisotropic spin-1/2 Heisenberg model*, with Hamiltonian given by

$$H = -J_{\parallel}\sum_{\langle ij\rangle} S_{iz}S_{jz} - \frac{1}{2}J_{\perp}\sum_{\langle ij\rangle}\left(S_{i+}S_{j-} + S_{i-}S_{j+}\right). \tag{1}$$

   Here S_{i+}, S_{i-}, and S_{iz} are the raising, lowering, and z-component of the spin operators for a spin-1/2 particle, as defined in class, $J_{\parallel}$ and $J_{\perp}$ are positive interaction energies, and the sums run over distinct pairs of nearest neighbor sites.

   (a). What is the ground state of this system, assuming that $J_{\parallel} > J_{\perp}$?

   Using the same approach as that done in class, obtain the spectrum for spin waves on a simple cubic lattice. Show that when $J_{|} = J_{\perp}$, this spectrum reduces to that of the isotropic spin-1/2 Heisenberg model on a simple cubic lattice (also obtained in class).

2. Consider the *isotropic* spin-1/2 Heisenberg model, for which the Hamiltonian is given by eq. (1) above with $J_{\parallel} = J_{\perp} = J$. It was shown in class that the number of spin wave excitations with wave vector $\mathbf{k}$ is $n_{\mathbf{k}} = 1/[\exp(\epsilon_{\mathbf{k}}/(k_BT) - 1]$, where $\epsilon_{\mathbf{k}} = (J/2)\sum_{\delta}[1 - \cos\mathbf{k}\cdot\delta)]$ is the energy of a spin wave with wave vector $\mathbf{k}$. Here δ is a vector connecting a given spin to one of its nearest neighbors. For example, in a simple cubic lattice $\delta = \pm a\hat{x}$, $\pm a\hat{y}$, and $\pm a\hat{z}$, where a is the lattice constant.

   (a). Show that the total number $\sum_{\mathbf{k}} n_{\mathbf{k}}$ of spin-wave excitations for a simple cubic lattice varies as $T^{3/2}$ at low temperatures T.

   (b). Show that this number diverges, even at low temperatures, for a two-dimensional square lattice. Hence, the spin-1/2 two-dimensional Heisenberg ferromagnet is unstable at any finite temperature.

3. Consider the one-dimensional nearest-neighbor spin-1/2 Heisenberg *antiferromagnet*, given by the Hamiltonian (1) with $J_{\|} = J_{\perp} = -J$ and $J > 0$. Show that the antiferromagnetic state $|\uparrow\downarrow\uparrow\downarrow ....\rangle$ is *not* an eigenstate of this Hamiltonian, and hence cannot be its ground state.

4. **Gibbs-Bogoliubov inequality**. Consider a classical system defined by some Hamiltonian H. The Helmholtz free energy is given by

$$F = -k_B T \ln Z. \tag{2}$$

Here the partition function is

$$Z = \int d\Gamma \exp(-\beta H), \tag{3}$$

where $\beta = 1/k_B T$ and $\int d\Gamma$ denotes an integral over the relevant phase space. (As an example, for the classical fluid considered in class, $\int d\Gamma$ means a 6N-dimensional integral over all the position and momentum coordinates of the system.

Now let $H = H_0 + V$, where H_0 is some unperturbed Hamiltonian, and V is a perturbation. The Gibbs-Bogoliubov inequality states that

$$F \leq F_0 + \langle V \rangle_0. \tag{4}$$

Here F_0 is the free energy of the unperturbed system, and $\langle V \rangle_0$ represents the expectation value of V with respect to a canonical ensemble defined by the Hamiltonian H_0.

To prove this theorem, consider a Hamiltonian $H(\lambda) = H_0 + \lambda V$, and the corresponding free energy $F(\lambda) = \int d\Gamma \exp(-\beta H(\lambda)$. Then the free energy corresponding to the Hamiltonian H is just $F(\lambda = 1)$. Now we can use the mean-value theorem of calculus to write

$$F(\lambda = 1) = F(\lambda = 0) + (1-0)\left(\frac{dF}{d\lambda}\right)_{\lambda=0} + \frac{1}{2}(1-0)^2 \left(\frac{d^2F}{d\lambda^2}\right)_{\lambda=\lambda_0}, \tag{5}$$

where $0 \leq \lambda_0 \leq 1$. This is just the statement that the Taylor series for a function becomes exact if the last term is evaluated at some value of the argument intermediate between 0 and 1.

To carry out the proof of the Gibbs-Bogoliubov inequality, proceed as follows:

(a). Show that

$$\left(\frac{dF}{d\lambda}\right)_{\lambda=0} = \langle V\rangle_0, \tag{6}$$

where

$$\langle V\rangle_0 = \frac{\int d\Gamma V \exp(-\beta H_0)}{\int d\Gamma \exp(-\beta H_0)}. \tag{7}$$

(b). Show that the last term on the right-hand side of eq. (5) is negative for any value of λ_0 between 0 and 1.

Thus, the left-hand side of eq. (5) is less than the sum of the first two terms on the right-hand side, which is equivalent to the Gibbs-Bogoliubov inequality. Q. E. D.