Physics 848: Problem Set 2

Due Tuesday, October 18 at 11:59 PM

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

1. (10 points). **Spin-spin correlation function for the Ising model in 1d.** Consider the ferromagnetic Ising model in 1D with zero applied magnetic field. The Hamiltonian is

$$H = -J \sum_{n=1}^{N-1} S_n S_{n+1}, \tag{1}$$

where S_n takes on the values ± 1, $J > 0$, and we assume FREE boundary conditions, so that S_1 and S_N are not attached to any neighbors.

(a) The partition function for this special case of $B = 0$ can be easily calculated by defining new variables $V_n = S_n S_{n+1}$, with n running from 1 to $N-1$ These V_n's also take on the allowed values ± 1 and are independent of one another. Hence, the partition function can be written $Q_N(T) = 2\sum_{V_1=\pm 1} \dots \sum_{V_{N-1}=\pm 1} \exp(-H/k_B T)$, where $H = -J\sum_{n=1}^{N-1} V_n$. The factor of 2 in front of the partition function allows for two possible orientations of the spin S_1. Since H is now the sum of independent variables, the partition function can be easily calculated. Use this simple transformation to calculate the partition function for a chain of N spins.

(b). Calculate the correlation function $\langle S_p S_q \rangle$, where $q > p$ but $|q - p| \ll N$. (p and q are site indices.) Hint: write $S_p S_q = (S_p S_{p+1})(S_{p+1} S_{p+2}) \dots (S_{q-1} S_q)$ and use the change of variables described in (a). Why is it possible to write $S_p S_q$ in this way?

(c). Show that, for $k_B T \ll J$, $\langle S_p S_q \rangle \sim \exp[-|p-q|/\xi(T)]$, where the correlation length $\xi(T) \sim \exp(2J/k_B T)/2$.

2. (20 points) **Mean-field theory for the XY model:** A mean-field theory for the XY model can be obtained by analogy with that of the

Ising model. To find the mean-field properties, consider the XY model Hamiltonian

$$H = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) - B \sum_i \cos\theta_i, \tag{2}$$

where B is the applied magnetic field, assumed to be in the x direction. i and j are site indices, and the first sum runs overall distinct pairs of nearest neighbor spins. We take the order parameter η to be the magnetization per spin, i. e.

$$\eta = \langle \cos\theta_i \rangle, \tag{3}$$

where $\langle ... \rangle$ denotes an average in the canonical ensemble. Note that because the coefficients J and B are independent of site, η should be independent of i. The exact expression for η in the canonical ensemble is

$$\eta = \frac{1}{Q_N} \int_0^{2\pi} d\theta_1 .... \int_0^{2\pi} d\theta_N \exp(-H/k_B T) \cos\theta_i, \tag{4}$$

where

$$Q_N = \int_0^{2\pi} d\theta_1 .... \int_0^{2\pi} d\theta_N \exp(-H/k_B T). \tag{5}$$

To obtain the critical temperature in the mean-field approximation, we assume that the ith spin is moving in a field equal to the applied field plus the mean-field of its z nearest neighbors. The interaction energy between the ith and jth spin is

$$-J \cos(\theta_i - \theta_j) = -J \left[\cos\theta_i \cos\theta_j + \sin\theta_i \sin\theta_j \right]. \tag{6}$$

We approximate the right-hand side of this equation as

$$-J \left[\cos\theta_i \langle \cos\theta_j \rangle + \sin\theta_i \langle \sin\theta_j \rangle \right] = -J\eta \cos\theta_j, \tag{7}$$

where the last equality comes from the fact that $\langle \sin\theta_j \rangle = 0$. Thus, in the mean-field approximation, η is given by the self-consistent equation

$$\eta = \frac{\int_0^{2\pi} \exp(-H_{MF}/k_B T) \cos\theta_i d\theta_i}{\int_0^{2\pi} \exp(-H_{MF}/k_B T) d\theta_i}, \tag{8}$$

where

$$H_{MF} = -(B + zJ\eta)\cos\theta_i. \qquad (9)$$

(a). Near the transition temperature T_c, η is expected to be small. Expand both the numerator and the denominator in powers of η, and find all terms through η^3 in the numerator and through η^2 in the denominator. Thus, obtain all terms in the ratio through η^3.

(b). Solve the resulting cubic equation for $B = 0$, and show that there exists a T_c such that this equation has real, non-zero solutions for η for $T < T_c$ but the only real solution for $T > T_c$ is $\eta = 0$. Find T_c in terms of z and J. Show that for $T < T_c$, $|\eta| \propto (T - T_c)^\beta$, and find the exponent β.

(c). For $T > T_c$ and $B \neq 0$, find η to first order in B. Show that $(\partial\eta/\partial B)_{B=0} \propto (T - T_c)^{-\gamma}$ and find γ.

Note that this solution fails badly in d = 1 and d = 2 because, as shown in class, the spontaneous magnetization in both cases vanishes for $T > 0$.

3. (20 pts.) **Properties of Spin Operators:** In this problem, you will prove some of the properties of spin operators stated in class, starting with the commutation relations $[S_x, S_y] = iS_z$, $S_y, S_z] = iS_x$, and $[S_z, S_x] = iS_y$. (Note: in this convention, the spin angular momentum operator is $\hbar$ multiplied by the spin operator.) Define the raising and lowering operators $S_+ = S_x + iS_y$ and $S_- = S_x - iS_y$, and the squared total spin angular momentum operator $S^2 = S_x^2 + S_y^2 + S_z^2$. Prove the following:

   (a). $[S_z, S^2] = 0$.

   (b). $[S_z, S_\pm] = \pm S_\pm$.

   (c). $[S_+, S_-] = 2S_z$.

   (d). $S_-S_+ = S^2 - S_z^2 - S_z$ and $S_+S_- = S^2 - S_z^2 + S_z$.

   (e). Since $[S_z, S^2] = 0$, we can find a complete set of states which are simultaneously eigenstate of S^2 and S_z. Denote these eigenstates as $|Sm\rangle$. Let the eigenvalue of S^2 be denoted $S(S+1)$ and that of S_z be denoted m. In this part, you will show that S is an integer or a half-integer, and that $-m \leq S \leq +m$.

(i). Since S^2 is the sum of three positive operators, its eigenvalue must be at least 0. Therefore, $S(S+1) \geq 0$. Use the same argument to show that the $\langle Sm|S_+S_-|Sm\rangle \geq 0$, and therefore that $S(S+1)-m^2-m \geq 0$. Show that this is equivalent to $(S+1/2)^2 \geq (m-1/2)^2$.

(ii) Use a similar argument to show that $S+1/2)^2 \geq (m+1/2)^2$.

(iii). Show that (i) and (ii) imply that $-S \leq m \leq +S$.

(iv). Use the result of part (a) to show that $S_zS_-|Sm\rangle = (m-1)S_-|Sm\rangle$. Thus, we can write $S_-|Sm\rangle = c|S, m-1\rangle$, where $|Sm\rangle$ and $|S, m-1\rangle$ are normalized to unity and c is some constant.

(v). Hence, show from (c) above that $\langle Sm|S_+S_-|Sm\rangle = |c|^2\langle S, m-1|S, m-1\rangle = [S(S+1) - m(m-1)]$.

Thus, if we choose the phase of $|S, m-1\rangle$ so that c is a real, positive constant, then you have shown that $S-|Sm\rangle = \sqrt{S(S+1) - m(m-1)}|S, m-1\rangle$. By a similar argument, it can be shown that $S_+|Sm\rangle = \sqrt{S(S+1_-m(m+1)}|S, m+1\rangle$.

Hence, it appears that if m is an eigenvalue of S_z, then so are $m+1$, $m+2$, etc. But you have already shown that $-S \leq m \leq +S$. Therefore, for some m that does not exceed S, the coefficient $\sqrt{S(S+1) - m(m+1)}$ must vanish, in order for the series of eigenstates to terminate with $m \leq S$. This vanishing clearly occurs for $m = S$. Thus, we must have $m = S$, $S-1$, $S-2$,... A similar argument shows that the lowest m value satisfies $\sqrt{S(S+1) - m(m-1)} = 0$ or $m = -S$. Thus m must also satisfy $m = -S$, $-S+1$, $-S+2$,... Both of these conditions can be satisfied only if S is an integer or a half-integer, in which case $m = -S$, $-S+1$, $-S+2$, ...$S-1$, S, as was to be proved.

Note: the last two paragraphs are purely explanatory, and do not ask you to do anything.