Ex5721: Ising antiferromagnet

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The problem:

Consider Ising model on a 2D lattice with antiferromagnet interaction ($\varepsilon = -\varepsilon_0$). You can regard the lattice as composed of two sublattices A and B, such that $M = \frac{1}{2}(M_A + M_B)$ is the averaged magnetizatin per spin, and $M_s = \frac{1}{2}(M_A - M_B)$ is the staggered magnetization.

(1) Explain the claim: for zero magnetic field ($h = 0$), Ising antiferromagnet is the same as Ising ferromagnet, where M_s is the order parameter.
(2) Given h and ε_0, find the coupled mean-field equations for M_A and M_B. Write the expression for $M_s(T)$ for $T \sim T_c$, based on the familiar solution of the ferromagnetic case.
(3) Find the critical temprature T_c for $h = 0$, and also for small h. Hints: for $h = 0$ use the same procedure of expanding $\arctan(x)$ as in ferromagnetic case, for small h you may use the most extreme simplification that does not give a trivial solution.
(4) Find the critical magnetic field h_c above which the system no longer acts as an antiferromagnet at zero temprature.
(5) Find an expression for the suseceptibility $\chi(T)$, expressed as a function of the staggered magnetization $M_s(T)$.
(6) In the region of $T \sim T_c$ give a linear approximation for $\frac{1}{\chi}$ as a function of the temprature.

The solution:

(1) The standart Ising Hamiltonian which also describes a ferromagnet is

$$\mathcal{H}^F = -\varepsilon \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i. \tag{1}$$

At zero field ($h = 0$) it reduces to

$$\mathcal{H}^F(h = 0) = -\varepsilon \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \tag{2}$$

there is one-to-one correspondence between microstates of equal energy in the zero field ferromagnet and antiferromagnet, these microstates are connected by the operation of reversing the spins on one sublattice, leaving those on the other sublattice unchanged, while changing the sign of the interaction,

$$\mathcal{H}^F(h = 0) = -(-\varepsilon) \sum_{\langle i,j \rangle} \sigma_i (-\sigma_j) = \mathcal{H}^{AF}(h = 0). \tag{3}$$

Thus it follows that in zero field the partition function for the antiferromagnet is equal to that for the ferrromagnet.

(2) Assume that in equilibrium we can regard the spins as quasi-independent, each experiencing an effective field $\bar{h}$, such that the effective Hamiltonian for the spin at site i and sublattice A is

$$\mathcal{H}^{(i)} = \varepsilon \sum_{\text{neighbors}} \langle \sigma_j \rangle \sigma_i - h\sigma_i = (c\varepsilon M_b - h)\sigma_i \equiv \bar{h}\sigma_i. \tag{4}$$

Thus the partition function is

$$Z = \sum_i e^{-\beta \mathcal{H}_i} = 2\cosh(\beta \bar{h}), \tag{5}$$

and the magnetization is

$$M_a = -\frac{\partial F}{\partial h} = -\tanh(\beta \bar{h}). \tag{6}$$

Doing the same procedure for sublattice B we get two coupled equations,

$$M_a = \tanh(\frac{1}{T}(h - T_c M_b)), \tag{7}$$

$$M_b = \tanh(\frac{1}{T}(h - T_c M_a)), \tag{8}$$

where $T_c = c\varepsilon$ and $c = 4$.

Taking the arctan of equations (7) and (8) and remembering that for $T \sim T_c$ at Ising model $M_a \simeq M_b \ll 1$ we can thus use the approximation $\arctan(x) \simeq x + \frac{1}{3}x^3$.

$$T \arctan(M_a) \simeq T(M_a + \frac{1}{3}M_a^3) \simeq TM_a + \frac{T_c}{3}M_a^3 = h - T_c M_b, \tag{9}$$

$$T \arctan(M_b) \simeq T(M_b + \frac{1}{3}M_b^3) \simeq TM_b + \frac{T_c}{3}M_b^3 = h - T_c M_a. \tag{10}$$

Adding and subtracting equations (9) and (10),

$$2h - T_c(M_a + M_b) = T(M_a + M_b) + \frac{T_c}{3}(M_a^3 + M_b^3), \tag{11}$$

$$T_c(M_a - M_b) = T(M_a - M_b) + \frac{T_c}{3}(M_a^3 - M_b^3). \tag{12}$$

Using $M = \frac{1}{2}(M_a + M_b)$ and $M_s = \frac{1}{2}(M_a - M_b)$ and doing some algebra we get

$$(T - T_c)M_s + \frac{1}{3}T_c(3M^2 M_s + M_s^3) = 0, \tag{13}$$

$$(T + T_c)M + \frac{1}{3}T_c(3M_s^2 M + M^3) = h. \tag{14}$$

The solutions are:

$$M_s = 0 \qquad \text{or} \qquad 3M^2 + M_s^2 = 3\left(\frac{T_c - T}{T}\right), \tag{15}$$

$$(2 + M_s^2)M + \frac{1}{3}M^3 = \frac{h}{T_c}. \tag{16}$$

Using equation (15) and the fact that for $T \sim T_c \quad M \ll 1$,

$$M_s = \sqrt{3\frac{T_c - T}{T}}. \tag{17}$$

(3) For $h = 0$: in the absence of magnetic field $M_s = 0$, thus using (17) we can see that $T_c = c\varepsilon$, in addition we have proven that $\mathcal{H}^{AF}(h = 0) = \mathcal{H}^F(h = 0)$.
For small h: from (13) we get

$$M_s(T - T_c(1 - M^2)) + \frac{1}{3}T_c M_s^3 = 0, \tag{18}$$

thus,

$$\tilde{T_c} = T_c(1 - M^2) = c\varepsilon(1 - M^2). \tag{19}$$

Now we will use (14) in order to find M, while $T \sim T_c \quad M_s^2, M^2 \ll 1$,

$$M = \frac{h}{2T_c}, \tag{20}$$

subtituting (20) into (19),

$$\tilde{T_c} = T_c\left(1 - \frac{h^2}{4T_c^2}\right). \tag{21}$$

Thus we can see that if we switch on the magnetic field the critical temprature is shifted to a lower temprature.

(4) Let us examine the energies of the ground state using mean field approximation where the spins are independent of each other, and therefore $\langle\sigma_i\sigma_j\rangle = \langle\sigma_i\rangle\langle\sigma_j\rangle$.
As we have shown in (3) for weak field Ising antiferromagnet is the same as Ising ferromagnet, thus the energy is $E = \langle\mathcal{H}\rangle = -\frac{1}{2}cN\varepsilon\langle\sigma\rangle^2$, where the half stands for double counting and c for the neighbors, for strong field $E = \frac{1}{2}cN\varepsilon\langle\sigma\rangle^2 - hN\langle\sigma\rangle$, at zero temprature $\langle\sigma\rangle = 1$, thus,

$$E(\uparrow\downarrow\uparrow\downarrow) = N(-\frac{1}{2}c\varepsilon), \quad \text{[for weak field]}, \tag{22}$$

$$E(\uparrow\uparrow\uparrow\uparrow) = N(\frac{1}{2}c\varepsilon - h), \quad \text{[for strong field]}. \tag{23}$$

Thus we can calculate the critical magnetic field from demanding $E(\uparrow\uparrow\uparrow\uparrow) = E(\uparrow\downarrow\uparrow\downarrow)$,

$$h_c = c\varepsilon \tag{24}$$

(5) As we defined $M = \frac{1}{2}(M_a + M_b)$, thus,

$$M = \frac{1}{2}\left(\tanh(\beta(h - T_c M_b)) + \tanh(\beta(h - T_c M_a))\right), \tag{25}$$

in order to find the suseceptibility we can expand the magnetization at (25) around $h = 0$ and the coefficient of the linear term will be χ,

$$M \simeq \frac{1}{2}\left(\tanh(-\beta T_c M_b) + \frac{\beta(h - T_c M_b)}{\cosh^2(-\beta T_c M_b)} + \tanh(-\beta T_c M_a) + \frac{\beta(h - T_c M_a)}{\cosh^2(-\beta T_c M_a)}\right), \tag{26}$$

in the absence of magnetic field, i.e. $h = 0 \quad M_a = -M_b$, thus for weak field $M_a \sim -M_b$ in addition $\tanh(x)$ is an odd function and $\cosh(x)$ is an even funaction, thus,

$$M \simeq \frac{1}{2}\left(\frac{2\beta h - \beta T_c(M_a + M_b)}{cosh^2(\beta T_c M_a)}\right) = \left(\frac{\beta h - \beta T_c M}{cosh^2(\beta T_c M_a)}\right) \simeq \left(\frac{\beta h - \beta T_c M}{cosh^2(\beta T_c M_s)}\right), \tag{27}$$

where the last transition was made by using the estimation that for weak field $M_s \simeq \frac{1}{2}2M_a = M_a$. Solving for M,

$$M = \frac{1}{T_c + T\cosh^2(\frac{T_c}{T}M_s(T))}h \equiv \chi h. \tag{28}$$

(6) For $T > T_c \quad M_s = 0$, thus,

$$\frac{1}{\chi} = T_c + T. \tag{29}$$

For $T < T_c$ but close to T_c we can use the approximation $\cosh^2(x) \simeq 1 + x^2$,

$$\frac{1}{\chi} = T_c + T\left(1 + \left(\frac{T_c}{T}\right)^2 3\left(\frac{T_c - T}{T}\right)\right), \tag{30}$$

since $T_c \sim T, \quad \left(\frac{T_c}{T}\right)^2 \to 1$,

$$\frac{1}{\chi} = T_c + T\left(1 + 3\left(\frac{T_c - T}{T}\right)\right) = 4T_c - 2T. \tag{31}$$

Finally,

$\frac{1}{\chi} = \begin{cases} T + T_c, & T > T_c \\ 4T_c - 2T, & T < T_c \end{cases}$

One can see that for $T > T_c$ the susceptibility obeys to Curie-Weiss law but with a negative intercept indicating negative exchange interactions