PHY 540 **Statistical Mechanics** Spring 2007

Homework 08 with Solutions

Problem 8.1. In class, we have discussed the modified mean-field approach to the Ising model, in which the average $s_0 = \langle s \rangle$ plays the role of the order parameter η. Use the results of our analysis to find coefficients a and b in the Landau expansion of free energy, and as many critical exponents as you can.

Solution: The modified mean-field theory reduces the initial Ising's expression for energy

$$E = -J \sum_{\{j,k\}} s_j s_k - h \sum_j s_j$$

to the following approximate form

$$E = -h_{\text{ef}} \sum_j s_j + \Delta E, \qquad \Delta E \equiv -JN \frac{z}{2} s_0^2, \qquad h_{\text{ef}} = h + h_0, \qquad h_0 = Jzs_0, \quad s_0 \equiv \langle s \rangle,$$

which differs from the non-interacting ("0D") case

$$E = -h \sum_j s_j$$

only by the additional term (the "Weiss molecular field" h_0) in the effective total field h_{ef}, and a "constant" (meaning non-thermodynamic) energy shift ΔE which may be directly carried over to all thermodynamic potentials. For the 0D case we have calculated the statistical sum (per unit particle)

$$Z = 2 \cosh \frac{h}{T}.$$

Hence for the modified mean-field theory at $h = 0$ we have

$$Z = 2 \cosh \frac{h_0}{T} = 2 \cosh \frac{Jzs_0}{T}.$$

The statistical sum is sufficient to calculate all thermodynamic properties of the system. In particular, free energy[1] per unit particle is

$$G = -T \ln Z + \frac{\Delta E}{N} = -T \ln \left(2 \cosh \frac{Jzs_0}{T} \right) - \frac{Jz}{2} s_0^2.$$

Expanding this expression into the Taylor series in small s_0 (i.e. at temperature below than, but close to the critical temperature $T_c = Jz$), we have

$$G(s_0) = G(0) + \frac{T_c}{2} \tau s_0^2 + \frac{T_c}{12} s_0^4 + ...,$$

where $G(0) = - T_c \ln 2$ and $\tau \equiv (T_c - T)/T_c << 1$. Identifying s_0 with the order parameter η and comparing the expression for G with the Landau expansion

[1] In the Ising problem, the Gibbs free energy G is equal to the Helmholtz free energy F.

$$G(\eta) = G(0) + a\tau\eta^2 + b\eta^4 + ...,$$

we get

$$a = \frac{T_c}{2}, \quad b = \frac{T_c}{12}.$$

We already know that in the mean-field theory the equilibrium value of the order parameter is

$$\eta = \sqrt{\frac{a}{b}\tau},$$

and the first three critical exponents are

$$\alpha = 0, \quad \beta = 1/2, \quad \gamma = 1,$$

thus satisfying the Essam-Fisher relation $\alpha + 2\beta + \gamma = 2$. In class, we have also used the expression for the Gibbs energy in finite external field

$$G(\eta) \approx G(0) + a\tau\eta^2 + b\eta^4 - h\eta,$$

to calculate the order parameter; in the high field limit:

$$\eta \approx \sqrt[3]{\frac{h}{4b}},$$

giving us one more critical index:

$$\delta = 3,$$

so that the Widom relation $\delta = (\beta + \gamma)/\beta$ is also satisfied. Actually, there is a very similar relation for another "high field exponent",[2] $1/\varepsilon = (\beta + \gamma)/\alpha$, giving

$$\varepsilon = 0.$$

The remaining two exponents related to the correlation radius require somewhat more complex calculations (see LL Sec. 146 and 148), giving finally

$$\nu = \frac{1}{2}, \quad \varsigma = 0.$$

Problem 8.2. In class we have calculated (using the transfer matrix approach) the statistical sum for the 1D Ising model. Using this solution, calculate all major thermodynamic characteristics of the system, including thermodynamic potentials and the specific heat *C*, as functions of temperature *T* and "magnetic field" *h*. Sketch the temperature dependence of the specific heat *C* for various values of the field *h* and give a physical interpretation of the result.

[2] I have not mentioned this relation in class, I will ask our grader to give the full credit for the correct calculation of the four critical exponents listed above (plus coefficients *a* and *b*).

Solution: In class, we have derived the following expression for the statistical sum of this system:

$$Z = \lambda_+^N, \quad \lambda_+ = \exp\{\beta J\}\left\{\cosh(\beta h) + \left[\sinh^2(\beta h) + \exp\{-4\beta J\}\right]^{1/2}\right\}, \quad \beta \equiv \frac{1}{T}.$$

From here we can get free energy per site

$$F = -\frac{T}{N}\ln Z = -T\ln\lambda_+,$$

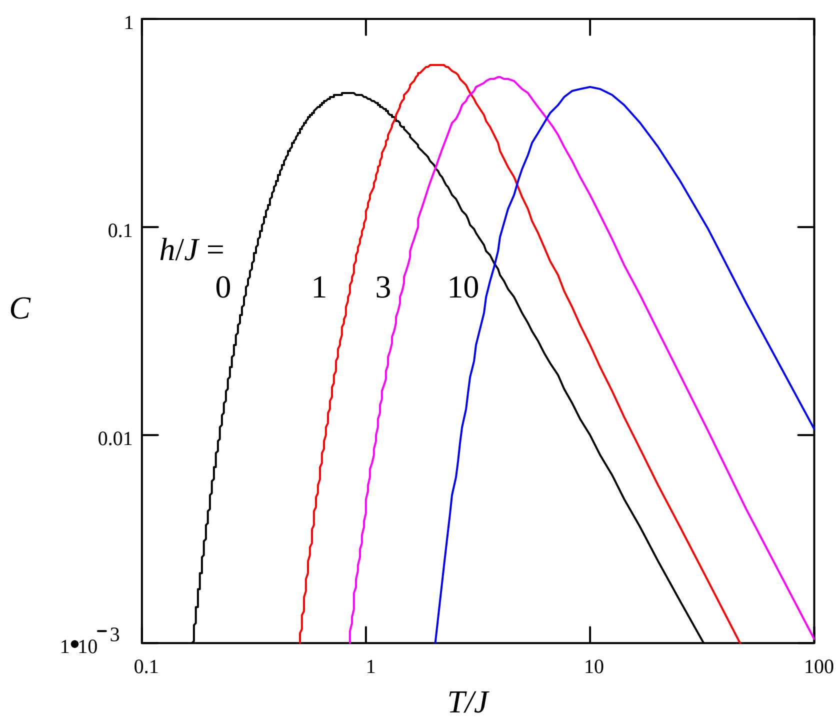
(average) internal energy per site

$$E = \frac{1}{N}\frac{\partial(\ln Z)}{\partial(-\beta)} = -\frac{\partial(\ln\lambda_+)}{\partial\beta},$$

and now use thermodynamic relations to calculate other entropy and specific heat:

$$S = \frac{E-F}{T} = \ln\lambda_+ - \beta\frac{\partial(\ln\lambda_+)}{\partial\beta}, \quad C \equiv \frac{\partial E}{\partial T} = \beta^2\frac{\partial^2(\ln\lambda_+)}{\partial\beta^2}.$$

(Note that since this model does not consider any volume change, we can take $W = E$ and $G = F$, and there is only one specific heat to speak about.) Figure below shows the numerical plot of the specific heat as a function of temperature, for several values of the ratio h/J.



At negligible magnetic field ($\beta h \ll 1$),

$$\lambda_+ = 2\cosh(\beta J), \quad F = -T\ln[2\cosh(\beta J)], \quad E = -J\tanh(\beta J), \quad C = \left(\frac{\beta J}{\cosh(\beta J)}\right)^2 .$$

The last formula shows that the specific heat vanishes both at $T \to 0$ and at $T \to \infty$, with a maximum with $C_{max} \sim 1$ at $T \sim J$ (see the plot above).This behavior is qualitatively similar to that of the usual 2-level system (formally corresponding to the 0D Ising model).

In the opposite limit when the energy h characterizing the external field is much higher than the energy scale T of thermal fluctuations, the above general formulas are reduced to

$$\lambda_+ \approx \exp\{\beta(J+h)\}, \quad F \approx E \approx -(J+h), \quad C \to 0.$$

These formulas describe a completely "polarized" system, with all spins are aligned by strong applied field. Such strong polarization effectively makes thermal excitations impossible; as a result, the specific heat tends to zero for any temperature. However, the plot above shows that such suppression of specific heat with the growth of the field is very gradual.