## Solutions to the problems in Chapter 24

24.4 Mean field theory

The antiferromagnetic two-dimensional Ising model on a square lattice. In this lattice, the number of nearest neighbours is $z = 4$. The Hamiltonian is supposed to be

$$\mathcal{H} = -\sum_{\langle \vec{R}\vec{R}'\rangle} J\,\sigma_{\vec{R}}\sigma_{\vec{R}'} - \sum_{\vec{R}} H\mu_{\mathrm{B}}\sigma_{\vec{R}} = -\frac{1}{2}\sum_{\vec{R}\vec{R}'} J\,\sigma_{\vec{R}}\sigma_{\vec{R}'} - \sum_{\vec{R}} H\mu_{\mathrm{B}}\sigma_{\vec{R}}, \qquad J < 0 \quad (1)$$

where $\mathcal{H} = \mathcal{E}$ in the usual representation of $\sigma_{\vec{R}} = \pm 1$. Because J is negative, the ground state is not the ferro- but the antiferromagnet. In the sums, $\vec{R}$ and $\vec{R}'$ are nearest neighbours, and the antiferromagnetic ground state is assumed to be determined by the mean field values

$$(\langle\sigma_{\vec{R}}\rangle, \langle\sigma_{\vec{R}'}\rangle) = \begin{cases} (\sigma_\uparrow, \sigma_\downarrow), & \vec{R} \subset \text{sublattice A} \\ (\sigma_\downarrow, \sigma_\uparrow), & \vec{R} \subset \text{sublattice B} \end{cases} \qquad (2)$$
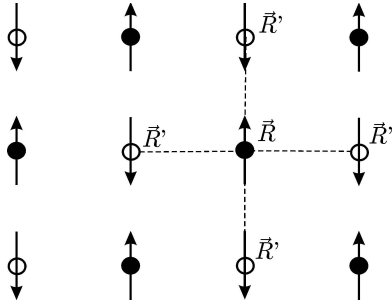
The two sublattices of the square lattice: A shown by filled and B by open circles. The figure shows the case, where the site at $\vec{R}$ belongs to the A-sublattice, in which case $\langle\sigma_{\vec{R}}\rangle = \sigma_\uparrow$. Its four nearest neighbours at positions $\vec{R}'$, then all belong to the B sublattice and $\langle\sigma_{\vec{R}'}\rangle = \sigma_\downarrow$.

(a) In the mean-field (MF) approximation we get, when inserting (2) in (1),

$$\mathcal{E} \stackrel{\mathrm{MF}}{=} -\frac{1}{2}\sum_{\vec{R}\vec{R}'} J\left(\sigma_{\vec{R}}\langle\sigma_{\vec{R}'}\rangle + \sigma_{\vec{R}'}\langle\sigma_{\vec{R}}\rangle - \langle\sigma_{\vec{R}}\rangle\langle\sigma_{\vec{R}'}\rangle\right) - H\mu_{\mathrm{B}}\sum_{\vec{R}} \sigma_{\vec{R}}$$

$$= -\sum_{\vec{R}\vec{R}'} J\,\langle\sigma_{\vec{R}'}\rangle\sigma_{\vec{R}} - H\mu_{\mathrm{B}}\sum_{\vec{R}}\sigma_{\vec{R}} + \tfrac{1}{2}NzJ\sigma_\uparrow\sigma_\downarrow \qquad (3)$$

$$= -\sum_{\vec{R}\subset A}^{N/2}\left(zJ\sigma_\downarrow + \mu_{\mathrm{B}}H\right)\sigma_{\vec{R}} - \sum_{\vec{R}\subset B}^{N/2}\left(zJ\sigma_\uparrow + \mu_{\mathrm{B}}H\right)\sigma_{\vec{R}} + \tfrac{1}{2}NzJ\sigma_\uparrow\sigma_\downarrow$$

Because of the MF-approximation, the total energy $\mathcal{E} = \sum_{\vec{R}}\mathcal{E}_{\vec{R}}$ is the sum of the individual contributions of each site, and the partition function of the total system

$$Z = \sum_{\text{all }\mathcal{E}} e^{-\beta\mathcal{E}} = \prod_{\vec{R}}\left(\sum_{\text{all }\mathcal{E}_{\vec{R}}} e^{-\beta\mathcal{E}_{\vec{R}}}\right) = \prod_{\vec{R}} Z_{\vec{R}} \qquad (4)$$

is reduced so to become the product of the partition functions $Z_{\vec{R}}$ for the individual sites, see for instance (6.40). For the sites, where $\vec{R}$ belongs to the sublattice A ($\uparrow$), we get, when omitting the constant energy term $\tfrac{1}{2}zJ\sigma_\uparrow\sigma_\downarrow$,

$$Z_\uparrow = \sum_{\sigma=\pm 1} e^{-\beta[-(zJ\sigma_\downarrow + \mu_{\mathrm{B}}H)\sigma]} = \sum_{\sigma=\pm 1} e^{\beta(zJ\sigma_\downarrow + \mu_{\mathrm{B}}H)\sigma} = 2\cosh\left[zJ\sigma_\downarrow + \mu_{\mathrm{B}}H\right] \quad (5)$$

which implies that

$$\langle \sigma_{\vec{R}} \rangle = \sigma_\uparrow = \frac{1}{Z_\uparrow} \sum_{\sigma=\pm 1} \sigma \, e^{\beta(zJ\sigma_\downarrow + \mu_B H)\sigma} = \tanh\left[\beta(zJ\sigma_\downarrow + \mu_B H)\right] \qquad (6)$$

Notice that the omission of a constant energy term does not affect the calculation of a thermal expectation value. $Z_\downarrow$ and $\sigma_\downarrow$ are determined equivalently

$$Z_\downarrow = 2\cosh\left[zJ\sigma_\uparrow + \mu_B H\right], \qquad \sigma_\downarrow = \tanh\left[\beta(zJ\sigma_\uparrow + \mu_B H)\right] \qquad (7)$$

and the (total) free energy is

$$\mathcal{F} = -\frac{N}{2}k_B T \left(\ln Z_\uparrow + \ln Z_\downarrow\right) + N\tfrac{1}{2}zJ\sigma_\uparrow \sigma_\downarrow =$$
$$-\frac{N}{2}k_B T \left\{\ln\left[2\cosh\left(zJ\sigma_\downarrow + \mu_B H\right)\right] + \ln\left[2\cosh\left(zJ\sigma_\uparrow + \mu_B H\right)\right]\right\} + \frac{N}{2}zJ\sigma_\uparrow \sigma_\downarrow$$
$$(8)$$

The constant energy term neglecting in the partition functions adds to $\mathcal{F}$.

(b) The self-consistent equations determining $\sigma_\uparrow$ and $\sigma_\downarrow$ are derived above.

(c) In the paramagnetic phase, $T > T_N$, $\sigma_\uparrow$ and $\sigma_\downarrow$ vanish in the limit $H \to 0$. Expanding tanh to leading order, $\tanh x \simeq x$, we get from (6) and (7)

$$\left.\begin{array}{l} \sigma_\uparrow = \tanh\left[\beta(zJ\sigma_\downarrow + \mu_B H)\right] \simeq \beta(zJ\sigma_\downarrow + \mu_B H) \\[2mm] \sigma_\downarrow = \tanh\left[\beta(zJ\sigma_\uparrow + \mu_B H)\right] \simeq \beta(zJ\sigma_\uparrow + \mu_B H) \end{array}\right\} \quad \sigma_\uparrow = \sigma_\downarrow = \frac{\mu_B H \beta}{1 - zJ\beta} \qquad (9)$$

The expectation values $\sigma_\uparrow$ and $\sigma_\downarrow$ are equal and are proportional to the field. The magnetization is $M = (N/V)\mu_B(\sigma_\uparrow + \sigma_\downarrow)/2$ and the susceptibility is defined as $\chi = M/H$ in the limit of zero field, and we find

$$\chi = \frac{N}{V}\frac{\mu_B^2}{k_B T - zJ} \equiv \frac{N}{V}\frac{\mu_B^2}{k_B(T - \Theta)}, \qquad \Theta = -\frac{z|J|}{k_B} = -T_N \qquad (10)$$

The paramagnetic Curie, or Curie–Weiss, temperature Θ is defined by (24.41), $\chi \propto (T - \Theta)^{-1}$. In the present system Θ is negative (J is negative), and $|\Theta|$ is, as we shall see, the same as the "Néel temperature", T_N, below which the system is antiferromagnetically ordered at zero field.

(d) The Néel temperature is the temperature below which the self-consistent equations for $\sigma_\uparrow$ and $\sigma_\downarrow$ have a non-zero solution at zero field. The solution is obtained by assuming $\sigma_\uparrow = -\sigma_\downarrow$, and $H = 0$, in which case we get

$$\sigma_\uparrow = \tanh\left[\beta(-z|J|)(-\sigma_\uparrow)\right] = \tanh(\beta z|J|\sigma_\uparrow) = \tanh(\alpha\sigma_\uparrow) \qquad (11)$$

This equation is the same as considered in the case of the ferromagnet, (24.56), and it has a non-zero solution, when the coefficient $\alpha \geq 1$. The Néel temperature T_N is the temperature at which $\alpha = z|J|\beta = 1$, or $T_N = z|J|/k_B$. The paramagnetic susceptibility, which diverges at the transition, is obtained by applying a field with the same symmetry as the ordered phase. The application of a "staggered" field, where $H_{\vec{R}} = +H$ at the A sites and $-H$ at the B sites determines straightforwardly (using $\sigma_\uparrow = -\sigma_\downarrow$) the staggered susceptibility to be

$$\chi_{\text{stag}} = \frac{N}{V}\frac{\mu_B(\sigma_\uparrow - \sigma_\downarrow)}{2H} = \frac{N}{V}\frac{\mu_B^2}{k_B(T - T_N)} \qquad (12)$$

which diverges at T_N.

(e) Spin-flip transition: In the ordered phase, the application of a small field along z, in the "up" direction, does not change $\sigma_\uparrow = 1$ or $\sigma_\downarrow = -1$. However, if the field becomes sufficiently large, the spins antiparallel to the field are going to flip so to become parallel to the field. This first-order spin-flip transition happens, when the Zeeman-energy gain is able to compensate for the loss of exchange energy.

Introducing dimensionless quantities, then

$$\sigma_\uparrow = \tanh\left(\frac{-\sigma_\downarrow + h}{t}\right), \quad \sigma_\downarrow = \tanh\left(\frac{-\sigma_\uparrow + h}{t}\right), \quad h = \frac{\mu_B H}{z|J|}, \quad t = \frac{T}{T_N} \quad (13)$$

In the limit of $t \to 0$, then the introduction of $\sigma_\uparrow = 1$ in the second equation implies $\sigma_\downarrow = -1$ if $1 > h > 0$ and $\sigma_\downarrow = 1$ if $h > 1$. The first equation then predicts $\sigma_\uparrow = 1$ in both cases, hence assuring that this is the self-consistent solution. Using $\ln[2\cosh x] = \ln[e^x + e^{-x}] \to \ln e^{|x|} = |x|$ for $x \to \pm\infty$, the free energy is found to be determined by

$$f = \frac{\mathcal{F}}{Nz|J|} = -\frac{t}{2}\left\{\ln\left[2\cosh\left(\frac{-\sigma_\downarrow + h}{t}\right)\right] + \ln\left[2\cosh\left(\frac{-\sigma_\uparrow + h}{t}\right)\right]\right\} - \frac{1}{2}\sigma_\uparrow\sigma_\downarrow$$

$$\to -\frac{t}{2}\left\{\frac{-\sigma_\downarrow + h}{t} + \left|\frac{-\sigma_\uparrow + h}{t}\right|\right\} - \frac{1}{2}\sigma_\uparrow\sigma_\downarrow = \begin{cases} -\frac{1}{2}, & 0 < h < 1 \\ -h + \frac{1}{2}, & h > 1 \end{cases}$$

$$(14)$$

Hence, the free energies of the antiferromagnetic phase $f = -1/2$ and of the spin-flipped phase $f = -h + 1/2$ are equal at the transition at $h = 1$. At a finite temperature the spin-flip transition is smeared out due to thermal effects. The figure below shows the numerical calculated "magnetization", $(\sigma_\uparrow + \sigma_\downarrow)/2$, as a function of the field h at various values of temperature t.
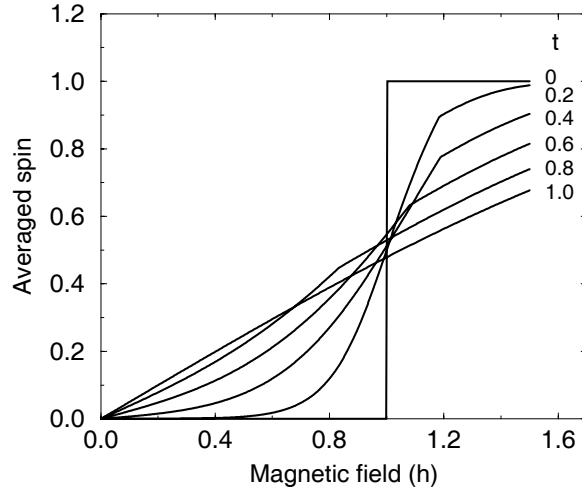
24.6 Superlattices

Model of Cu_3Au – In the fcc lattice, the sites in the centers of the six faces are named A_s and the 8 corners are named B_s as indicated on the figure by, respectively, black and white spheres. There is $8/8 = 1$ B_s site and $6/2 = 3$ A_s sites per unit cell. The distance between nearest neighbours is $a/\sqrt{2}$, and the coordination number is $z = 12$. The kind of nearest neighbours of the two kind of sites are

A_s-site: 8 A_s sites and 4 B_s sites.

B_s-site: 12 A_s sites.
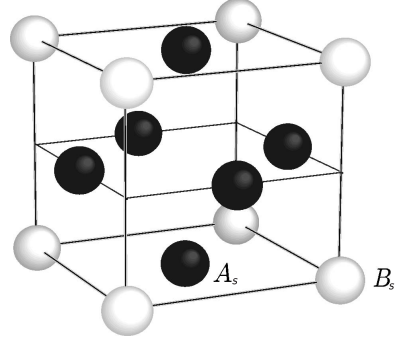
The correct solution to the equations (24.62) and (24.63) is not (24.64), but

$$f(\sigma_{\vec{R}}, \sigma_{\vec{R}'}) = \frac{\epsilon_{BB} - \epsilon_{AA}}{4}(\sigma_{\vec{R}} + \sigma_{\vec{R}'}) - \frac{2\epsilon_{AB} - \epsilon_{AA} - \epsilon_{BB}}{4}\sigma_{\vec{R}}\sigma_{\vec{R}'} \qquad (24.64')$$

when leaving out the constant term $C_1 = (2\epsilon_{AB} + \epsilon_{AA} + \epsilon_{BB})/4$. This modification affects the definition of the effective parameters in (24.67), which should read

$$\mu_B H = \mu - \frac{\epsilon_{BB} - \epsilon_{AA}}{2}\, z\,, \qquad J = \frac{2\epsilon_{AB} - \epsilon_{AA} - \epsilon_{BB}}{4} \qquad (24.67')$$

(a) In the present system we have a 3:1 mixture of A and B atoms. The effective Hamiltonian equals the energy minus the chemical potential times the difference between the numbers of B and A atoms, is (leaving out the constant contribution)

$$\mathcal{H} = \mathcal{E} - \mu \sum_{\vec{R}} \sigma_{\vec{R}} = -J \sum_{\langle \vec{R}\vec{R}' \rangle} \sigma_{\vec{R}}\sigma_{\vec{R}'} - \mu_B H \sum_{\vec{R}} \sigma_{\vec{R}} \qquad (1)$$

We are going to use the same choice as Marder, that $\sigma_{\vec{R}} = 1$ or -1 signifies a site occupied by, respectively, a B or an A atom. With this choice, the effective energy parameters are those given by $(24.67')$ above. In the mean-field approximation

$$\mathcal{H} \overset{\text{MF}}{=} -J \sum_{\langle \vec{R}\vec{R}' \rangle} \left(\sigma_{\vec{R}}\langle\sigma_{\vec{R}'}\rangle + \sigma_{\vec{R}'}\langle\sigma_{\vec{R}}\rangle - \langle\sigma_{\vec{R}}\rangle\langle\sigma_{\vec{R}'}\rangle \right) - \mu_B H \sum_{\vec{R}} \sigma_{\vec{R}} = \sum_{\vec{R}} \mathcal{H}_{\vec{R}} \qquad (2)$$

where

$$\sum_{\langle \vec{R}\vec{R}' \rangle} \left(\sigma_{\vec{R}}\langle\sigma_{\vec{R}'}\rangle + \sigma_{\vec{R}'}\langle\sigma_{\vec{R}}\rangle \right) = \frac{1}{2}\sum_{\vec{R}\vec{R}'} \left(\sigma_{\vec{R}}\langle\sigma_{\vec{R}'}\rangle + \sigma_{\vec{R}'}\langle\sigma_{\vec{R}}\rangle \right) = \sum_{\vec{R}} \sigma_{\vec{R}} \left(\sum_{\vec{R}'\,(\text{nn})} \langle\sigma_{\vec{R}'}\rangle \right)$$

$$= \sum_{\vec{B}_s}^{N} \sigma_{\vec{B}_s}\left(12\,\langle\sigma_{\vec{A}_s}\rangle \right) + \sum_{\vec{A}_s}^{3N} \sigma_{\vec{A}_s}\left(8\,\langle\sigma_{\vec{A}_s}\rangle + 4\,\langle\sigma_{\vec{B}_s}\rangle \right)$$

$$\tag{3}$$

Here N is the number of unit cells (or B_s sites), and $\sigma_{\vec{R}} = \sigma_{\vec{A}_s}$ $(\sigma_{\vec{B}_s})$, if $\vec{R} = \vec{A}_s$ $(\vec{B}_s)$ is the position of an A_s (B_s) site. The (grand) partition function of the total system is the product of the individual partition functions for each site, because $\mathcal{H} = \sum_{\vec{R}} \mathcal{H}_{\vec{R}}$, and in the case of an A_s site (omitting the constant energy term)

$$Z_{A_s} = \sum_{\sigma=\pm 1} e^{\beta\left[J\left(8\langle\sigma_{\vec{A}_s}\rangle + 4\langle\sigma_{\vec{B}_s}\rangle\right) + \mu_B H\right]\sigma} \qquad (4)$$

implying that

$$\langle \sigma_{\vec{A}_s} \rangle = \frac{1}{Z_{A_s}} \sum_{\sigma=\pm 1} \sigma \, e^{\beta\left[J\left(8\langle\sigma_{\vec{A}_s}\rangle+4\langle\sigma_{\vec{B}_s}\rangle\right)+\mu_{\mathrm{B}}H\right]\sigma}$$

$$= \tanh\left\{\beta\left[8\,J\,\langle\sigma_{\vec{A}_s}\rangle + 4\,J\,\langle\sigma_{\vec{B}_s}\rangle + \mu_{\mathrm{B}}H\right]\right\} \tag{5}$$

and equivalently

$$\langle\sigma_{\vec{B}_s}\rangle = \tanh\left\{\beta\left[12\,J\,\langle\sigma_{\vec{A}_s}\rangle + \mu_{\mathrm{B}}H\right]\right\} \tag{6}$$

(b) $\sigma_{\vec{R}} = +1$ for the B atoms and the number of these atoms is equal the number of unit cells N, whereas the number of A atoms is $3N$. These conditions imply

$$\sum_{\vec{R}} \sigma_{\vec{R}} = \begin{cases} N - 3N = -2N \\[2mm] \sum_{\vec{B}_s}^{N} \sigma_{\vec{B}_s} + \sum_{\vec{A}_s}^{3N} \sigma_{\vec{A}_s} = N\langle\sigma_{\vec{B}_s}\rangle + 3N\langle\sigma_{\vec{A}_s}\rangle \end{cases} \Rightarrow \quad \langle\sigma_{\vec{B}_s}\rangle = -2 - 3\langle\sigma_{\vec{A}_s}\rangle \tag{7}$$

(c) The chemical potential, or effectively $\mu_{\mathrm{B}}H$, has to be adjusted so that the two equations (5) and (6) are in accordance with the relation $\langle\sigma_{\vec{B}_s}\rangle = -2 - 3\langle\sigma_{\vec{A}_s}\rangle$. The effective Zeeman term may be eliminated:

$$\tanh^{-1}\langle\sigma_{\vec{A}_s}\rangle - \tanh^{-1}\langle\sigma_{\vec{B}_s}\rangle = \beta\left[8\,J\,\langle\sigma_{\vec{A}_s}\rangle + 4\,J\,\langle\sigma_{\vec{B}_s}\rangle + \mu_{\mathrm{B}}H\right]$$

$$-\beta\left[12\,J\,\langle\sigma_{\vec{A}_s}\rangle + \mu_{\mathrm{B}}H\right] = 4\beta J\left(\langle\sigma_{\vec{B}_s}\rangle - \langle\sigma_{\vec{A}_s}\rangle\right) = -8\beta J\left(1 + 2\langle\sigma_{\vec{A}_s}\rangle\right) \tag{8}$$

Introducing an effective order parameter Q and $J = -|J|$, we finally get

$$f(Q) \equiv \tanh^{-1}\left(\frac{Q+1}{2}\right) + \tanh^{-1}\left(\frac{3Q-1}{2}\right) = 8\beta|J|Q, \quad Q = -1 - 2\langle\sigma_{\vec{A}_s}\rangle \tag{9}$$

In the disordered phase both the A_s and the B_s sites are occupied by an A atom with the probability $\frac{3}{4}$ or $\langle\sigma_{\vec{A}_s}\rangle = \langle\sigma_{\vec{B}_s}\rangle = (-1)\frac{3}{4} + (+1)\frac{1}{4} = -\frac{1}{2}$. This result is in accordance with (7) and $Q = -1 - 2\langle\sigma_{\vec{A}_s}\rangle = 0$. In the completely ordered phase at zero temperature, all A (B) atoms are placed on the A_s (B_s) sites implying that $\langle\sigma_{\vec{A}_s}\rangle = -1$ and $\langle\sigma_{\vec{B}_s}\rangle = 1$ and hence $Q = 1$.

Order parameter (Q)

The numerical solution of (9) is discussed in a Mathematica program. The system orders at a first-order transition, when $f(Q) = Q\,f'(Q)$ [the line $y = \alpha Q$ with $\alpha = f'(Q_c)$ is parallel to the tangent of $f(Q)$ at $Q = Q_c$, and this line just touches $f(Q)$ at $Q = Q_c$, when $f(Q_c) = \alpha Q_c$. This then becomes a solution to (9) if choosing $\alpha = 8\beta|J|$]. The solution is $Q = Q_c = 0.3455$ and defining the effective temperature scale $t = (8\beta|J|)^{-1}$ then Q jumps from zero to Q_c at the temperature $t = t_c = 1/f'(Q_c) = 0.4143$. The calculated variation of Q as a function of t is shown in the figure.

Temperature (t)