Solutions exam st2 Fall/Winter 2012

1. Virial expansion

(a) The expansion of $1/(1-D\lambda)$ is

$$\frac{1}{(1-D\lambda)} = 1 + D\lambda + D^2\lambda^2 + \ldots \tag{1}$$

therefore

$$\frac{\lambda}{(1-D\lambda)} = \lambda + D\lambda^2 + D^2\lambda^3 + \ldots \tag{2}$$

(b) We have

$$\begin{aligned} B_2(T) &= -\int_0^D (-1)\,\mathrm{d}r - \int_D^\infty 0\,\mathrm{d}r && (3)\\ &= D - 0 && (4)\\ &= D. && (5)\end{aligned}$$

(c) $B_2(T)$ is obviously equal to the coefficient of λ^2 of (a), i.e. D .

(d) In this case we have to study the integral

$$\begin{aligned} B_2(T) &= -\int_0^\infty (e^{-\beta A/r^\alpha} - 1)\,\mathrm{d}r && (6)\\ &= -\int_0^R (e^{-\beta A/r^\alpha} - 1)\,\mathrm{d}r - \int_R^\infty (e^{-\beta A/r^\alpha} - 1)\,\mathrm{d}r && (7)\end{aligned}$$

where $R \gg 1$. When $r \to 0$ we have $-r^{-\alpha} \to -\infty$, and thus $e^{-\beta A/r^\alpha} \to 0$. Therefore the first integral is limited for all values of α . On the other hand, when $r \gg 1$ we can expand the exponential to get

$$e^{-\beta A/r^\alpha} - 1 \approx 1 - \frac{A\beta}{r^\alpha} - 1 = -\frac{A\beta}{r^\alpha}. \tag{8}$$

In this case Eq. 6 is

$$B_2(T) = \text{something limited } + \int_R^\infty \beta A/r^\alpha\,\mathrm{d}r \tag{9}$$

which exist only for $\alpha > 1$ (already for $\alpha = 1$, the integral goes as a logarithm, and $\log(x) \overset{x\to\infty}{\to} \infty$. For $\alpha < 1$ the integral goes as a positive power of x , which is also ∞ in the limit $x \to \infty$.)

(e) Since ions interact with a $1/r$ potential we expect that the virial expansion would not work.

(f) Small values of α mean that there is a long-ranged interaction between particles. As many particles feel each other, mean-field theory is a good alternative.

2. Ferromagnetism

(a) Mean-field Hamiltonian:

$$H_{\mathrm{MF}}\left(\{s_i\}\right) = -\left(mB + Jz\left\langle s\right\rangle \sum_i s_i\right)$$

(b) Mean-field partition function:

$$Z_{\mathrm{MF}} = \sum_{\{\sigma_i=\pm 1\}} e^{-\beta H_{\mathrm{MF}}(\{\sigma_i\})} = \sum_{\{\sigma_i=\pm 1\}} \prod_i e^{\beta(mB+Jz\langle\sigma\rangle)\sigma_i}$$

and thus

$$Z_{\mathrm{MF}} = \left(e^{\beta(mB+Jz\langle\sigma\rangle)} + e^{-\beta(mB+Jz\langle\sigma\rangle)}\right)^N = \left[2\cosh\left(\beta\left(Jz\left\langle\sigma\right\rangle + mB\right)\right)\right]^N$$

(c) mean-field free energy:

$$F_{\mathrm{MF}} = -k_B T \ln Z_{\mathrm{MF}} = -k_B T N \ln\left(2\cosh\left(\beta\left(Jz\left\langle\sigma\right\rangle + mB\right)\right)\right)$$

(d) mean-field magnetization per spin:

$$\left\langle\sigma\right\rangle = -\frac{1}{N}\frac{\partial F_{\mathrm{MF}}}{\partial B} = \tanh\left(\beta\left[Jz\left\langle\sigma\right\rangle + mB\right]\right)$$

(e) $d = 1$

(f) $d = 2$, self-duality

1. Adsorption to a surface

(a) The possible values of n_i are either 0 (empty site) or 1 (filled site).

$$H = -\varepsilon \sum_{i=0}^{M} n_i - K \sum_{\langle i,j\rangle} n_i n_j.$$

Notice the minus sign, which ensures that for $\varepsilon, K > 0$ the energy is lowered when the atoms stick to the surface, and to each other.

(b) This is a proof by construction. Given the possible values of n_i, one can make the change of variables $n_i = (\sigma_i + 1)/2$, with $\sigma_i = \pm 1$. Replacing this in the Hamiltonian and expanding the brackets leads to:

$$H = -\frac{\varepsilon}{2}\sum_{i=0}^{M}\sigma_i - \frac{\varepsilon}{2}\sum_{i=0}^{M} 1 - \frac{K}{4}\sum_{\langle i,j\rangle}\sigma_i\sigma_j - \frac{K}{4}\sum_{\langle i,j\rangle}\sigma_i - \frac{K}{4}\sum_{\langle i,j\rangle}\sigma_j - \frac{K}{4}\sum_{\langle i,j\rangle} 1.$$

First of all, we can ignore all the constant (independent of σ) terms, since the energy is always defined up to a constant. Secondly, the sums over nearest neighbors which depend on a single spin variable can be converted into sums over all spins by simply multiplying with the coordination number of the lattice, z. In the case of a square lattice $z = 2$. The result is:

$$H = -\frac{\varepsilon}{2}\sum_{i=0}^{M}\sigma_i - \frac{K}{4}\sum_{\langle i,j\rangle}\sigma_i\sigma_j - \frac{Kz}{4}\sum_{i=0}^{M}\sigma_i - \frac{Kz}{4}\sum_{i=0}^{M}\sigma_i,$$

meaning that the Ising magnetic field can be written as $mB = (\varepsilon + Kz)/2$, and the spin-spin interaction as $J = K/4$.

(d) One expects that in the low temperature limit the system is in an ordered phase in which the energy is minimized. As such, all sites will be occupied and the probability of occupation will be $\langle n_i\rangle = 1$. In the high temperature regime, thermal fluctuations will dominate, and each site will be occupied randomly, with a 50% probability (like in the Ising model in that case where half of the spins points up, the other half down). Therefore, in this limit, $\langle n_i\rangle = 1/2$.

(e) One can apply the usual prescription to compute the average occupation number of site i. After canceling out all possible terms, one has:

$$\langle n_i\rangle = \frac{\sum n_i \exp(\beta\varepsilon n_i)}{\sum \exp(\beta\varepsilon n_i)} = \frac{\exp(\beta\varepsilon)}{1+\exp(\beta\varepsilon)}.$$

In the high temperature limit, $\beta \to 0$ and $\langle n_i\rangle \to 1/2$, while for low temperatures, $\beta \to \infty$ and $\langle n_i\rangle \to 1$, as expected.