Session 11: solutions

Exercise 1

a) The correct variables are $\{n_i\}$ $n_i = 0,1$ $\forall i$

with $n = +1 \rightarrow$ full site

$n = 0 \rightarrow$ empty site

b) $$H = -\varepsilon \sum_{\langle i,j \rangle} n_i n_j + \mu \sum_i n_i$$

c) We must map the variables n_i into variables s_i with $s_i = \pm 1$.

Map $s_i = +1 \iff n_i = +1$

$s_i = -1 \iff n_i = 0$

The relation is

$$n_i = \frac{1}{2}(s_i + 1)$$

Then

$$H = -\varepsilon \sum_{\langle i,j \rangle} \frac{1}{4}(s_i + 1)(s_j + 1) + \mu \sum_i \frac{1}{2}(s_i + 1) =$$

$$= -\frac{\varepsilon}{4} \sum_{\langle i,j \rangle} s_i s_j + \left(\frac{\mu}{2} - \frac{\varepsilon z}{4}\right) \sum_i s_i + \text{const}$$

with z the coordination number of the lattice

Then the mapping with the Ising model is

$$J = \frac{\varepsilon}{4} \qquad h = -\frac{\mu}{2} + \frac{\varepsilon z}{4}$$

Exercise 2

Here we go straigth to the mapping:

$s_i = +1 \longrightarrow$ type A

$s_i = 0 \longrightarrow$ vacancy

$s_i = -1 \longrightarrow$ type B

of course, other choices are legitimate

then, let's write the chemical potential term:

$$\sum_i \left\{ \frac{\mu_A}{2} \underbrace{s_i(s_i+1)}_{\substack{=2 \text{ only if } s_i=+1, \\ \text{otherwise it is } 0}} + \frac{\mu_B}{2} \underbrace{s_i(s_i-1)}_{\substack{=2 \text{ only if } s_i=-1, \\ \text{otherwise it is } 0}} \right\} =$$

$$= \sum_i \left\{ \frac{\mu_A}{2} s_i^2 + \frac{\mu_A}{2} s_i + \frac{\mu_B}{2} s_i^2 - \frac{\mu_B}{2} s_i \right\} =$$

$$= \frac{\mu_A + \mu_B}{2} \sum_i s_i^2 + \frac{\mu_A - \mu_B}{2} \sum_i s_i$$

Now we have learned the trick, we can write the interaction term

$$\sum_{\langle i,j\rangle}\left\{-\frac{\varepsilon_{AA}}{4}s_i(s_i+1)s_j(s_j+1)-\frac{\varepsilon_{BB}}{4}s_i(s_i-1)s_j(s_j-1)+\right.$$

$$\left.-\frac{\varepsilon_{AB}}{4}s_i(s_i+1)s_j(s_j-1)\right\} =$$

$$=\sum_{\langle i,j\rangle}\left\{-\frac{\varepsilon_{AA}}{4}s_i^2s_j^2-\frac{\varepsilon_{AA}}{4}(s_i^2s_j+s_is_j^2)-\frac{\varepsilon_{AA}}{4}s_is_j+\right.$$

$$-\frac{\varepsilon_{BB}}{4}s_i^2s_j^2+\frac{\varepsilon_{BB}}{4}(s_i^2s_j+s_is_j^2)-\frac{\varepsilon_{BB}}{4}s_is_j+$$

$$\left.-\frac{\varepsilon_{AB}}{4}s_i^2s_j^2+\frac{\varepsilon_{AB}}{4}(\underbrace{s_i^2s_j-s_is_j^2}_{\text{this is }=0\text{ by exchange symmetry between } i \text{ and } j})+\frac{\varepsilon_{AB}}{4}s_is_j\right\}$$

Putting everything together:

$$H=-\frac{\varepsilon_{AA}+\varepsilon_{BB}+\varepsilon_{AB}}{4}\sum_{\langle i,j\rangle}s_i^2s_j^2-\frac{\varepsilon_{AA}-\varepsilon_{BB}}{4}\sum_{\langle i,j\rangle}(s_i^2s_j+s_is_j^2)+$$

$$-\frac{\varepsilon_{AA}+\varepsilon_{BB}-\varepsilon_{AB}}{4}\sum_{\langle i,j\rangle}s_is_j+\frac{\mu_A+\mu_B}{2}\sum_i s_i^2+\frac{\mu_A-\mu_B}{2}\sum_i s_i$$

This is the most general Hamiltonian with spin 1 and is called the

Blume-Emery-Griffith model.