E5651: Ising in interaction with lattice gas

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The problem:

Consider a one dimensional Ising model of spins $\sigma_i = \pm 1, i = 1, 2, 3, ..., N$ and circular boundary condition ($\sigma_{N+1} = \sigma_1$). Between each two spins there is a site for an additional atom, which if present decreases the coupling J to $J(1 - \lambda)$. The Hamiltonian is then

$$H = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1} (1 - \lambda n_i)$$

where $n_i = 0$ or 1 and there are $M = \sum_{i=1}^{N} n_i$ atoms ($M < N$), i.e. on average $\langle n_i \rangle = M/N$.

(1) Evaluate the partition sum by allowing all configurations of spins and of atoms. Calculate the free energy.

(2) If the atoms are stationary impurities one needs to evaluate the free energy F for some random configuration of the atoms and then average F over all configurations. Evaluate the average F. Find the entropy difference between the result calculated from the averaged F and from the F calculated in (1).

The solution:

(1) The partition function is:

$$Z = \sum_{\sigma_1=\pm1} \sum_{\sigma_2=\pm1} ... \sum_{\sigma_n=\pm1} e^{-\beta(-J\sum_{i=1}^{N} \sigma_i \sigma_{i+1}(1-\lambda n_i))}$$

We define

$$s_i = \sigma_i \sigma_{i+1}$$

So the partition function can be writen as seen in class:

$$Z = \sum_{s_1=\pm1} \sum_{s_2=\pm1} ... \sum_{s_n=\pm1} e^{-\beta(-J\sum_{i=1}^{N} s_i(1-\lambda n_i))}$$

We are going to solve this case, according to the solution of the 1D Ising Model, Using the Transfer matrices formalism:

$$Z = \sum_{\sigma_1=\pm1} \sum_{\sigma_2=\pm1} ... \sum_{\sigma_n=\pm1} < \sigma_1 | T_{\sigma_1 \sigma_2} | \sigma_2 >< \sigma_2 | T_{\sigma_2 \sigma_3} | \sigma_3 > ... < \sigma_n | T_{\sigma_n \sigma_{n+1}} | \sigma_{n+1} >$$

The transfer matrix for two spins without an atom between is:

$$T_i = \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix}$$

The transfer matrix for two spins with an atom between is:

$$T_i' = \begin{pmatrix} e^{\beta J(1-\lambda)} & e^{-\beta J(1-\lambda)} \\ e^{-\beta J(1-\lambda)} & e^{\beta J(1-\lambda)} \end{pmatrix}$$

Both matrices commute So the multiplication order does not matter:

$$[T_i, T_i^{'}] = 0$$

Reminder: The trace of matrix doesn't change upon diagonalization.
After changing to the diagonalized base, we get for a single configuration:

$$Z = Tr(T'^{M} T^{N-M})$$

$$= Tr(\begin{pmatrix} 2cosh(\beta J)^{N-M} & 0 \\ 0 & 2sinh(\beta J)^{N-M} \end{pmatrix} \begin{pmatrix} 2cosh(\beta J(1-\lambda))^{M} & 0 \\ 0 & 2sinh(\beta J(1-\lambda))^{M} \end{pmatrix})$$

Notice that a combinatorial factor is introduced into the partition function, in order to count the different configurations possible, for a given M. Assuming $N \to \infty$ we can neglect the smaller eigenvalue so:

$$Z = (\begin{matrix} N \\ M \end{matrix}) 2cosh(\beta J)^{N-M} 2cosh(\beta J(1-\lambda))^{M}$$

The free energy is therefore:

$$F = -\tau lnZ = -\tau ln((\begin{matrix} N \\ M \end{matrix})) - \tau(N-M)ln(2cosh(\beta J)) - \tau M ln(2cosh(\beta J(1-\lambda))) =$$

$$-\tau(ln(n!) - ln(m!) - ln((n-m)!)) - \tau(N-M)ln(2cosh(\beta J)) - \tau M ln(2cosh(\beta J(1-\lambda)))$$

(2) For any configuration with exactly M impurities, the partition function is:

$$Z = 2cosh(\beta J)^{N-M} 2cosh(\beta J(1-\lambda))^{M}$$

As the number of impurities is fixed, the combinatorial factor is not needed.
The free energy for any configuration with M impurities is:

$$F = -\tau lnZ = -\tau l(N-M)ln(2cosh(\beta J)) - \tau M ln(2cosh(\beta J(1-\lambda)))$$

The average free energy for a given M is:

$$< F >= \frac{\sum_{configurations} F_{conf}}{\sum_{configurations}} = \frac{(\begin{matrix} N \\ M \end{matrix}) \times -\tau l(N-M)ln(2cosh(\beta J)) - \tau M ln(2cosh(\beta J(1-\lambda)))}{(\begin{matrix} N \\ M \end{matrix})}$$

$$< F >= -\tau l(N-M)ln(2cosh(\beta J)) - \tau M ln(2cosh(\beta J(1-\lambda)))$$

The entropy difference between the two calculations:

$$\triangle S = -\frac{\partial F}{\partial \tau} + \frac{\partial < F >}{\partial \tau} = ln((\begin{matrix} N \\ M \end{matrix}))$$