Homework Assignment 3, Special topics in Phys. Chem.(Fall 2008)

The partition function for the one-dimensional Ising magnet (or Ising spin) in an external magnetic field (H) is

$$Q = \sum_{s_1, s_2, \ldots s_N = \pm 1} \exp\left[\sum_{i=1}^{N} (h s_i + K s_i s_{i+1})\right] \tag{1}$$

where $h = \beta \mu H$, $K = \beta J$ and we are using periodic boundary conditions i.e., $s_1 = s_{N+1}$.

(a) Show that Q can be expressed as

$$Q = \mathrm{Tr}(\mathcal{T}^N) \tag{2}$$

where $\mathcal{T}$ is the 2×2 matrix

$$\mathcal{T} = \begin{pmatrix} \exp(-h + K) & \exp(-K) \\ \exp(-K) & \exp(h + K) \end{pmatrix},$$

[*Hint* $\sum_{i=1}^{N} s_i = s_1 + s_2 + s_3 + s_4 + \cdots s_N = \frac{1}{2}(s_N + s_1) + \frac{1}{2}(s_1 + s_2) + \cdots + \frac{1}{2}(s_{N-1} + s_N)$]

(b) By noting that the trace of a matrix is independent of representation, show that Q can be expressed as

$$Q = \lambda_+^N + \lambda_-^N, \tag{3}$$

where λ_+ and λ_- are the larger and smaller eigenvalues, respectively, of the matrix $\mathcal{T}$.

(c) Determine these two eigenvalues, and show that in the thermodynamic limit ($N \to \infty$)

$$\frac{\log Q}{N} = \log \lambda_+ = K + \log\left\{\cosh(h) + [\sinh^2(h) + e^{-4K}]^{1/2}\right\} \tag{4}$$

This method for computing a partition function is called the "trasfer matrix method." In the class, we learned other example of using transfer matrix method for helix-coil transition. The problem of Ising spin and helix-coil transition is *isomorphic* because the correspondence between these two model can be established by making the change of variables $n_i = (s_i + 1)/2$. The "spin-up state" ($s_i = +1$) corresponds to an ordered region (helix, $n_i = 1$), and "spin-down" state ($s_i = -1$) corresponds to a disordered region (coil, $n_i = 0$).

(d) Evaluate the average magnetization and show that the magnetization vanishes as $h \to 0^+$. [*Hint*: You can determine $\langle s_i \rangle$ by differentiating $N^{-1} \log Q$ with respect to h.]