Ex5645: Potts Model in One Dimension

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The problem:

A set of N atoms is arranged on a one-dimensional chain. Each atom has p possible orientations, labelled by $\sigma = 1, 2, ..., p$. Two neighboring atoms σ_i and σ_j have a negative interaction energy $-\varepsilon$ if they are in the same orientation, and zero otherwise. It is useful to define bond variables $s_i = \sigma_{i+1} - \sigma_i \mod (p)$.

(1) The partition function $Z_{\text{chain}}(\beta)$ of an open chain can be written as $Z = Aq^{N-1}$. Write what are A and q. Tip: the partition sum factorizes in the "bond" representation.

(2) The partition function $Z_{\text{ring}}(\beta)$ of a closed chain, with periodic boundary conditions, can be written as $Z = \text{trace}(T^N)$. Write what is the matrix T for $p = 4$.

(3) Find what are the eigenvalues of the transfer matrix T for general p, and deduce an explicit expression for $Z_{\text{ring}}(\beta)$. Tip: The T matrix is diagonal in the "momentum" representation.

(4) Find the energy per atom at the $N \to \infty$ limit. Write the result as $E(T)/N = \epsilon f(\epsilon - \mu)$. Provide expressions for μ and for $f()$ using p and the temperature T.

The solution:

1. The Hamiltonian for this model is:

$$\mathcal{H} = -\varepsilon \sum_{\langle i,j \rangle} \delta_{\sigma_i,\sigma_j} \,, \tag{1}$$

where $\delta_{\sigma_i,\sigma_j}$ is Kronecker's delta:

$$\delta_{\sigma_i,\sigma_j} = \begin{cases} 1, & \sigma_i = \sigma_j \\ 0, & otherwise \end{cases} \tag{2}$$

Introducing the bond variables $s_i = \sigma_{i+1} - \sigma_i$, we can rewrite the Hamiltonian in the following form:

$$\mathcal{H} = -\varepsilon \sum_{i=1}^{N-1} \delta_{s_i,0} \,. \tag{3}$$

Instead of summing over spin orientations, we can sum over bonds. The partition function is given by:

$$Z = \sum_{\sigma_1} ... \sum_{\sigma_N} e^{\beta\varepsilon \sum_{\langle i,j \rangle} \delta_{\sigma_i,\sigma_j}} = \sum_{\sigma_1=1}^{p} \sum_{s_i(\cdot)} e^{\beta\varepsilon \sum_{i=1}^{N-1} \delta_{s_i,0}} = \sum_{\sigma_1=1}^{p} \sum_{s_i(\cdot)} \prod_{i=1}^{N-1} e^{\beta\varepsilon\delta_{s_i,0}} = \sum_{\sigma_1=1}^{p} \prod_{i=1}^{N-1} \sum_{s_i(\cdot)} e^{\beta\varepsilon\delta_{s_i,0}} \tag{4}$$

The exponent in the product is 1 if $s_i \neq 0$ and $e^{\beta\varepsilon}$ if $s_i = 0$. The final expression sums the energy contributions from the bonds relative to the first spin which can be found in p orientations. For each s_i there is one state which contributes to the energy and $p - 1$ states

that do not contribute to the energy.
So we get:

$$Z = \sum_{\sigma_1=1}^{p} \left(p - 1 + e^{\beta\varepsilon}\right)^{N-1} = p\left(p - 1 + e^{\beta\varepsilon}\right)^{N-1} . \tag{5}$$

Therefore: $A = p$ and $q = p - 1 + e^{\beta\varepsilon}$.

2. For periodic bounday conditions $\sigma_{N+1} = \sigma_1$. The Hamiltonian is:

$$\mathcal{H} = -\varepsilon \sum_{i=1}^{4} \delta_{s_i,0} \,, \tag{6}$$

which means that the partition function factorized:

$$Z = \sum_{s_i(\cdot)} e^{\beta\varepsilon \sum_{i=1}^{4} \delta_{s_i,0}} = \mathrm{Tr}\left(T^N\right) . \tag{7}$$

Diagonal matrix elements - spins in the same orientation (contribution of $e^{\beta\epsilon}$)
Off-Diagonal matrix elements - not in the same orientation (contribution of $e^{\beta 0} = 1$)
Therefore T is the following matrix:

$$\begin{pmatrix} e^{\beta\varepsilon} & 1 & 1 & 1 \\ 1 & e^{\beta\varepsilon} & 1 & 1 \\ 1 & 1 & e^{\beta\varepsilon} & 1 \\ 1 & 1 & 1 & e^{\beta\varepsilon} \end{pmatrix} = \mathrm{Ones}_{4\times 4} + \left(e^{\beta\varepsilon} - 1\right) I_{4\times 4}$$

3. In general (p orientations):

$$T = \left(e^{\beta\varepsilon} - 1\right) I_{p\times p} + \mathrm{Ones}_{p\times p} \tag{8}$$

The first term is diagonalized
The second term is ones matrix with $Dim(Ones) = p$, so the eigenvalues are:
1. p (Degeneration 1)
2. 0 (Degeneration $p - 1$)

Diagonalizing T we get the following eigenvalue matrix:

$$\begin{pmatrix} e^{\beta\varepsilon} + p - 1 & 0 & \dots & 0 \\ 0 & e^{\beta\varepsilon} - 1 & 0 & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & e^{\beta\varepsilon} - 1 \end{pmatrix}$$

The partition function:

$$Z = \mathrm{Tr}\left(T^N\right) = \left[e^{\beta\varepsilon} + p - 1\right]^N + (p-1)\left[e^{\beta\varepsilon} - 1\right]^N . \tag{9}$$

4. In the limit of $N \to \infty$ we can neglect the smaller eigenvalues and have:

$$\ln Z \approx N \ln\left(e^{\beta\varepsilon} + p - 1\right) . \tag{10}$$

The energy per atom is:

$$\frac{\langle E\rangle}{N} = -\frac{1}{N}\frac{\partial \ln Z}{\partial \beta} \approx -\frac{1}{e^{\beta\varepsilon} + p - 1}\varepsilon e^{\beta\varepsilon} = -\varepsilon \frac{1}{1 + e^{-\beta(\varepsilon-\mu)}} = \varepsilon f\left(\epsilon - \mu\right) . \tag{11}$$

Where we defined: $\mu = \ln(p-1)/\beta$ and $f\left(\epsilon - \mu\right) = -\left(1 + e^{-\beta(\varepsilon-\mu)}\right)^{-1}$.