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:

Alert: over complicated perpective on trivail diagonalization in item 3

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 the usual Kronecker delta and it is 1 if $\sigma_i = \sigma_j$, and 0 otherwise. Introducing the bond variables $s_i = \sigma_{i+1} - \sigma_i$, we can rewrite the Hamiltonian in the following form:

$$\mathcal{H} = -\varepsilon \sum_{i=1}^{N-1} \delta_{s_i,0} \,. \tag{2}$$

The partition function is therefore,

$$Z = \sum_{\sigma(\cdot)} e^{\beta\varepsilon \sum_{\langle i,j \rangle} \delta_{\sigma_i,\sigma_j}} = \sum_{\sigma_1=1}^{p} \sum_{s_i(\cdot)} e^{\beta\varepsilon \sum_{i=1}^{N-1} \delta_{s_i,0}} = \sum_{\sigma_1=1}^{p} \sum_{s_i(\cdot)} \prod_{i=1}^{N-1} e^{\beta\varepsilon \delta_{s_i,0}} \,. \tag{3}$$

Notice that the exponent in the product is 1 if $s_i \neq 0$ and $e^{\beta\varepsilon}$ if $s_i = 0$, so in a sense the product 'counts' the number of bonds which contribute to the energy. The sum over s_i factorized as s_i and s_j are independent. There are $p - 1$ exponents which do not contribute to the energy and one which does (per s_i). So we get

$$Z = \sum_{\sigma_1=1}^{p} \left(p - 1 + e^{\beta\varepsilon} \right)^{N-1} = p \left(p - 1 + e^{\beta\varepsilon} \right)^{N-1} \,. \tag{4}$$

We then see that $A = p$ and $q = p - 1 + e^{\beta\varepsilon}$.

2. As already stated, the Hamiltonian is:

$$\mathcal{H} = -\varepsilon \sum_{i=1}^{4} \delta_{s_i,0} \,, \tag{5}$$

which means that the partition function factorized, again, and it is:

$$Z = \sum_{s_i(\cdot)} e^{\beta\varepsilon \sum_{i=1}^{4} \delta_{s_i,0}} = \sum_{s_1=-3}^{3} \left(T^N\right)_{s1s1} = \mathrm{Tr}\left(T^N\right) \,. \tag{6}$$

Here T is the following matrix:

$$\begin{pmatrix} e^{\beta\varepsilon} & 1 & 1 & 1 \\ 1 & e^{\beta\varepsilon} & 1 & 1 \\ 1 & 1 & e^{\beta\varepsilon} & 1 \\ 1 & 1 & 1 & e^{\beta\varepsilon} \end{pmatrix} = \left(e^{\beta\varepsilon} - 1\right) I_{4\times 4} + \mathrm{One}_4 \,,$$

where One_4 is a 4×4 matrix full of 1's, and I is the identity matrix.

3. In the general case:

$$T = \left(e^{\beta\varepsilon} - 1\right) I_{p\times p} + \mathrm{One}_p = \left(e^{\beta\varepsilon} - 1\right) I_{p\times p} + |\psi\rangle\langle\psi| \,, \tag{7}$$

where $|\psi\rangle$ is the vector $(1, 1, \ldots, 1)$. Notice that $|\psi\rangle$ is an eigenvector of T with an eigenvalue $\left(e^{\beta\varepsilon} - 1\right) + \sum_{i=1}^{p} 1 = e^{\beta\varepsilon} + p - 1$. Notice that this matrix is symmetric, which means that every other eignenvector which has different eigenvalue is orthogonal to $|\psi\rangle$[1] so if $|\phi\rangle$ is another eigenvector we have $T|\phi\rangle = \left(e^{\beta\varepsilon} - 1\right)|\phi\rangle$. This means that every other eigenvalue is $e^{\beta\varepsilon} - 1$. In fact, diagonalizing T we get:

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

which means that:

$$Z = \mathrm{Tr}\left(T^N\right) = \left[e^{\beta\varepsilon} + p - 1\right]^N + (p-1)\left[e^{\beta\varepsilon} - 1\right]^N \,. \tag{8}$$

In the case of $p = 4$ we get:

$$Z = \left[e^{\beta\varepsilon} + 3\right]^N + 3\left[e^{\beta\varepsilon} - 1\right]^N \,. \tag{9}$$

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:

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

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

[1] Quick proof: $\lambda_1\langle\psi,\phi\rangle = \langle T\psi,\phi\rangle = \langle\psi, T^{\mathrm{T}}\phi\rangle = \lambda_2\langle\psi,\phi\rangle \Rightarrow (\lambda_1 - \lambda_2)\langle\psi,\phi\rangle = 0 \Rightarrow \langle\psi,\phi\rangle = 0$