E5971: Potts model in one dimension

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The problem:

A set of N atoms, each with p states, is arranged on a 1d chain with periodic boundary conditions. The atom at the i-th site is in a state n_i that is chosen from the set $\{1, 2, ..., p\}$.

Two neighboring atoms at sites i and j (where $j = i + 1$), respectively, have an interaction energy $-J$ ($J > 0$) if they are in the same state, i.e. $n_i = n_j$, and 0 interaction otherwise.

The Hamiltonian is therefore

$$\mathcal{H} = -J \sum_{<ij>} \delta_{n_i,n_j}$$

where δ_{n_i,n_j} is the Kronecker symbol, and the boundary conditions are $n_{N+1} = n_1$. The summation is being done only over nearest neighbours, i.e. over $< ij >$ satisfying $j = i + 1$.

(At all items consider the limit $N \to \infty$.)

(1) Derive the free energy of the system for $p = 2$.

(2) Derive the free energy of the system for a general p.

(3) Find the energy E at the low and high temperature limits and interpret the results.

The solution:

(1) First, we shall calculate the partition function by summing over all states:

$$Z = \sum_r e^{-\beta E_r} = \sum_{n_1=1}^{p} \times \sum_{n_2=1}^{p} \times ... \times \sum_{n_N=1}^{p} e^{\beta J \sum_{i=1}^{p} \delta_{n_i,n_{i+1}}} =$$

$$= \sum_{n_1=1}^{p} \times \sum_{n_2=1}^{p} \times ... \times \sum_{n_N=1}^{p} e^{\beta J \delta_{n_1,n_2}} e^{\beta J \delta_{n_2,n_3}} ... e^{\beta J \delta_{n_N,n_{N+1}}}$$

We shall now define the transfer matrix T, and use the Dirac notation to denote its (i,j) element:

$T_{ij} =< n_i|T|n_j >= e^{\beta J \delta_{n_i,n_j}}$

Using this definition and the boundary condition $n_{N+1} = n_1$, we get

$$Z = \sum_{n_1=1}^{p} \times \sum_{n_2=1}^{p} \times ... \times \sum_{n_N=1}^{p} < n_1|T|n_2 >< n_2|T|n_3 > ... < n_N|T|n_{N+1} >$$

$$= \sum_{n_1=1}^{p} < n_1|T^N|n_1 >= trace(T^N) = \sum_{j=1}^{p} \lambda_j^N$$

Where the λ's are the eigenvalues of the transfer matrix T.

In the case of p=2, we get

$$T = \begin{pmatrix} e^{\beta J} & 1 \\ 1 & e^{\beta J} \end{pmatrix}$$

And by demanding

$$Det \begin{pmatrix} e^{\beta J} - \lambda & 1 \\ 1 & e^{\beta J} - \lambda \end{pmatrix} = 0$$

We get the eigenvalues:

$\lambda_+ = e^{\beta J} + 1$
$\lambda_- = e^{\beta J} - 1$

From which we can derive the free energy:

$\ln(Z) = \ln(\lambda_+^N + \lambda_-^N) = \ln(\lambda_+^N(1 + \frac{\lambda_-^N}{\lambda_+^N}))$

In the thermodynamic limit $N \to \infty$ we get

$\ln(Z) = \ln(\lambda_+^N) = N\ln\lambda_+ = N\ln(e^{\beta J} + 1)$

Thus we get the free energy for the case p=2:

$F = -NT \times \ln(e^{\beta J} + 1)$

(2) For a general p, the problem is finding the eigenvalues of the T matrix, which has now $p * p$ elements. Since we consider the thermodynamic limit only, it will be enough to find the largest eigenvalue of the T matrix.

$$T = \begin{pmatrix} e^{\beta J} & 1 & 1 & ... \\ 1 & e^{\beta J} & 1 & ... \\ 1 & 1 & e^{\beta J} & ... \\ ... & ... & ... & ... \end{pmatrix}$$

In order to find the eigenvalues of the T matrix, we write down the vectorial equation

$Ta = \lambda a$

where a is a column vector consisting of p components $a_1, a_2, ..., a_p$.

Multiplying the column vector a by T from the left, we obtain p linear equations:

for each j, we get

$$(e^{\beta J} - 1)a_j + \sum_{i=1}^{p} a_i = \lambda a_j$$

Assuming that the vector a is not the trivial zero solution, there is at least one component a_j NOT equal to zero. Thus, we can conclude that there are two ways of solving the eigenvalue equation:

(a) A solution where

$$\sum_{i=1}^{p} a_i = 0$$

and

$$\lambda = e^{\beta J} - 1$$

(b) A solution where

$$\sum_{i=1}^{p} a_i \neq 0$$

which implies that $a_j \neq 0$ for ANY j. Thus, we get

$$\lambda = e^{\beta J} - 1 + \frac{1}{a_j} \sum_{i=1}^{p} a_i$$

Since λ cannot depend on our selection of j here, we deduce that for this solution all a_j are equal, and hence we get

$$\lambda = e^{\beta J} - 1 + p$$

Which is the LARGEST eigenvalue.

Solution (a) ($\lambda = e^{\beta J} - 1$) has a $p - 1$ degeneration, and solution (b) ($\lambda = e^{\beta J} - 1 + p$) has no

degeneration - only a vector with p equal entries has this eigenvalue.

After finding the largest eigenvalue, we can find $\ln(Z)$ in the thermodynamic limit $N \to \infty$:

$\ln(Z) = \ln((largest - eigenvalue)^N) = N \times \ln(e^{\beta J} - 1 + p)$

And thus we obtain the free energy for a general p in the thermodynamic limit:

$F = -NT \times \ln(e^{\beta J} - 1 + p)$

(3) The energy E will be found by differentiating $\ln(Z)$ with respect to β:

$E = -\frac{\partial \ln(Z)}{\partial \beta} = -NJ\frac{e^{\beta J}}{e^{\beta J} - 1 + p}$

In the limit of low temperature ($T << J$), the system approaches the energy $E = -NJ$.

In this limit there is no external energy coming from thermal fluctuations, and thus the system will be in equilibrium when all atoms will be in the same state. Another interpertation - at low temperature the entropy has no effect over the free energy, and thus the minimum of the free energy F will also be the minimum of the energy E.

In the limit of high temperature ($T >> J$) the system approaches the energy $-\frac{N}{p}J$.

The thermal fluctuatuions will be so strong that the system's behavior will be totally random - there will be no significance to the interaction energy J, each atom could be at any one of the states with equal probability $\frac{1}{p}$, and the number of J-interactions will correspondingly be $\frac{N}{p}$. Thus, the energy of the system in this limit will be $-\frac{N}{p}J$.

As a general comment, it should be noted that the properties of the largest eigenvalue and of the corresponding eigenvectors when T is a non-negative real square matrix is being described more generally in the Perron-Frobenius theorem.