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CALCULATION OF THE FREE ENERGY IN A SIMPLE MODEL

A.K. Kwaśniewski

Abstract:

The free energy per site is calculated, for the one-dimensional periodic chain, in an arbitrary external magnetic field.
This chain is a one-dimensional counterpart of the two-dimensional, three state Potts models.

The use of generalized Clifford algebras, has recently resulted in revealing new perspectives for calculation of the partition function for Potts models [1,2].

At the same time the main algebraic obstacle for straightforward generalizations of the known in the Ising case model methods - seems to be localized now. Therefore it is useful to get further experience, while calculating the partition function for the one-dimensional counterparts of both standard and planar Potts models.

These are one-dimensional periodic chains with partition functions defined as follows:

$$Z_N = \sum_{\{\mu\}} \exp\{a \sum_{i=1}^{N} \delta(\mu_i - \mu_{i+1}) + B \sum_{i=1}^{N} \mathrm{Re}\, \mu_i\} , \tag{1}$$

$$Z'_N = \sum_{\{\mu\}} \exp\{a \sum_{i=1}^{N} \mathrm{Re}(\mu_i \bar{\mu}_{i+1}) + B \sum_{i=1}^{N} \mathrm{Re}\, \mu_i , \tag{2}$$

where $\mu_i \in \{\omega^k\}_{k=0}^{2}$, $\omega = \exp(i\, \frac{2\pi}{3})$ and $\mu_{N+1} = \mu_1$, $a \neq 0$, $a, B \in \mathbb{R}$.

The transfer matrices L and L′ are given correspondingly by:

$$L(a) = \begin{pmatrix} e^a & 1 & 1 \\ 1 & e^a & 1 \\ 1 & 1 & e^a \end{pmatrix} \begin{pmatrix} e^B & 0 & 0 \\ 0 & e^{B\mathrm{Re}\omega} & 0 \\ 0 & 0 & e^{B\mathrm{Re}\omega} \end{pmatrix} , \tag{3}$$

$$L'(a) = e^{a\mathrm{Re}\omega} L(a - \mathrm{Re}\omega) . \tag{4}$$

Due to (4) it is sufficient to calculate Z_N partition function only.
We shall look for eigenvalues of L(a), and for that to do let us introduce the following notation:

$$e^a = \alpha\ ,\quad b_o^2 = e^B\ ,\quad b^2 = e^{BRe\omega}\ ,\qquad x_o = \alpha - \lambda b_o^{-2} \equiv \alpha - \lambda\beta .$$

$$x = \alpha - \lambda b^{-2} \equiv \alpha - \lambda\beta .$$

Note that $\beta_o\beta^2 = 1$.
Define now for the moment the A & B matrices:

$$A = \begin{pmatrix} \alpha & 1 & 1 \\ 1 & \alpha & 1 \\ 1 & 1 & \alpha \end{pmatrix} \quad , \qquad B = \begin{pmatrix} b_o & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & b \end{pmatrix} .$$

Then one easily sees that the spectrum of L(a) is that of BAB, what amounts to looking for the roots of det(BAB - λI), where

$$\det(BAB - \lambda I) = \begin{vmatrix} x_o & 1 & 1 \\ 1 & x & 1 \\ 1 & 1 & x \end{vmatrix} = (x - 1)(xx_o + x_o - 2) . \tag{5}$$

Hence the first eigenvalue of L(a) is equal to

$$\lambda_o = (\alpha - 1)b^2 . \tag{6}$$

The other two are to be found from

$$\lambda^2 - [\alpha\beta^2 + (\alpha + 1)\beta_o\beta]\lambda + \beta[\alpha(\alpha + 1) - 2] . \tag{7}$$

Denote the coefficient of λ by A_1 while $A_2 = \beta[\alpha(\alpha+1) - 2]$. Then we see that L(a) has two more eigenvalues as

$$\Delta = A_1^2 - 4A_2 = [\alpha\beta^2 - (\alpha+1)\beta\beta_o]^2 + 8\beta > 0 \tag{8}$$

for any a and B. Thus we obtain:

$$\lambda_1 = \tfrac{1}{2}[\alpha\beta^2 + (\alpha + 1)\beta_o\beta + \sqrt{\Delta}\,] . \tag{9}$$

$$\lambda_2 = \tfrac{1}{2}[\alpha\beta^2 + (\alpha + 1)\beta_o\beta - \sqrt{\Delta}\,] . \tag{10}$$

It follows from (9) that $\lambda_1>0$ independently of a and B. Meanwhile $\lambda_2 \gtrless 0$ depending on the values of a only, i.e.

$$\lambda_1 > \lambda_2 > 0 \quad \text{for } a > 0, \text{ and}$$
$$\lambda_2 < 0, \; \lambda_1 > |\lambda_2| \quad \text{for } a < 0. \qquad (11)$$

In order to prove (11) it is enough to notice that

$b^2\lambda_1\lambda_2 = \alpha(\alpha + 1) - 2$ and that $\alpha > 1$ for $a > 0$, while $\alpha < 1$ for $a < 0$.

The inequality $\lambda_1 > |\lambda_2|$ for any α is obvious in virtue of (9) and (10).
As the next important step we prove:

LEMMA 1.

Let $B \geq 0$ and $a \neq 0$, then $\lambda_1 > |\lambda_o|$ ∎.

Proof:

$$\frac{\lambda_1^2}{\lambda_o^2} > \frac{\lambda_1|\lambda_2|}{\lambda_o^2} = \beta^3 \left|\frac{\alpha + 2}{\alpha - 1}\right| > 1 \quad ∎$$

Now we are in a position to extend the validity of the above Lemma - to arbitrary B.

LEMMA 2.

For any B and $a \neq 0$, $\lambda_1 > |\lambda_o|$. ∎

Proof:

At first we prove that the continuous function of B: $f(B) = \lambda_1 - |\lambda_o|$ never takes the zero value. The thesis to be proved then follows from Lemma 1.

Let $a>0$. Then $\alpha>1$ and let $\lambda_1-|\lambda_o|=\lambda_1-\lambda_o=0$. This is equivalent to $\beta_o=\beta$ i.e. $B=0$ and this leads to contradiction as for $B=0$, $\alpha+2=\lambda_1\neq\lambda_o=\lambda_2=\alpha-1$.
Let now $a<0$, then $\alpha<1$ and let $\lambda_1-|\lambda_o| = \lambda_1 + \lambda_o = 0$. Then $xx_o+x_o-2 = 0$ for $\lambda =-\lambda_o$ (see (5)). This is equivalent to $x_o = 1$ or explicitly: $\alpha^2+\alpha^2\kappa-\alpha\kappa-1=0$; $\kappa=\beta_o\,\beta^{-1}>0$. However, this proves the contradiction as for $0<\alpha<1$ $\alpha^2-1 + \kappa(\alpha^2-\alpha) < 0$. ∎

From what was proved it follows directly that the free energy per site - $f(a,B)$ - for the model defined by (1), reads:

$$\boxed{f(a,B) = -kT \ln \lambda_1} \quad . \qquad (12)$$

The free energy thus is a continuous function of all its arguments.
The further, implicite dependence of f on temperature T is through parameters a and B which naturally incorporate the 1/kT factor.
The 5-state model is to be presented in a forthcoming paper.

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REFERENCES

TRUONG T.T., FUB-TKM Sept.85/25(1985) Berlin
KWASNIEWSKI A.K., J.Phys.A (in press), ITP UWr 84/621 (1984) Wrocław

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