WSAA 14

A. K. Kwaśniewski

Calculation of the free energy in a simple model

In: Zdeněk Frolík and Vladimír Souček and Marián J. Fabián (eds.): Proceedings of the 14th Winter School on Abstract Analysis. Circolo Matematico di Palermo, Palermo, 1987. Rendiconti del Circolo Matematico di Palermo, Serie II, Supplemento No. 14. pp. [231]–234.

Persistent URL: http://dml.cz/dmlcz/701898

Terms of use:

© Circolo Matematico di Palermo, 1987

Institute of Mathematics of the Czech Academy of Sciences provides access to digitized documents strictly for personal use. Each copy of any part of this document must contain these *Terms of use*.

This document has been digitized, optimized for electronic delivery and stamped with digital signature within the project *DML-CZ: The Czech Digital Mathematics Library* http://dml.cz

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:

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

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.

$$\begin{aligned} &\lambda_1 > \lambda_2 > 0 \qquad \text{for} \quad a > 0, \text{ and} \\ &\lambda_2 < 0 \,, \; \lambda_1 > |\lambda_2| \qquad \text{for } a < 0 \,. \end{aligned} \tag{11}$$

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

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

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 $xx_o^2+x_o-2 = 0$ 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:

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

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.

Acknowledgments:

The author expresses his thanks to Prof. F. Calogero and to Dr. D. Levi for their hospitality and help during the author's stay at the University of Rome.

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

ISTITUTO DI FISICA; UNIVERSITA DI ROMA; PIAZZALE ALDO MORO 2, I-00 185 ROMA, ITALY *)

*) Work performed under the exchange agreement between University of Rome and University of Wrocław.