We investigate recently proposed method for locating critical temperatures and introduce some modifications which allow to formulate exact criterion for any self-dual model. We apply the modified method for the Ashkin-Teller model and show that the exact result for a critical temperature is reproduced. We test also a two-layer Ising model for the presence of eventual self-duality.

1. Introduction

The recent proposition of the analytical method for locating critical temperatures in some spin systems employs moments of the transfer matrix \( T \). Let us remind briefly its basic assumptions.

For a \( d \)-dimensional spin system we define the characteristic function of rank \( n \)

\[
\rho_n(\beta) = \lim_{L \to \infty} \left( \frac{\text{Tr} T^n}{T^n} \right)^{\frac{1}{L^d}}
\]

where \( T \) is a transfer matrix of our system with linear size \( L \). The latter quantity was introduced for regularization purposes. The dependence on the inverse temperature \( \beta = 1/T \) is hidden in the definition of the transfer matrix \( T \). The same method relies on the hypothesis that the location of a maximum of the function \( \rho \) occurs at a critical point ("maximum criterion")

\[
\beta_c = \beta_{\text{max}}.
\]

It remains to test this very attractive hypothesis in practice. Among others an important question is: how big is the class of models for which the relation (1) indeed holds for any \( n \) ? A conjecture was given, that a maximum rule is at least valid for self-dual systems. Indeed it was checked directly for simple self-dual systems like Ising and \( q \) state Potts models on a square lattice \( \square \).

Recently Souza et al. have analyzed the Ashkin-Teller model \( \square \). However in particular case of the isotropic Ashkin-Teller, where the phase structure is determined from the self-duality condition, the predicted critical temperature is a good numerical estimation of the exact value.

In this paper we introduce some modifications which allow to formulate exact criterion for any self-dual model. We show it on the Ashkin-Teller model as an example. Apart from determining critical temperatures our method can be used to test the existence of duality transformations for more complicated models. We investigate a certain kind of duality relation in the two-layer Ising model and show that it is not self-dual.

2. Application to the Ashkin-Teller model

The Ashkin-Teller model \( \square \) is defined by the Hamiltonian

\[
H = -J_0 - J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - J' \sum_{\langle i,j \rangle} s_i s_j - J_4 \sum_{\langle i,j \rangle} s_i \sigma_i s_j \sigma_j
\]

with two Ising-like variables \( s_i \) and \( \sigma_i \) located on the same site \( i \) of a quadratic lattice. In some sense the AT model interpolates between the Ising \( (J_4 = 0) \) and 4-state Potts model \( (J = J' = J_4) \). In general its phase structure is rather complicated and can not be simply obtained.

In the simpler isotropic AT model \( (J = J') \) the duality transformation provides for \( J \geq J_4 \) the position of a critical point. It is convenient to
introduce dimensionless coefficients

\[ K_0 = \beta J_0, \quad K = \beta J, \quad K_4 = \beta J_4 \]  \hspace{1cm} (4)

and the quantities

\[ \omega_0 = \exp(2K + K_4 + K_0), \quad \omega_2 = \exp(-K_4 + K_0), \quad \omega_3 = \exp(-2K + K_4 + K_0). \]  \hspace{1cm} (5)

Then the partition function for the isotropic AT model is invariant

\[ Z(\omega'_0, \omega'_2, \omega'_3) = Z(\omega_0, \omega_2, \omega_3) \]  \hspace{1cm} (6)

under the duality transformation

\[ \omega'_0 = \frac{1}{2}(\omega_0 + 2\omega_2 + \omega_3), \quad \omega'_2 = \frac{1}{2}(\omega_0 - \omega_3), \quad \omega'_3 = \frac{1}{2}(\omega_0 - 2\omega_2 + \omega_3). \]  \hspace{1cm} (7)

The critical temperature is known from the self-duality condition

\[ \omega_0 = 2\omega_2 + \omega_3. \]  \hspace{1cm} (8)

From definition (6) follows that

\[ \rho_n(\beta) = \lim_{L \to \infty} \left( \frac{Z^i_n}{Z_n} \right)^{\frac{1}{n}} \]  \hspace{1cm} (9)

where \( Z_1 \) and \( Z_n \) are the partition functions of a chain of length \( L \) and of such \( n \) coupled chains respectively. In our example the characteristic function \( \rho \) depends on two couplings \( K \) and \( K_4 \) (as can be easily noticed \( K_0 \) does not appear in the final result). Therefore we may expect similar to (3) invariance for the function \( \rho \)

\[ \rho_n(K', K_4') = \rho_n(K, K_4) \]  \hspace{1cm} (10)

where \( K' \) and \( K_4' \) are the dual couplings to \( K \) and \( K_4 \) respectively.

For simpler models (like Ising or Potts) the function \( \rho \) depends only on one coupling or equivalently on \( \beta \). Then it can be easily shown that if there is only one maximum of \( \rho \) at some \( \beta_{\text{max}} \) it must coincide with the self-dual point \( \beta_{\text{max}} = \beta^* \). The same is not true in our case. In fact the straight line parametrized by

\[ K = \beta J, \quad K_4 = \beta J_4 \]  \hspace{1cm} (11)

is not consistent with the duality transformation i.e. the dual image of a point \((K, K_4)\) taken from line (11) does not lie necessarily on this line. Our proposition of the modified criterion employs the duality transformation to find the proper direction for passing the self-dual curve. Since we are mainly interested in the behavior of the function \( \rho \) near the real critical point it is sufficient to consider the linearized duality transformation in a vicinity of some self-dual point \((K^{*}_0, K^*, K_4^*)\). Let us denote the vector \( k^T = (K_0 - K^*_0, K - K^*, K_4 - K_4^*) \) and its image under the duality transformation as \( k' \). Then

\[ k' = Mk \]  \hspace{1cm} (12)

where the transformation matrix \( M \) is:

\[ 
\begin{pmatrix}
1 & \frac{a^2}{a^2 - b} & b^2 \\
0 & -a & -ab \\
0 & \frac{a^2b - b}{a} & a^2
\end{pmatrix}
\]  \hspace{1cm} (13)

with \( a = \sinh 2K^* \) and \( b = \cosh 2K^* \). The matrix \( M \) has three eigenvectors: two with eigenvalue 1 and one with \(-1\). The latter eigenvector

\[ e^T_3 = \left( \frac{2 \cosh 2K^*}{\cosh 4K^* - 3}, \frac{-\sinh 4K^*}{3 - \cosh 4K^*}, 1 \right) \]  \hspace{1cm} (14)

is interesting since it corresponds to approaching the self-dual curve from both sides and provides the valid parametrization (analogous to (11)) in the modified criterion

\[ K_4 = \frac{3 - \cosh 4K^*}{\sinh 4K^*}(\beta - K^*) + K^*_4, \quad K = \beta, \]  \hspace{1cm} (15)

where \( J = 1 \) is assumed.

Of course the arguments given above are not a rigorous mathematical proof. In particular the assumption that for modified criterion the function \( \rho \) has only one maximum has to be checked directly for a given model. For the AT model few lowest moments can be easily computed numerically. Table.1 contains the critical temperatures obtained from the \( \rho_2 \) function in the original and modified method. In accord to (3) original criterion is exact only for \( J_4 = 0 \) (two decoupled Ising models) and for \( J_4 = 1 \) (four state Potts model). The modified method gives exact results for \( J_4 \leq 1 \) up to rounding errors of order of \( 10^{-8} \).
For $J_4 > 1$ the self-dual curve (8) is not longer a critical line. In fact the phase structure is more complicated with two second order phase transitions. Our criterion predicts the existence of only one phase transition exactly on the self-dual curve.

3. Application to the two-layer Ising model

It is very interesting to apply the modified criterion to other models (not necessarily self-dual) for which the original maximum rule does not give exact answers. The two-layer Ising model is an important example. Its Hamiltonian resembles that for the AT model

$$H = -J \sum_{(i,j)} \sigma_i \sigma_j - J \sum_{(i,j)} s_i s_j - J_2 \sum_i s_i \sigma_i .$$  

(16)

The main difference is in the form of the interaction term and in the interpretation of spin variables $s$ and $\sigma$ which are now assigned to two distinct layers. Neither the duality transformation nor the exact critical temperature is known for this model. One can still attempt to determine the slope of the straight line in the modified criterion from the condition

$$\beta_{\text{crit}} = \beta_{\text{max}} .$$  

(17)

A priori, it is not even certain wheather the relation (17) can be satisfied at all. We found that we were able to estimate the slope numerically for few lowest moments (Table 2). For $\beta_{\text{crit}}$ ($J = J_4 = 1$) we take the value 0.2760, the result of Monte Carlo simulations [3]. Since it is not exact, with the statistical errors on the last decimal digit, for comparison the results for two other possible values of $\beta_{\text{crit}}$ are also given. The resulting slopes depend on $n$ which is exactly what we expect for not self-dual models. Since we do not have at our disposal sufficiently precise estimations of the real critical temperature it is premature to present similar values for other critical points ($K, K_2$). However it is rather obvious that the results would not differ qualitatively.

In conclusion, the method of moments is very closely related to self-duality of a given model. For any self-dual model there is a unique direction in the space of parameters which allows to construct exact criterion. Conversely if the direction does not depend on $n$ then this is a strong argument for the existence of a self-duality relation in a model.

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**Table 1**

Comparison of different estimations of the critical temperature for the isotropic Ashkin-Teller with $J = 1$: $\beta_{\text{crit}}$ (exact value), $\beta_{\text{max}}$ (original criterion), $\hat{\beta}_{\text{max}}$ (modified criterion).

| $J_4$ | $\beta_{\text{crit}}$ | $\beta_{\text{max}}$ | $\hat{\beta}_{\text{max}}$ |
|------|----------------|----------------|--------------------|
| 0.00 | 0.44068679 | 0.44068679 | 0.44068679 |
| 0.10 | 0.41215166 | 0.41150224 | 0.41215166 |
| 0.20 | 0.38799451 | 0.38716551 | 0.38799451 |
| 0.30 | 0.36721416 | 0.36642983 | 0.36721416 |
| 0.40 | 0.34402080 | 0.34400572 | 0.34400572 |
| 0.50 | 0.3315396 | 0.3313596 | 0.3313596 |
| 0.60 | 0.3183130 | 0.3183130 | 0.3183130 |
| 0.70 | 0.30618959 | 0.30618959 | 0.30618959 |
| 0.80 | 0.2947908 | 0.2947908 | 0.2947908 |
| 0.90 | 0.28421612 | 0.28421611 | 0.28421611 |
| 1.00 | 0.2745307 | 0.2745307 | 0.2745307 |

**Table 2**

Slopes of the lines (see eq. (15)) in the modified criterion for the two-layer Ising model.

| $\beta_{\text{crit}}$ | n=2 | n=3 | n=4 | n=5 |
|----------------|----|----|----|----|
| 0.2755 | 0.6399 | 0.5969 | 0.5915 | 0.5929 |
| 0.2760 | 0.6233 | 0.5746 | 0.5647 | 0.5625 |
| 0.2765 | 0.6067 | 0.5526 | 0.5382 | 0.5324 |