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Nuclear Physics B (Proc. Suppl.) 119 (2003) 855–857

NUCLEAR PHYSICS B
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New algorithm of the high-temperature expansion for the Ising model in three dimensions

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New algorithm of the finite lattice method is presented to generate the high-temperature expansion series of the Ising model. It enables us to obtain much longer series in three dimensions when compared not only to the previous algorithm of the finite lattice method but also to the standard graphical method. It is applied to extend the high-temperature series of the simple cubic Ising model from β^{26} to β^{46} for the free energy and from β^{25} to β^{32} for the magnetic susceptibility.

1. INTRODUCTION

The finite lattice method[1–3] is a powerful tool to generate the exact high- and low-temperature series and other exact expansion series for the spin models in the infinite volume limit. In the graphical method, one has to list up all the relevant diagrams and count the number they appear. In the finite lattice method we can skip these jobs and reduce the main task to the calculation of the partition function for the finite size lattices, which can be done efficiently using the site-by-site integration[4,5] without the graphical technique.

It has been extremely effective primarily in two dimensions, but unfortunately it has worked out the series only in some limited cases in three dimensions. This is because in two dimensions the CPU time and the computer memory needed to obtain the series to order N increase exponentially with N, while they grow up exponentially with N^2 in three dimensions. Here we present a new algorithm of the finite lattice method in which the CPU time and the computer memory increase exponentially with $N \log N$. It enables us to generate much longer series of the high-temperature expansion for the Ising model in three dimensions when compared not only to the previous algorithm of the finite lattice method but also to the graphical method.

Although our main target is in three dimensions, the new algorithm of the finite lattice method applies in arbitrary dimensions, so we describe it in two dimensions for convenience in the next two sections.

2. FINITE LATTICE METHOD

In the finite lattice method to generate the high-temperature series for the free energy in two dimensions we calculate the partition function $Z(l_x \times l_y)$ for the finite size lattices with $2(l_x + l_y) \leq N$ and define recursively[2]

$$\phi(l_x \times l_y) = \log\left[Z(l_x \times l_y)\right] - \sum_{\substack{l'_x \leq l_x, l'_y \leq l_y, \\ l'_x + l'_y \neq l_x + l_y}} \phi(l'_x \times l'_y) \,. \qquad (1)$$

Here we use the notation for the lattice size such that the 1×1 lattice means the unit square composed of 2×2 sites. The Boltzmann factor for each bond is expressed as

$$\exp\left(\beta s_k s_{k'}\right) = \cosh\left(\beta\right)\left(1 + t s_k s_{k'}\right), \qquad (2)$$

with $\beta = J/k_B T$ and $t = \tanh\left(\beta\right)$. We define the bond configuration as the set of bonds to which

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0920-5632/03/$ – see front matter
doi:10.1016/S0920-5632(03)01701-8

the factor $ts_k s_{k'}$ in (2) is assigned while the factor 1 is assigned to the other bonds. Non-vanishing contribution to the partition function comes only from the bond configuration in which the bonds form one or more closed loops. Each of the closed loops is a polymer in the standard cluster expansion[6]. Then the Taylor expansion of $\phi(l_x \times l_y)$ with respect to t includes the contribution from all the clusters of polymers in the standard cluster expansion that can be embedded into the lattice of $l_x \times l_y$ but cannot be embedded into any of its rectangular sub-lattices $l'_x \times l'_y$ and it starts from the term t^n with $n = 2(l_x + l_y)$, which comes from the cluster of a single polymer (one closed loop of bonds) that have two intersections with any line perpendicular to the lattice bonds. The expansion series of the free energy density in the infinite volume limit is given by

$$f = \sum_{2(l_x+l_y)\leq N} \phi(l_x \times l_y) \tag{3}$$

3. NEW ALGORITHM

In the standard algorithm of the finite lattice method the full partition function for the finite size lattice is calculated with all the bond configurations taken into account. In order to obtain the series to a given order, however, it is enough to consider only a restricted number of the bond configurations. Let us consider the anisotropic model of the simple cubic Ising model with $\beta_i = J_i/k_BT$ and $t_i = \tanh(\beta_i)$ $(i = x, y)$. To obtain the series for $\phi(l_x \times l_y)$ to order $N_y = 2l_y + \Delta N_y$ in t_y we introduce[7] in the new algorithm $\phi(l_x \times l_y, \Delta N_y)$ defined recursively by

$$\begin{aligned}\phi(l_x \times l_y, \Delta N_y) &= \log[Z(l_x \times l_y, \Delta N_y)] \\ &\quad - \sum_{\substack{l'_x \leq l_x, l'_y \leq l_y, \\ l'_x + l'_y \neq l_x + l_y}} \phi(l'_x \times l'_y, \Delta N_y)\ .\end{aligned} \tag{4}$$

Here the partition function $Z(l_x \times l_y, \Delta N_y)$ is calculated only with the bond configurations taken into account that have orders n_{yi} in t_y for the i-th layer perpendicular to the y-direction satisfying

$$\sum_{i=1}^{l_y} \max(n_{yi}, 2) \leq 2l_y + \Delta N_y\ . \tag{5}$$

We neglect every bond configuration for the partition function that has $\sum_{i=1}^{l_y} \max(n_{yi}, 2) > 2l_y + \Delta N_y$ among the configurations that have $\sum_{i=1}^{l_y} n_{yi} \leq 2l_y + \Delta N_y$. It is easy to prove that any of the neglected configuration does not contribute to $\phi(l_x \times l_y)$ in the order lower than or equal to $N_y = 2l_y + \Delta N_y$. For such a configuration at least one of the n_{yi}'s should be zero, so they are disconnected configuration(composed of more than one polymer) or they can be embedded into a rectangular sub-lattice of $l'_x \times l'_y$ with $l'_y < l_y$ and in either case they do not contribute to $\phi(l_x \times l_y)$ in the order lower than or equal to $N_y = 2l_y + \Delta N_y$. They contribute to $\phi(l_x \times l_y)$ only in higher order than $N_y = 2l_y + \Delta N_y$ by constituting the connected cluster of polymers together with the polymers coming from other configurations that have $n'_{yi} \geq 2$ for the layer i with $n_{yi} = 0$. Examples of the bond configurations are shown in Figure 1 for $l_x = 4$, $l_y = 5$. The example (a) has $\{n_{yi}\} = \{2, 2, 4, 2, 2\}$ and should be taken into account for $\Delta N_y = 2$, while the example (b) has $\{n_{yi}\} = \{0, 4, 4, 0, 2\}$ and should be neglected for the same $\Delta N_y = 2$, in spite of the fact that the total order of (b) in t_y is smaller than $2l_y + \Delta N_y$.

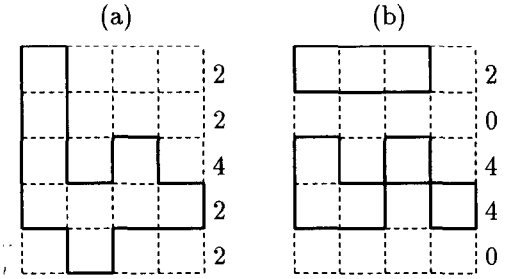

Figure 1. Examples of the bond configurations.

The contribution of the bond configuration with $\{n_{yi}\}$ to the partition function of the finite size lattice can be calculated by the transfer matrix formalism as

$$Z(\{n_{yi}\}) = V_{0,j_1} t_y^{n_{y1}} V_{j_1,j_2} t_y^{n_{y2}} \cdots t_y^{n_{yl_y}} V_{j_{l_y},0}\ . \tag{6}$$

Here $V_{j_i,j_{i+1}}$ is the transfer matrix element with incoming n_{yi} spins and outgoing $n_{y\,i+1}$ spins.

The summations over the spin locations $j_1, j_2, \cdots$ of the $n_{y1}, n_{y2}, \cdots$ spins, respectively, are assumed in the right hand side of (6).

In three dimensions, which is our main target, the transfer matrix element itself can be regarded as the partition function in two dimensions and can be calculated efficiently by the site-by-site construction[4,5]. In the new algorithm most of the CPU time should be used for the calculation of these transfer matrix elements, and the total CPU time to generate the series to order N can be estimated to increase exponentially with the leading term of the exponent proportional to $N \log N$.

4. RESULT

The new algorithm is applied to generate the high-temperature series of the simple cubic Ising model for the free energy[7] to β^{46} and for the magnetic susceptibility[8] to β^{32}. The obtained series agree with the previous series to β^{26} for the free energy[9], which was obtained by the previous algorithm of the finite lattice method, and to β^{25} for the susceptibility[10], which was obtained by the graphical method. It should be commented that the previous algorithm of the finite lattice method can generate the susceptibility series only to β^{13}.

Preliminary analysis of the free energy series using the inhomogeneous differential approximation and the ratio method biased by the value of the critical point β_c gives the estimation of the critical exponent for the specific heat as $\alpha = 0.104(1)$ and $\alpha = 0.108(1)$ corresponding to the result of $\beta_c = 0.22165459(10)$ and $\beta_c = 0.2216595(15)$,respectively, of the recent two Monte Carlo simulations[11,12]. Unfortunately the free energy series can give the estimate of the critical point itself only in poor precision. The analysis of the susceptibility series by the ratio method gives the estimate of the critical point as $\beta_c = 0.2216550(5)$ and the critical exponent as $\gamma = 1.2370(2)$. This estimation for the critical exponent do not use the value of the critical point as the input. It is consistent with the recent estimate $\gamma = 1.2371(4)$ obtained from the high-temperature series of the generalized Ising model [13].

5. DISCUSSION

We have presented the new algorithm of the finite lattice method for the high-temperature expansion of the Ising model. It has been applied to the high-temperature expansion of the free energy and the magnetic susceptibility for the simple cubic Ising model. It can be applied to the high-temperature expansion of other quantities such as the correlation length and it can also be applied to the models with continuous spin variables such as the XY model in three dimensions. We note that the dimensionality of the lattice is not restricted to three as can seen by the fact that the description of the new algorithm in section 3 was given in two dimensions. Furthermore the basic idea of the new algorithm can be used in the low-temperature expansion for the spin models. We can expect that the new algorithm will enable us to generate the series for these models that are much longer than the presently available series.

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