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COMPUTATIONAL ASPECTS OF THE DIFFERENTIAL OPERATOR TECHNIQUE FOR ISING MODEL[1]

S. Mockovčiak, M. Jaščur
Department of Theoretical Physics and Geophysics, Faculty of Natural Sciences, P. J. Šafárik University, Moyzesova 16, 041 54 Košice, Slovakia

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A method for step application of binomial expressions, containing the Kaneyoshi differential operator, is introduced. This method substantially simplifies computations in one- and two-spin cluster effective-field theory approximations for arbitrary number of neighbours. As an example the critical temperature of the site-diluted spin-1 Ising model is calculated.

1. Introduction

Over the last fifteen years the properties of magnetic systems have been studied partly by a method proposed by Honmura and Kaneyoshi [1]. The method is based on using of the exact Callen's identities [2] for a single spin and averaging via differential operator technique. Later, Bobák and Jaščur [3] generalized the method for the case of pair neighbouring spins and then also utilized differential operator technique. Both one- and two-spin cluster formulations lead to substantial improvement over the standard mean-field theory. Moreover, the differential operator method has been successfully used in developing of the effective-field renormalization group approach [4-9].

In all cases the differential operator technique and the full decoupling for thermal average of spin-variable products lead to the evaluation of expressions

$$\prod_i \{F_i[\cosh(t_i D_i)]; \sinh(t_i D_i); m; q; p; ...\}^{z_i} f(x_1, ..., x_i, ...)\Big|_{\text{all } x_i=0}, \qquad (1)$$

where the operator F_i is as a rule of the binomial form $(a + mb)$. $D_i = \partial/\partial x_i$ is the differential operator, $m = \langle\langle S_k \rangle\rangle_c$, $q = \langle\langle S_k^2 \rangle\rangle_c$ are both thermal and configurational average of Ising spin variables and their powers, p represents for the site-diluted systems the concentration of magnetic atoms. z_i is an integer, dependent on the coordination number of the studied structure,

$$t_i = \frac{J_i}{k_B T} \qquad (2)$$

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is the temperature parameter and J_i stands for the exchange interaction between spins in ith equivalent positions.

The conventional attempt to expression (1) is to calculate whole operator $\prod_i F_i$ and then to apply it to the function $f(x_1, ..., x_i, ..)$. This attempt, however, becomes rapidly very tedious in treating more complicated problems, such as problems with higher coordination number ($z > 4$) or higher spins, problems with next-nearest neighbour interaction and in general also the applications of two-spin cluster approximation. The main aim of this work is to show how we can avoid this shortcoming.

2. Step Application of F_i

The essence of our method is to evaluate each operator $(F_i)^{z_i}$ (with moderate z_i) independently. This evaluation gives in (1) terms

$$\Big[\sum_{\mu=0}^{z_i} c_\mu^c \cosh(\mu t_i D_i)\Big] \times \Big[\sum_{\nu=1}^{z_j} c_\nu^s \sinh(\nu t_j D_j)\Big] f(x_1, ..., x_i, ..., x_j, ..)\Big|_{\text{all } x=0}, \tag{3}$$

and after the application of operators $\cosh(\mu t_i D_i)$ and $\sinh(\nu t_i D_i)$ we have finally

$$\frac{1}{4} \sum_{\mu=-z_i}^{z_i} c_\mu^c \sum_{\nu=-z_j}^{z_j} c_\nu^s f(x_1, ..., x_i + \mu t_i, ..., x_j + \nu t_j, ...)\Big|_{\text{all } x=0}, \tag{4}$$

At this stage the problem is already possible to solve by using a computer. For that purpose we need to calculate the coefficients c_μ^c and c_ν^s that satisfy the following relation:

$$c_\mu^c = c_{-\mu}^c, \quad c_\nu^s = -c_{-\nu}^s, \quad c_0^s = 0. \tag{5}$$

As far as we put the factor $1/2$ in the front of the sum, we must be carefull with the c_0^c which occurs in the sum one time only.

3. Examples. Critical Temperature of the Site-Diluted Spin-1 Ising Model

3.1. Two-Spin Cluster Approximation for $z = 4$

For this problem the following equations can be obtained:

$$m = p^2[F_x(D_x, m, q)F_y(D_y, m, q)]^{z-1} f(x, y)|_{x,y=0} + p(1-p)[F_x(D_x, m, q)]^{z-1} f_2(x)|_{x=0} \tag{6}$$

$$q = p^2[F_x(D_x, m, q)F_y(D_y, m, q)]^{z-1} g(x, y)|_{x,y=0} + p(1-p)[F_x(D_x, m, q)]^{z-1} g_2(x)|_{x=0} \tag{7}$$

For details see [7]. Here

$$F_i(D_i, m, q) = [(1-q) + q\cosh(D_i t) + m\sinh(D_i t)] \tag{8}$$

and functions $f(x, y), g(x, y), f_2(x), g_2(x)$ will be given below.

The second-order phase transition line is defined by limit $m \to 0$ and it is determined by the relation

$$1 = 3[2p^2 A_x^3(t, q)A_y^2(t, q)B_y(t)f(x, y)|_{x,y=0} + p(1-p)A_x^2(t, q)B_x(t)f_2(x)|_{x=0}] \tag{9}$$

where t is the critical temperature parameter (2) and

$$q = p^2[A_x(t, q)A_y(t, q)]^3 g(x, y)|_{x,y=0} + p(1-p)A_x^3(t, q)g_2(x)|_{x=0}, \tag{10}$$

with operators

$$A_i = (1-q) + q\cosh(D_i t), \qquad B_i = \sinh(D_i t) \qquad i = x, y \tag{11}$$

and with functions (see[7]):

$$\begin{aligned}
f(x, y) &= f_1(x, y)/f_0(x, y) \\
g(x, y) &= g_1(x, y)/f_0(x, y) \\
f_0(x, y) &= 1 + 2[e^t\cosh(x+y) + e^{-t}\cosh(x-y) + \cosh x + \cosh y] \\
f_1(x, y) &= 2e^t\sinh(x+y) + \sinh x + \sinh y \\
g_1(x, y) &= 2[e^t\cosh(x+y) + e^{-t}\cosh(x-y)] + \cosh x + \cosh y
\end{aligned} \tag{12}$$

$$f_2(x) = \frac{2\sinh x}{1 + 2\cosh x} \qquad g_2(x) = \frac{2\cosh x}{1 + 2\cosh x}.$$

Using the method, given in Section II one finds explicit form for the equations (9) and (10):

$$1 = \frac{6}{4}p^2 \sum_{\mu=-3}^{3}\sum_{\nu=-3}^{3} c_\mu^c c_\nu^s f(\mu t, \nu t) + \frac{3}{2}p(1-p)\sum_{\nu=-3}^{3} c_\nu^s f_2(\nu t) \tag{13}$$

$$q = \frac{1}{4}p^2 \sum_{\mu=-3}^{3}\sum_{\rho=-3}^{3} c_\mu^c c_\rho^c g(\mu t, \rho t) + \frac{1}{2}p(1-p)\sum_{\mu=-3}^{3} c_\mu^c g_2(\mu t), \tag{14}$$

where

$$\begin{array}{llll}
c_0^c = 2[(1-q)^3 + \frac{3}{2}(1-q)q^2] & c_1^c = 3q(1-q)^2 + \frac{3}{4}q^3 & c_2^c = \frac{3}{2}(1-q)q^2 & c_3^c = \frac{q^3}{4} \\
c_0^s = 0 & c_1^s = (1-q)^2 + \frac{q^2}{4} & c_2^s = q(1-q) & c_3^s = \frac{q^2}{4}
\end{array}$$

3.2. Two-Spin Cluster Approximation for $z = 6$

From equations (6) and (7), that are valid in this case, we obtain the following expressions

$$1 = \frac{10}{4}p^2 \sum_{\mu=-5}^{5}\sum_{\nu=-5}^{5} c_\mu^c c_\nu^s f(\mu t, \nu t) + \frac{5}{2}p(1-p)\sum_{\nu=-5}^{5} c_\nu^s f_2(\nu t) \tag{15}$$

and

$$q = \frac{p^2}{4} \sum_{\mu=-5}^{5}\sum_{\rho=-5}^{5} c_\mu^c c_\rho^c g(\mu t, \rho t) + \frac{1}{2}p(1-p)\sum_{\mu=-5}^{5} c_\mu^c g_2(\mu t), \tag{16}$$

where

$c_0^c = 2[(1-q)^5 + 5(1-q)^3q^2 + \frac{15}{8}(1-q)q^4]$ $\quad c_0^s = 0$

$c_1^c = 5q(1-q)^4 + \frac{15}{2}(1-q)^2q^3 + \frac{5}{8}q^5$ $\quad c_1^s = (1-q)^4 + \frac{3}{2}(1-q)^2q^2 + \frac{q^4}{8}$

$c_2^c = 5q^2(1-q)^3 + \frac{5}{2}(1-q)q^4$ $\quad c_2^s = 2q(1-q)^3 + (1-q)q^3$

$c_3^c = \frac{5}{2}(1-q)^2q^3 + \frac{5}{16}q^5$ $\quad c_3^s = \frac{3}{2}q^2(1-q)^2 + \frac{3}{16}q^4$

$c_4^c = \frac{5}{8}q^4(1-q)$ $\quad c_4^s = \frac{1}{2}(1-q)q^3$

$c_5^c = \frac{q^5}{16}$ $\quad c_5^s = \frac{q^4}{16}$

In both cases the concentation dependence of the critical temperature (or the curve t^{-1} vs. p) can be immediately calculated from (13), (14) for $z = 4$ and from (15), (16) for $z = 6$, respectively.

The transition temperature decreases with decreasing p and reduces to zero at the critical concentration p_c. We received t_c^{-1} equal to 2.1491 and 3.4995 at $p = 1$ (pure Ising model) for $z = 4$ and $z = 6$, respectively. The critical concentration p_c is 0.4069 for square and 0.2725 for simple cubic lattices.

4. Conclusions

In this work we have shown how to simplify tedious algebraic calculations in the framework of differential operator method. From the examples presented in Section III we can see that the increasing coordination number z has the minimal effect on the growth of calculations, except the coefficients c^c and c^s. The present method completely avoids operations with many terms in sums and consequently allows to apply differential operator method to physical problems that are practically untractable by another way [4,5].

In Tucker et al. [10] the effective field equations for Ising model having all possible single–ion and nearest-neighbour pair interactions are derived for all spin values from $S = 1/2$ to $S = 5/2$. Our method represents an alternative approach to evaluation of a set of coupled equations (23) from [10] for single-site cluster theory. It is applicable to two–site clusters and bond diluted Ising systems [5] as well. On the other hand, for single–site clusters, our method is much less general than that of Tucker et al.

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