Excluded Volume Effects for Frequency Moments of the Spin Autocorrelation Function of the Heisenberg Model on a Square Lattice at High Temperatures

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The expansion coefficients in powers of time (or frequency moments) of the spin autocorrelation function are represented at the simple self-consistent approximation as a sum of weighted trees on a Bethe lattice. Using the computer numeration and the Monte Carlo method for self-avoidingly embedding these trees on the square lattice, we estimate the moments and the convergence radius of the expansion. We show that the moments decrease and the radius increases in consequence of the volume exclusion.

Excluded volume effects are well known to modify properties of large clusters[1–3] modelled usually by lattice animals (i.e., connected clusters embeddable in a regular lattice). They are the same for both real and formal clusters. The real clusters are polymer molecules[1, 3] and percolation clusters.[2] The formal clusters are formed in high-temperature[4] and short-time[5] expansions. In their turn peculiarities of the large clusters determine properties of singularities of the expanded functions. Since the time expansions are not so well known as temperature ones they are necessary to be reported in detail.

We consider the isotropic Heisenberg model on a regular lattice at high temperatures.[5–11] The Hamiltonian of the model is given by

$$\mathscr{H} = -\sum_{i,j} J_{ij}(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z) \tag{1}$$

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where J_{ij} is equal to J when i and j are the nearest-neighbour lattice sites and zero otherwise, S_i^α is the α-component ($\alpha = x, y, z$) of the vector spin operator at the lattice site i, $S = 1/2$. We calculate the time-dependent autocorrelation function $F(t)$, which is defined by

$$F(t) = Sp\{\exp(i\mathcal{H}t)\, S_0^\alpha \exp(-i\mathcal{H}t)\, S_0^\alpha\}/Sp\{(S_0^\alpha)^2\} \qquad (2)$$

The function (2) may be expanded in powers of time

$$F(t) = \sum_{n=0}^{\infty} (-1)^n M_{2n} t^{2n}/(2n)! \qquad (3)$$

where the expansion coefficients are defined by the $2n$-fold commutator:

$$M_{2n} = Sp\{[\mathcal{H}, [\mathcal{H}, ... [\mathcal{H}, S_0^\alpha]...]\, S_0^\alpha\}/Sp\{(S_0^\alpha)^2\} \qquad (4)$$

On the other hand M_{2n} are moments of the spectral density of the autocorrelation function (2).[12]

The calculation rules of the multiple-fold commutations in (4) have been considered in many works.[5–11] From a geometrical point of view this procedure has a similarity with cluster growth processes.[1–3, 13, 14] In fact, if the interaction of spin operator pair in the Hamiltonians in (4) is presented by a bond between appropriate lattice sites then each commutation adds the bond to the existing cluster. Using the well-known properties of the Pauli matrices we have following results. The growing cluster is a bond one with operators S_i^α or $(S_i^\alpha)^2 = 1/4$ at their sites. Let name the first sites as active ones and another sites as nonactive ones. Thus each commutation adds the bond at an active site of the cluster. If the free end of the bond is placed on an unoccupied lattice site then the cluster size increases on one active site. If the free end of the bond is placed on a cluster site then the commutation result depends on the projection of the site spin operator. It may be zero or the site activity may be changed: the active site becomes the nonactive one and vice versa. It should be noted that the total ensemble of clusters is generated because in (4) the Hamiltonians have the sum of all bonds and projections.

Among the clusters of this ensemble only ones with nonzero traces give contributions to the moments (4). These are the clusters with the active initial site 0 and with nonactive all another sites. Then M_{2n} can be obtained as a sum over connected graphs with $2n$ bonds and $n + 1$ or fewer sites one of which is the initial site 0. The equal graphs constructed by different ways come as different terms of the sum. The replacement of multiple

bonds by single bonds transforms this sum to the one over basic graphs g (bond lattice animals):[5]

$$M_{2n} = J^{2n} \sum_g N(g) \, K_{2n}(g) \tag{5}$$

where $N(g)$ is the number of different ways that the given graph g may be self-avoidingly embedded on a lattice, $J^{2n} K_{2n}(g)$ is the contribution of the given graph to the moment ($K_{2n}(g)$—the spin weight coefficient). If in an approximate theory one neglects the excluded volume effects then the moment values and properties of the autocorrelation function (2) change. In the present paper the attempt of estimating these changes is made.

The second moment or the mean-square frequency is given by

$$M_2 = 2J^2 Z$$

where Z is a number of nearest neighbours, in particular $Z = 2d$ for the simple cubic lattice of the dimension d. Calculation of high order moments is a very difficult problem. Up to now only few first moments have been calculated: up to $n = 15$ at $d = 1$,[9] up to $n = 4$ at $d = 3$,[5] up to $n = 5$ at $d = 2$[8] and $d = \infty$.[11] The sizes of clusters corresponding to these moments are not enough for discovering the excluded volume effects. Therefore for the moments we use below approximate expressions obtained on the basis of the self-consistent approach of Resibois–DeLeener–Blume–Hubbard.[6, 7] Recently[11] we have shown that at $d \to \infty$ this approach becomes correct and lattice trees give the main contribution in the sum (5). In the present work we pass from the trees on the infinite-dimensional cubic lattice to trees on the Bethe lattice[1, 2, 13, 14] of coordination number Z. Then the computer simulation method is used to calculate the decrease of the moments of the spin system on the square lattice after excluding of the contribution corresponding to the trees with intersected branches. The moments up to 24 order are calculated by a method of exact enumeration of all trees whereas the higher moments up to 40 order are approximate calculated by a Monte Carlo method. In the end of the paper the radius of convergence of the series (3) is estimated on the found moments.

We shall first consider the self-consistent equation for $F(t)$ obtained by Resibois–DeLeener–Blume–Hubbard.[6, 7] As it has been shown by us[11] this equation reduces at $d \to \infty$ to the equation for the correlation function of a magnetic moment moving in the Gaussian fluctuating magnetic field, the correlation function of which expresses in terms of $F(t)$. The complicated form of this nonlinear integral equation is caused by the noncommutativity of magnetic moment rotations around different instant orientations of the magnetic field fluctuating in time. For qualitative analysis of

the effects interesting us we shall make use the simple approximate self-consistent equation of Blume–Hubbard[7]

$$F(t) = \exp\left\{ -M_2 \int_0^t (t - t') F(t') dt' \right\} \tag{6}$$

where the exponent is the first term of the usual cumulant expansion. The simplification of Eq. (6) is reached at the expense of neglect of the non-commutativity of the rotations or neglect of change of the field orientation. The physical motivation of such approximation obtaining the title of the adiabatic theory of the line shape[12] is the slowness of a velocity of the field orientation change compared to the Larmor frequency.

Let us now examine Eq. (6) as an equation for the generating function of moment clusters in the sum (5). For this purpose we consider the spin system on a Bethe lattice of coordination number Z. In this case possible graphs in (5) are root trees. Since each added site should be deactivated the maximal possible size of the trees is equal to $n + 1$ sites for the $2n$-order moment and these trees are built of double bonds. It is clear that the deactivation of sites must be carry out sequentially from an end of a branch to the root. To estimate the number of these maximal trees let us assume that an adding and a deactivating of sites on different branches are independent. Let $w_1(n)$ be a number of trees of $n + 1$ sites and n double bonds when the root has only one neighbour. Then we have

$$w_1(n) = \sum \frac{(2n - 2)!}{(2n_1)!\,(2n_2)!\cdots(2n_{Z-1})!}\, w_1(n_1)\, w_1(n_2)\cdots w_1(n_{Z-1}) \tag{7}$$

where the summation is over all possible distributions of $2n - 2$ bonds among $Z - 1$ branches grown from the site nearest to the root. Introducing the generating function

$$W_1(x) = \sum_{n=0}^{\infty} w_1(n)\, x^{2n}/(2n)! \tag{8}$$

we can obtain from (7) the equation

$$W_1(x) = 1 + a^2 \int_0^x dx_1 \int_0^{x_1} dx_2 [\, W_1(x_2)]^{Z-1} \tag{9}$$

where $a^2 = 1$. Using $W_1(x)$ we can obtain generating functions for the number of trees when the root has Z neighbours

$$W_Z(t) = [\, W_1(t)]^Z \tag{10}$$

In order to consider the limiting case $Z \to \infty$ let us introduce $y = xZ^{1/2}$ in (9). Then in this limit (10) reduces to

$$W_Z(y) = \exp\left\{ a^2 \int_0^y dy_1 \int_0^{y_1} dy_2\, W_Z(y_2) \right\} \qquad (11)$$

It is easy to see that (11) is identical to (6) if $y = itZ^{1/2}$ and $a^2 = 2$. When we pass from $a^2 = 1$ to $a^2 = 2$ the number of trees with $n+1$ sites increases by the factor of 2^n. It is the consequence of the presence of three spin projections in the Hamiltonian (1). Therefore one tree can be constructed by many ways differed one from another by a set of spin projection operators and by their connection order. The value 2^n is the maximal value of this factor. For some trees this factor is smaller since some combinations of spin operators give zero results. The relation $a^2 = 1$ corresponds to the existence of a single combination for each tree.

Thus with the help of Eq. (9) and (10) we can calculate approximately the summary spin weight coefficient of all maximal root trees with n bonds on the Bethe lattice of coordination number Z (as in (5) we now return from the double bonds to single bonds). The spin weight coefficient $K_{2n}(g)$ for each such a tree is the product of the weight coefficients K_s of its sites

$$K_s = a^{2n_s} \frac{(2n_s)!}{(2n_1)!\,(2n_2)! \cdots (2n_k)!} \qquad (12)$$

where $n_1, n_2,..., n_k$ are the numbers of bonds in k branches grown from a given site, $n_s = n_1 + n_2 + \cdots + n_k$. We shall assume $a^2 = 2$ in the following.

We now transfer the trees from the $Z = 4$ Bethe lattice on a square one. The part of the trees can be embedded on the square lattice only at repeated use of the same sites, i.e., at allowing of self-intersections. The another trees can be embedded without self-intersections. To introduce the excluded volume effects for the moments we must discard the contribution of the trees with self-intersections in (5). Such a calculation of M_{2n} by exact computer enumerations is carried out via the following scheme. A n-bond tree is self-avoidingly embedded on the square lattice. The spin weight coefficient $K_{2n}(g)$ is calculated for this tree. All various such n-bond trees are enumerated and their spin weight coefficients are put together. This sum is M_{2n}/J^{2n}. The results have been obtained up to $n = 12$ and are given in Table 1.

To estimate the higher order moments a Monte Carlo method will be used. But at the beginning we rewrite Eq. (4) in the form

$$M_{2n} = J^{2n}(n+1)\, N_n \bar{K}_{2n}, \qquad \bar{K}_{2n} = \sum_g K_{2n}(g)\, N(g)/[(n+1)\, N_n] \qquad (13)$$

where N_n is the full number of lattice trees with n bonds and multiplicand $n + 1$ is the number of ways of choosing the initial site (root) on a tree. The formula (13) is still exact since we have produced identical transformations. The next step we can replace exact value $\bar{K}_{2n}$ with the its approximate value found by the Monte Carlo method. For this purpose we construct trees g_i with n bonds by connecting sequentially bonds choosing at random. A tree is deleted if it has a closed loop of bonds. In order to transform the sum over the different trees in (13) to the sum over the N constructed random trees with n bonds it is necessary to take into account that the same tree g can be constructed by $P_n(g)$ ways. Using $P_n(g)$ we obtain

$$\bar{K}_{2n} = \sum_{i=1}^{N} K_{2n}(g_i) \, P_n^{-1}(g_i) \Big/ \sum_{i=1}^{N} P_n^{-1}(g_i) \tag{14}$$

Above we have defined the evaluation rule for the weight factor $K_{2n}(g)$—the number of different ways in which the tree g with n double bonds can be constructed. The evaluation rule of the weight factor $P_n(g)$—the number of different ways to construct the ordinary tree[14] with n single bonds—turns out from the rule for $K_{2n}(g)$ after replacing all numbers $2n_k$ by n_k and $a^2 = 1$ in (12).

The values of moments up to 40 order calculated using (13) and (14) are also given in Table 1. In Eq. (13) the values N_n have been taken from the work:[15] at $n < 15$—the exact values, and at $n \geqslant 15$—the approximate values from the asymptotic expression

$$N_n \sim A n^{-1} \lambda^n (1 + B n^{-\Delta})$$

where $\lambda = 5.142$, $A = 0.527$, $B = -0.376$, $\Delta = 1.34$. We have generated $N = 10^6$ for $n \leqslant 12$, $N = 10^5$ for n from 13 to 15, and $N = 10^3$ for $n = 20$. One can see from Table 1 that the values M_{2n} obtained by the Monte Carlo method at $n \leqslant 12$ agree up to well with those obtained by exact enumeration method. The error about 30% for M_{40} was estimated by treating the data consisted of 20 parts.

We now turn to the analysis of possible changes in dynamical properties of the spin system caused by the excluded volume effects. In the previous works[10, 11] we have shown that in the limit $d \to \infty$ the solution of the nonlinear integral equation obtained for the autocorrelation function in the self-consistent approach has the important property—the existence of singular points on the imaginary time axis. The solution of the equation (9) also has singularities (Eq. (9) can be transformed to the differential one by differentiating twice and solving in quadratures).

Table 1. Values of M_{2n}/M_2^n for the $Z = 4$ Bethe Lattice and for the Square (sq) Lattice Calculated by the Exact Enumeration of Trees (Exact) and the Monte Carlo (MC) Method

n	Bethe	sq (exact)	sq (MC)
2	3	3	3.004
3	15.75	15.75	15.748
4	126	124	123.902
5	1429.31	1338.81	1338.25
6	2.183×10^4	1.866×10^4	1.867×10^4
7	4.318×10^5	3.222×10^5	3.229×10^5
8	1.074×10^7	6.702×10^6	6.695×10^6
9	3.280×10^8	1.643×10^8	1.636×10^8
10	1.207×10^{10}	4.671×10^9	4.649×10^9
11	5.269×10^{11}	1.520×10^{11}	1.543×10^{11}
12	2.689×10^{13}	5.605×10^{12}	5.517×10^{12}
13	1.588×10^{15}		2.294×10^{14}
14	1.074×10^{17}		1.170×10^{16}
15	8.249×10^{18}		6.081×10^{17}
20	1.168×10^{29}		7.014×10^{26}

Let us approximately calculate the autocorrelation function (2) of the spin system on the Bethe lattice by the use of Eqs. (9) and (10) with $x = itJ$ and $a^2 = 2$ (it is easy to see that the change of value a^2 is equal to the change of the time scale). In the neighbourhood of the two closest singularities at $\pm i\tau_c$

$$F_Z(t) \approx C(it \pm \tau_c)^{-2m} \tag{15}$$

where

$$m = Z/(Z-2), \qquad C = (2m^2/M_2)^m, \qquad \tau_c = \tau_\infty \frac{\Gamma(1/2 - 1/Z)}{\sqrt{\pi}\, \Gamma(1 - 1/Z)} \tag{16}$$

$\Gamma(x)$ is gamma-function, $\tau_\infty = \pi(2M_2^2)^{1/2}$ is the coordinate of singularities in the limit $Z \to \infty$ found in the work[7] for the equation (6). The coordinate of the closest singular point determines the convergence radius of time-power series of the considered function. It should be noted that at $Z = 2$ this radius defined by (16) becomes infinite in full accordance with the theorem of Araki[16] for one-dimensional systems.

On the other hand the convergence radius of the series (3) can be defined by the moments calculated above and given in Table 1. We first

calculate this radius using the Cauchy formula as the limit at $n \to \infty$ of the sequence of the values

$$\tau_n = [(2n)!/M_{2n}]^{1/2n} \tag{17}$$

The results are shown on the Fig. 1. To decrease the slope of the sequences of points for convenience of the analysis we move on from (17) to the formula

$$\tau_n = \left[\frac{2C \cdot \Gamma(2n + 2m)}{M_{2n}\Gamma(2m)} \right]^{1/(2n + 2m)} \tag{18}$$

taking into account the behaviour of the functions (15) in the neighbourhoods of the singular points. This formula is obtained by equating the coefficient before t^{2n} in (3) and in the short-time expansion

$$C(it + \tau_c)^{-2m} + C(it - \tau_c)^{-2m} = \sum_{n=0}^{\infty} (-t^2)^n \frac{2C \cdot \Gamma(2n + 2m)}{\Gamma(2m)(2n)!} \tau_c^{-2(n+m)}$$

The new sequences recalculated with $m = 2$ are also shown on the Fig. 1. The sequence for the Bethe lattice becomes parallel to the abscissa as expected.

The sequence for the square lattice remains the slope that may be testify to the greater value m in this case. To decrease the slope we increase m up to 4 and accordingly the coefficient C changes. Using new sequence the estimation

$$\tau_c \approx \tau_{20} = 5.4/\sqrt{M_2} \tag{19}$$

is obtained. The comparison of (19) with the result

$$\tau_c = 3.71/\sqrt{M_2}$$

found from (16) at $Z = 4$ shows that the convergence radius increases about in 1.5 times in consequence of the volume exclusion.

This result is obtained using the approximate values of moments. To calculate the exact values of moments using the formula (5) or (13) it is necessary to take into account, at first, the change of the spin weight coefficient of the lattice trees, secondly, contributions of lattice animals (graphs) with loops. As a consequence the moments vary but in our opinion the fast growth of their values with order resulting to the divergence of time-power series retain. Moreover the excluded volume effects on the exact moments may be weaken because multiple interactions with the same spin are
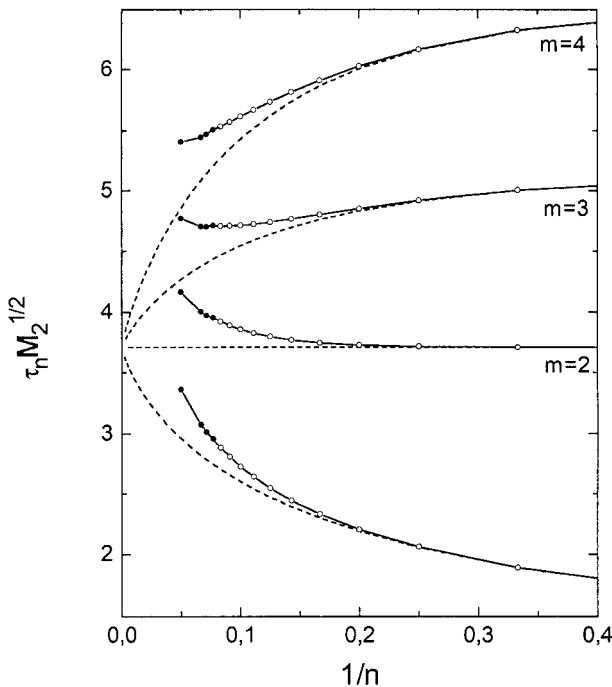
Fig. 1.   Sequences of estimates for the convergence radius versus $1/n$ according to equations (17) and (18) with $m = 2 \div 4$. Open and solid circles represent respectively the exact enumeration of trees and the Monte Carlo data for the square lattice, dashed lines represent the data for the $Z = 4$ Bethe lattice.

allowed (of course with other spin coefficients than above at intersections of the tree branches). We have discarded the multiple interactions in order to clarify the fundamental question on the convergence of the series or on the existence of the singular points of the autocorrelation function. As it is well known from the theory of critical phenomena[17] singularities are possible only at infinite systems, i.e., only at involving of an infinite number of spins. In this sense the repeated use of the same spin is useless though it varies the coordinate of similar singularity.

Thus the introduction of excluded volume effects leads to decreasing of the moments of the spin autocorrelation function and to increasing of the convergence radius of the its time power series. Nevertheless, on the our estimate, the radius value remains finite. Then the singular points of the autocorrelation function of the two-dimensional Heisenberg spin system are placed at a finite time distance like ones of the infinite dimensional system but not at infinite time distance taking place for an one-dimensional

system. So in a dynamical theory of spin systems it is necessary to take into consideration such singular points.

ACKNOWLEDGMENTS

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