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SINGULAR POINTS OF TIME-DEPENDENT CORRELATION FUNCTIONS OF SPIN SYSTEMS ON LARGE-DIMENSIONAL LATTICES AT HIGH TEMPERATURES

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Time-dependent autocorrelation functions are investigated for the Heisenberg model with spins 1/2 on d-dimensional simple cubic lattices of large dimensions d at infinite temperature. The autocorrelation function on the imaginary time axis is interpreted as the generating function of bond trees constructed with double bonds. These trees provide the leading terms with respect to $1/d$ for the time-expansion coefficients of the autocorrelation function. The correction terms from branch intersections to the generating function in the Bethe approximation are derived for these trees. A procedure is suggested for finding the correction to the coordinate of the singular point of the generating function (i.e., to the reciprocal of the branch growth-rate parameter) from the above correction terms without calculating the number of trees. The leading correction terms of order $1/\sigma^2$ (where $\sigma = 2d - 1$) are found for the coordinates of the singular points of the autocorrelation function in question and for the generating function of the trees constructed with single bonds in the Eden model.

1. Introduction

The strong dependence of singularity characteristics describing phase transitions and other critical phenomena on the space dimension d is generally recognized and comprehensively studied. The dependence of analytic properties of dynamic correlation functions of quantum spin systems at high temperatures on d is not nearly so thoroughly investigated. It was proved that in the one-dimensional case, these functions have no singular points at a finite distance in the plane of the complex temporal variable [1]. On the other hand, it was established that the autocorrelation function of the Heisenberg magnet on an infinite-dimensional lattice at an infinite temperature has singular points on the imaginary time axis at a finite distance from the origin [2]. No rigorous results are known for systems of an arbitrary dimension d.

The power series method is a powerful tool for investigating singularities of functions. These series include high-temperature expansions in phase transition theory, generating functions for clusters, i.e., lattice configurations ("animals"), in polymer and percolation theory, and finally the power series (with respect to time) studied in this paper for spin correlation functions. The coefficients in the series or, equivalently, the spectral moments can be represented as a sum of lattice configurations with bonds [3, 4]. In the limit $d \to \infty$, trees that are constructed on the lattice using double bonds remain in this sum [2, 4], and the correlation function on the imaginary time axis can be interpreted as the generating function for these trees. In contrast to the trees in polymer and percolation theory [5, 6], the weighting factor involves the number of ways the given tree can be constructed. Similar properties are characteristic of trees in the Eden model [7] that are constructed with single bonds and are therefore simpler.

In passing to spin systems on hypercubic lattices of a high, but finite, dimension, the contribution to the moments from the trees with double bonds are not unique but still remain leading. Representing time correlation functions by these trees permits investigating the possible changes in analytic properties of these

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functions under the variation of the space dimension. First, with decreasing space dimension d, a constraint on the number of branches issuing from a single tree vertex appears. The related increase in the coordinate of the nearest singular point of the autocorrelation function was found in [4] in the Bethe approximation, which had earlier been applied to trees with single bonds [5, 7]. Another consequence of the finiteness of d is the strengthening of the influence of the intersection of tree branches (the excluded volume effect). This effect was studied using the computer simulation method for two- and three-dimensional lattices in [4]. To take these effects on lattices of higher dimension into account, the method of expansion with respect to the reciprocal of the space dimension ($1/d$ or $1/\sigma$, where $\sigma = 2d - 1$) was used [6, 8–10]. In polymer theory, several $1/\sigma$-expansion terms were found for the growth-rate parameters of lattice configurations and trees [6, 9, 10], that is, for the reciprocals of the coordinates of singular points of generating functions. In this paper, we find the leading correction terms of order $1/\sigma^2$ to the coordinates of the nearest singular points of the abovementioned autocorrelation function and to the generating function of trees in the Eden model. The corrections of order $1/d$ to the root mean square cluster radius were previously calculated in the Eden model [11, 12]. We do not know of any papers with corrections to the cluster growth-rate parameter.

In Sec. 2, we describe the spin model in question and state the combinatorial problem. Section 3 is devoted to deriving formulas for the corrections from the branch intersection to the generating function for trees constructed with double bonds. These formulas are used to calculate the corrections to the coordinates of the nearest singular points of generating functions in Sec. 4. Accordingly, Secs. 4.1 and 4.2 deal with calculations for trees constructed with single and double bonds. In the appendix, the suggested approach is verified using lattice configurations.

2. Model

We consider the time-dependent autocorrelation function of a spin located at one of the lattice points of a d-dimensional simple hypercubic lattice at an infinite temperature,

$$F(t) = \frac{\mathrm{Sp}\{e^{i\varkappa t} S_0^\alpha e^{-i\varkappa t} S_0^\alpha\}}{\mathrm{Sp}\{(S_0^\alpha)^2\}}, \tag{2.1}$$

where $\varkappa$ is the Hamiltonian in the isotropic Heisenberg model with the nearest-neighbor interaction J and S_0^α is the α-component ($\alpha = x, y, z$) of the vector spin operator at the lattice point 0, $S = 1/2$. Function (2.1) can be expanded as a power series,

$$F(t) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} M_{2n} t^{2n}, \tag{2.2}$$

where the nth expansion coefficient is found via the $2n$-fold commutator,

$$M_{2n} = \frac{\mathrm{Sp}\{[\varkappa, [\varkappa, \ldots [\varkappa, S_0^\alpha] \ldots] S_0^\alpha]\}}{\mathrm{Sp}\{(S_0^\alpha)^2\}}. \tag{2.3}$$

As is known, M_{2n} is the moment of the $2n$th order for the spectral density of autocorrelation function (2.1).

The calculation rules for multiple commutators in (2.3) were thoroughly studied (see, e.g., [2, 3, 13–16]). From the geometric standpoint, they have much in common with the case of the growth process of a polymer molecule or a cluster [7, 17]. Indeed, if the bond between the lattice points occupied by the spins is associated with each pair of interacting spins in the Hamiltonian, then each commutation adds a bond to the already constructed cluster. The well-known properties of the Pauli matrices lead to the following results: the cluster is constructed of bonds, and the operators S_i^α and $(S_i^\alpha)^2 = 1/4$ are located at its lattice points. Accordingly, the corresponding lattice points are termed active and inactive. Each commutation

adds a new bond to one of the active lattice points of the cluster. If the free end of a bond falls on an unoccupied lattice point, then the cluster increases by an active lattice point. And if the free end of a bond falls on an lattice point that was already added to the cluster, then the result of the commutation depends on the projection of the spin operator of this lattice point. This result can be zero or can manifest itself in a change of the activity of the lattice point under consideration, namely, an active lattice point can become inactive and vice versa. We note that the complete set of all possible clusters is constructed simultaneously because the Hamiltonians in formula (2.3) involve the sums over all bonds and projections. As a rule, in cluster growth problems, the growth of one cluster or a limited number of clusters is considered [17].

Not all clusters in the above set but only those having a nonzero spur contribute to moment (2.3). In the latter clusters, the initial lattice point 0 is active, and all the other lattice points are inactive. As a result of the necessary deactivation of the added lattice points, $2n$ bonds in the M_{2n} representing bond graphs join at most $n+1$ lattice points, one of which is the initial lattice point 0. In this case, identical graphs constructed differently are different terms in the sum. After the multiple bonds are replaced by single ones, this sum reduces to that over the base graphs g [3], i.e., over lattice configurations of bonds,

$$M_{2n} = J^{2n} \sum_g N(g) K_{2n}(g), \tag{2.4}$$

where $N(g)$ is the number of arrangements without self-intersections for the given configuration on the lattice and $J^{2n}K_{2n}$ is the contribution to the moment corresponding to the configuration.

In the limit $d \to \infty$, the leading contributions to sum (2.4) come from rooted trees with the maximum possible number of lattice points ($n+1$ for M_{2n}) [2, 4]. However, even for them, attempts to calculate the weighting factors K_{2n} fail. At the same time, some bounds for the magnitudes of the moments can be indicated in this limit [2]. An upper bound is given by the moments of the solution of the Blume–Hubbard equation [16],

$$F(t) = \exp\left\{-2J^2 Z \int_0^t (t-t')F(t')\,dt'\right\}, \tag{2.5}$$

where the first term of the cumulant expansion remains in the exponential function and $Z = 2d$ is the number of nearest neighbors. A lower bound is found from the solution of the Resibois–De Leener equation [15]. A cruder lower bound can be obtained using the solution of Eq. (2.5) with a halved coefficient in the integral.

To elucidate the indicated relation between the moments, we make the change of variable $Jt = i\tau$ in Eq. (2.5) and interpret the result as an equation for the generating function of the number of rooted trees. For this, we consider an auxiliary spin system on the Bethe lattice with coordination number $Z = \sigma+1$. The possible configurations in sum (2.4) are rooted trees. Because every added lattice point must be deactivated, the trees with the maximum possible number of lattice points (which are the only ones considered in what follows) are constructed with double bonds. It is clear that if the addition of new lattice points is performed consecutively, then the deactivation of the lattice points must also be consecutive but in the reverse direction (from the branch end to the root).

We take the trees in which at most a single neighboring lattice point can be connected with the root (the so-called trees with a pendant root) and let $w_1(2n)$ denote the number of these trees containing $n+1$ lattice points and n double bonds. We suppose that both the construction and the deactivation of different tree branches are performed independently. Then the number of trees is given by the relation

$$w_1(2n) = \sum \frac{(2n-2)!}{(2n_1)!\,(2n_2)!\ldots(2n_\sigma)!} w_1(2n_1)w_1(2n_2)\ldots w_1(2n_\sigma), \tag{2.6}$$

where the summation extends over all possible distributions of $2n-2$ bonds among the σ branches issuing from the lattice point nearest to the root. We introduce the generating function

$$F_1(\tau) = \sum_{n=0}^{\infty} w_1(2n) \frac{\tau^{2n}}{(2n)!} \tag{2.7}$$

to obtain the equation

$$F_1(\tau) = 1 + \int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \left[F_1(\tau_2)\right]^\sigma \tag{2.8}$$

from (2.6).

We can use $F_1(\tau)$ to find the generating function for the number of trees for which the root has Z neighbors,

$$F_Z(\tau) = \left[F_1(\tau)\right]^Z. \tag{2.9}$$

To pass to the limit $Z \to \infty$, we introduce the variable $y = \tau\sqrt{Z}$ in (2.8). Then function (2.9) becomes

$$F_\infty(y) = \exp\left\{ \int_0^y dy_1 \int_0^{y_1} dy_2\, F_\infty(y_2) \right\} \tag{2.10}$$

in this limit.

We return to the variable $t = y/\left(iJ\sqrt{Z}\right)$ in (2.10), which results in Eq. (2.10) with a halved exponent. Therefore, the number of trees with n double bonds in case (2.5) is 2^n times as great. This increase occurs because the interaction between every pair of lattice-point spins in the Hamiltonian $\varkappa$ in (2.4) is a sum of three terms containing the x-, y-, and z-components of the spin operators of these lattice points. A given tree can be constructed in many ways differing in the sequences of projections of spin operators. Because the commutator of projections on the same axis vanishes and the choice of the operator projections in the deactivation is unambiguous, the maximum number of ways a tree with n double bonds can be constructed is 2^n. The case where the coefficient in front of the integral in (2.10) is equal to unity corresponds to the choice of a unique set of operators for each tree. The actual coefficient lies between these extreme values and depends on the structure of the tree and on the sequence of operations in its construction because some combinations of spin projections give a zero result in the exact calculation of commutators.

We now analyze the analytic properties of autocorrelation function (2.1) for a d-dimensional system. For this, we use equations in the dimensionless form, (2.7)–(2.10). To return to real time, the change of variable $\tau = itJp$ is performed. The agreement with Eq. (2.5) is attained for $p = 2$. The choice of a different value of p changes the time scale but does not change the properties of the functions. Equation (2.8) is equivalent to the second-order differential equation

$$\ddot{F}_1(\tau) = \left[F_1(\tau)\right]^\sigma, \tag{2.11}$$

which can be solved in quadratures. Its solution has the nearest singular points with coordinates $\pm\tau_b$ on the imaginary time axis,

$$\tau_b = \tau_\infty \frac{\Gamma(1/2 - 1/Z)}{\sqrt{\pi}\,\Gamma(1 - 1/Z)} \approx \tau_\infty \left(1 + \frac{2\log 2}{Z}\right), \tag{2.12}$$

where $\Gamma(x)$ is the gamma function, $\tau_\infty = y_\infty/\sqrt{Z}$, and $y_\infty = \pi/\sqrt{2}$ is the coordinate of the nearest singularity of the solution of limiting equation (2.10) [16],

$$F_\infty(y) = \frac{1}{\cos^2\left(y/\sqrt{2}\right)}. \tag{2.13}$$

(For Eq. (2.5), we have $t_\infty = i\tau_\infty/(J\sqrt{2})$.) In the neighborhood of the singularity, we obtain

$$F_1(\tau) \approx A_1(\tau_b - \tau)^{-2/k} \tag{2.14}$$

for the leading term of the solution, where

$$k = \sigma - 1 = Z - 2, \qquad A_1 = \left\{\frac{2Z}{k^2}\right\}^{1/k}.$$

We therefore see that in the Bethe approximation, the singular points of autocorrelation functions are retained on the imaginary time axis with increasing d although their coordinates increase. We recall that in the derivation of Eq. (2.11), only the trees that have the maximum number of lattice points and are constructed with double bonds are preserved in sum (2.4). In the Bethe approximation, we take an important constraint into account: for finite dimensions d, at most σ branches issue from each lattice point of the tree. The effect of another constraint forbidding the intersection of branches of these trees (the so-called excluded volume effect) is considered in the subsequent sections. For comparison, we now present similar results in the Bethe approximation for trees constructed with single bonds. There are two known types of these trees. As in our study, the trees in the Eden model [7] are distinguished by the sequence of added bonds, i.e., by how they are constructed, whereas in the theory of branching molecules [5, 9, 10] and percolation theory [5], the trees are distinguished only by the topology and their arrangement on the lattice.

We begin with the Eden model. We introduce the generating function for the number v_n of such trees with a pendant root,

$$E_1(x) = \sum_{n=0}^{\infty} v_n \frac{x^n}{n!}. \tag{2.15}$$

This function satisfies the equation

$$E_1(x) = 1 + \int_0^x dx_1 \left[E_1(x_1)\right]^\sigma \tag{2.16}$$

because the relation for v_n is obtained from (2.6) by replacing all the numbers $2n_i$ with n_i. Equation (2.16) is equivalent to the differential equation

$$\frac{dE_1(x)}{dx} = \left[E_1(x)\right]^\sigma \tag{2.17}$$

having the solution

$$E_1(x) = (1 - kx)^{-1/k}. \tag{2.18}$$

Formula (2.18) coincides with the corresponding result in [7], which was obtained differently.

The generating function for the ordinary lattice trees [5, 6, 9, 10] with a pendant root is given by the expression

$$G_1(x) = \sum_{n=0}^{\infty} T_n x^n, \tag{2.19}$$

where T_n is the number of such trees that satisfy the algebraic equation

$$G_1(x) = 1 + x\left[G_1(x)\right]^\sigma, \tag{2.20}$$

whose solution has a singularity for

$$x_b = \frac{(1 - 1/\sigma)^k}{\sigma}. \tag{2.21}$$

At the singular point, we have

$$G_1(x_b) = \frac{\sigma}{\sigma - 1} = (x_b\sigma)^{-1/k}, \tag{2.22}$$

and the relation

$$G_1(x) \approx \frac{\sigma}{k} - \left[2\sigma k^{-3}\frac{x_b - x}{x_b}\right]^{1/2} \tag{2.23}$$

holds in its neighborhood.

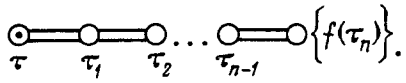
3. Corrections to the generating function from the intersection of tree branches

We now transfer the trees constructed on the Bethe lattice to the simple hypercubic lattice. Part of them can be arranged only with repeated use of the same lattice points and bonds, i.e., by admitting self-intersections. The other part of the trees can be arranged without self-intersections. The simplest loop formed under branch intersection is a square. A tree of n double bonds each of which is located in the new dimension can be arranged on the lattice in d^n ways (to within a numerical coefficient). Because the directions of the opposite sides of the square coincide, the number of ways the tree whose branches form the square can be arranged is d^2-fold smaller. It is clear that the losses are still greater for a loop consisting of a greater number of components [8, 9].

We find the first correction from the simplest tree intersection to the generating function for trees with a pendant root. To write this correction, we transform Eq. (2.8). Its original form reflects the fact that all trees can be sorted by the number of branchings from the lattice point nearest to the root. Differently, the trees can be sorted by the number of bonds in a direction chosen on the Bethe lattice. We consider the most general case, in which a chain of n components in the chosen direction can terminate not only with a free end but also with a fragment (e.g., a loop) described by a function $f(\tau)$. The generating function for trees including such a loop has the form

$$\begin{aligned} L_n(\tau, f) = &\int_0^{\tau} d\tau_1' \int_0^{\tau_1'} d\tau_1 \left[F_1(\tau_1)\right]^k \int_0^{\tau_1} d\tau_2' \int_0^{\tau_2'} d\tau_2 \left[F_1(\tau_2)\right]^k \times \cdots \\ &\cdots \times \int_0^{\tau_{n-1}} d\tau_n' \int_0^{\tau_n'} d\tau_n \left[F_1(\tau_n)\right]^k f(\tau_n), \\ L_0(\tau, f) = &f(\tau). \end{aligned} \tag{3.1}$$

For clarity, we represent this function by the diagram



(3.2)

The double line in the diagram shows the occupied bond to which the double integral in (3.1) corresponds, and the function $\left[F_1(\tau_p)\right]^k$ at the lattice point p and the root are accordingly indicated by the empty circle and dotted circles.

Introducing the formal parameter θ to define the number of bonds and adding together the contributions in (3.1) for the chains of different lengths in the chosen direction, we obtain the corresponding generating function

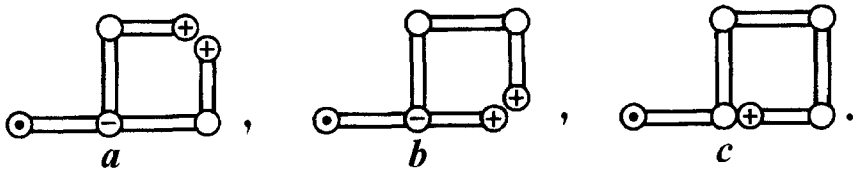
$$L(\theta, \tau, f) = \sum_{n=0}^{\infty} \theta^n L_n(\tau, f) \tag{3.3}$$

satisfying the equation

$$L(\theta, \tau, f) = f(\tau) + \theta \int_0^{\tau} d\tau_1' \int_0^{\tau_1'} d\tau_1 \left[F_1(\tau_1)\right]^k L(\theta, \tau_1, f). \tag{3.4}$$

It can be easily seen that Eq. (3.4) with $\theta = 1$ and $f(\tau) = 1$ becomes Eq. (2.8) because $L(1, \tau, 1) = F_1(\tau)$. In this case, expression (3.3) is an iterative series for (2.8) resulting from consecutive iterations in the chosen direction.

The generating function for trees containing other configurations of chains can be constructed similarly. For example, the three possible versions of the intersection of two branches issuing from the lattice point nearest to the root can be represented by the three diagrams



(3.5)

The circles with plus and minus signs indicate that the corresponding exponents of the function $F_1(\tau)$ are $k+1$ and $k-1$, and the two neighboring circles at a vertex of the square denote the intersection.

Using function (3.1) with $f(\tau) = F_1(\tau)$, we can write the explicit expressions for diagram (3.5) in the form

$$\int_0^\tau d\tau_1' \int_0^{\tau_1'} d\tau_1 \left[F_1(\tau_1)\right]^{k-1} L_a(\tau_1, F_1) L_b(\tau_1, F_1). \tag{3.6}$$

The following products stand under the integral sign in (3.6):

1. $\left[L_2(\tau_1, F_1)\right]^2$ for (3.5a),
2. $L_3(\tau_1, F_1) L_1(\tau_1, F_1)$ for (3.5b), and
3. $L_4(\tau_1, F_1) L_0(\tau_1, F_1)$ for (3.5c).

For each specific square on the lattice, there is one diagram of type (3.5a) and two diagrams each of types (3.5b) and (3.5c) differing in the permutation of the long and short chains forming the square. We let $P_q(\tau)$ denote the sum of the contributions from one loop of q components. For a square, we have

$$P_4(\tau) = \left[L_2(\tau, F_1)\right]^2 + 2L_3(\tau, F_1) L_1(\tau, F_1) + 2L_4(\tau, F_1) L_0(\tau, F_1). \tag{3.7}$$

This sum can be expressed via auxiliary function (3.3) with $f(\tau) = F_1(\tau)$, which is denoted by

$$\Phi(\theta, \tau) \equiv L(\theta, \tau, F_1).$$

Squaring the sum in (3.3), we can easily verify that sum (3.7) is the coefficient before θ^4 in $\left[\Phi(\theta, \tau)\right]^2$. It is convenient to rewrite Eq. (3.4) for the above function in the form of the second-order differential equation

$$\ddot{\Phi}(\theta, \tau) = \left[F_1(\tau)\right]^\sigma + \theta \left[F_1(\tau)\right]^k \Phi(\theta, \tau) \tag{3.8}$$

with the initial conditions $\Phi(\theta, 0) = 1$ and $\dot{\Phi}(\theta, 0) = 0$.

The loop with intersection can be located on the tree at an arbitrary distance from the root and go in any direction. For the loop attached to the root by a chain of n components, we should take

$$f(\tau) = \int_0^\tau d\tau_1' \int_0^{\tau_1'} d\tau_1 \left[F_1(\tau_1)\right]^{k-1} P_q(\tau_1) \tag{3.9}$$

in expression (3.1). Because the lattice points and the directions are identical, the summation in a direction reduces to the multiplication of contribution (3.1) from chains of n components by the additional factor σ^n. The summation over the lengths of the chains leading to the loop can then be performed using Eqs. (3.3) and (3.4) with $\theta = \sigma$ and the function $f(\tau)$ defined by (3.9).

Using the function $\Phi(\theta, \tau)$, the desired expression $R_4(\tau)$ can be obtained as the coefficient before θ^4 in the expansion of the function $R(\theta, \tau) \equiv L(\sigma, \tau, f)$ serving as the solution of Eq. (3.4) for $\theta = \sigma$ and

$$f(\tau) = \int_0^\tau d\tau_1' \int_0^{\tau_1'} d\tau_1 \left[F_1(\tau_1)\right]^{k-1} \left[\Phi(\theta, \tau_1)\right]^2. \tag{3.10}$$

It is convenient to rewrite Eq. (3.4) for $R(\theta,\tau)$ with the function f defined by formula (3.10) in the form of the second-order differential equation

$$\ddot{R}(\theta,\tau) = \left[F_1(\tau)\right]^{k-1}\left[\Phi(\theta,\tau)\right]^2 + \sigma\left[F_1(\tau)\right]^k R(\theta,\tau) \tag{3.11}$$

with the initial conditions $R(\theta,0) = \dot{R}(\theta,0) = 0$.

Finally, to obtain the ultimate expression for the correction from the simplest intersection of tree branches, $R_4(\tau)$ should be summed over all positions of the square near the given lattice point. The number of these positions is

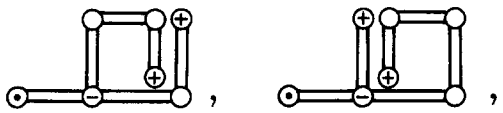
$$N_4 = \frac{k^2}{2}. \tag{3.12}$$

We have excluded the bond leading from the root to the given lattice point from the set of available bonds because the number in question is less than $Z(Z-2)/2$ [9].

The results for some other more complex configurations [9] formed under intersection of tree branches can also be obtained in this way. In particular, the contribution to the generating function from a branch intersection in the form of a loop with six components can be found as the coefficient before θ^6 in the expansion of $R(\theta,\tau)$. The number of such loops for a single lattice point is

$$N_6 = (\sigma-1)\left[(\sigma-2)(2\sigma-3) - \frac{1}{2}\right]. \tag{3.13}$$

To calculate the corrections of the next order of smallness with respect to $1/\sigma$, the corrections of the corresponding order to the leading correction term that are given by the simple configurations should be taken into account apart from the addition of the leading correction term from the complex configurations. For example, the representation of $P_4(\tau)$ in form (3.7) is exact in the leading order σ^{-2} if two lattice points coincide in the intersection. But if two bonds are imposed at the point of intersection,



(3.14)

then this contribution to $P_4(\tau)$ is taken into account twice. Therefore, to an accuracy of $1/\sigma^3$, the expression

$$2L_3(\tau,F_1)L_2(\tau,F_1) + 2L_4(\tau,F_1)L_1(\tau,F_1) \tag{3.15}$$

should be subtracted from sum (3.7). Naturally, the corrections from (3.12) should not be forgotten either. The above procedure is demonstrated in the appendix for an example of lattice configurations that were studied earlier using some other methods [8–10].

4. Calculating coordinates of singular points

4.1. Trees constructed with single bonds. We first apply the above formulas to the simple case of trees in the Eden model. As can be easily seen by comparing expressions (2.16) and (2.17) with (2.8) and (2.11), the formulas required for this case can be derived from those in the foregoing section by replacing the second derivatives and the double integrals with first derivatives and onefold integrals. Solving the equations thus obtained from Eqs. (3.8) and (3.11), we find

$$R(\theta,x) = \frac{1}{k}y^{-\sigma/k}\int_y^1 y_1^{2/k}\left[\Phi(\theta,x_1)\right]^2 dy_1, \tag{4.1}$$

$$\Phi(\theta,x) = \frac{y^{-1/k} - \theta y^{-\theta/k}}{1-\theta}, \tag{4.2}$$

where $y = 1 - kx$. Calculating the integral in (4.1), we obtain

$$R(\theta, x) = \left\{1 - y - 2\theta\frac{1 - y^{1+(1-\theta)/k}}{1 + (1-\theta)/k} + \theta^2\frac{1 - y^{1+2(1-\theta)/k}}{1 + 2(1-\theta)/k}\right\}\frac{1}{k(1-\theta)^2 y^{\sigma/k}}. \tag{4.3}$$

The coefficient of $R_q(x)$ before θ^q in expansion (4.3) yields the generating function for the number of trees with a single branch intersection in the form of a simple loop of q components. For the square we are interested in, it follows that

$$\begin{aligned} R_4(x)\left(ky^{\sigma/k}\right) = {} & 5(1-y) - 2k(1+k)^{-4}(4k^3 + 15k^2 + 20k + 10)\left(1 - y^{1+1/k}\right) + \\ & + k(2+k)^{-3}(3k^2 + 16k + 24)\left(1 - y^{1+2/k}\right) - 2(1+k)^{-3}(3k^2 + 8k + 6)y^{1+1/k}\log y + \\ & + 4(2+k)^{-2}(k+3)y^{1+2/k}\log y + (1+k)^{-2}\left(2 + \frac{3}{k}\right)y^{1+1/k}\log^2 y - \\ & - 2(2+k)^{-1}k^{-1}y^{1+2/k}\log^2 y - (1+k)^{-1}k^{-2}3^{-1}y^{1+1/k}\log^3 y. \end{aligned} \tag{4.4}$$

We multiply (4.4) by the number N_4 (see (3.12)) of positions of the square near the given lattice point and subtract it from (2.18) to obtain

$$E_1(x) = (1 - kx)^{-1/k} - \frac{k^2 R_4(x)}{2} + \cdots \tag{4.5}$$

for the generating function of trees with a pendant root with inclusion of the first correction for the tree intersection.

Based on two terms in expansion (4.5), we determine the coordinate x_c of the singular point. This coordinate enters the asymptotic formula for the number of trees. A procedure for calculating a similar parameter for lattice configurations by finding the number of clusters of a greater size was suggested in [9]. The determination of these numbers is a complicated problem in itself. As we show, its solution can be avoided, and the idea of the method in [9] can be used to determine the desired parameter x_c directly from the generating function. This approach was verified for lattice configurations studied earlier [9, 10]. We now apply it to the trees in the Eden model, Eq. (4.5).

We have $x_c = x_b = 1/k$ in the Bethe approximation (2.18). Forbidding branch intersections increases the coordinate, i.e.,

$$x_c = x_b + \delta x_c.$$

We regard the generating function as being dependent on the two parameters x and x_c and expand it with respect to the small parameter δx_c,

$$E_1(x, x_c) = E_1(x, x_b) + \delta x_c \left.\frac{\partial E_1(x, x_c)}{\partial x_c}\right|_{x_c = x_b} + \ldots. \tag{4.6}$$

Comparing (4.5) with (4.6) and setting

$$\left.\frac{\partial E_1(x, x_c)}{\partial x_c}\right|_{x_c = x_b} = \frac{\partial E_1(x, x_b)}{\partial x_b} = -kx(1 - kx)^{-\sigma/k},$$

we obtain

$$\delta x_c = \left\{R_4(x)\frac{ky^{\sigma/k}}{2x}\right\}_{x = x_b} = [8\sigma^3 + 7\sigma^2 + 4\sigma + 1]k\sigma^{-4}Z^{-3}.$$

It follows that

$$x_c = x_b(1 + 8\sigma^{-2}) \tag{4.7}$$

in the leading order with respect to $1/\sigma$.

4.2. Trees constructed with double bonds. For trees with double bonds (in contrast to those with single bonds), the attempts to analytically solve the equations derived in Sec. 3 fail. However, the correction to the coordinate of the singular point we are interested in is determined by the behavior of the function in the neighborhood of this point, in which the leading terms of the solution can be found rather simply.

Substituting (2.14) in Eq. (3.11), we find the leading term of the solution in the neighborhood of the singularity,

$$R(\theta,\tau) \approx C\left(1-\frac{\tau}{\tau_b}\right)^{-1-2/k}, \tag{4.8}$$

where

$$C = \frac{\tau_b}{3+4/k}\int_0^{\tau_b}\left(1-\frac{\tau}{\tau_b}\right)^{2+2/k}\left[F_1(\tau)\right]^{k-1}\left[\Phi(\theta,\tau)\right]^2 d\tau. \tag{4.9}$$

Because the attempt to find the function $\Phi(\theta,\tau)$ fails to calculate the correction R_4 from the simplest branch intersection in the form of a square, we substitute the function $P_4(\tau)$ (see (3.7)) for $\Phi(\theta,\tau)$ in (4.9). We then pass to the dimensionless variables $\varphi = \pi\tau/(2\tau_b)$ in (4.9) and in the multiple integrals in (3.7). This results in

$$R_4 = \frac{\tau_b^{10}}{3+4/k}\left(\frac{\pi}{2}\right)^{11}\int_0^{\pi/2}\left(\frac{\pi}{2}-\varphi\right)^{2+2/k}\left[F_1\left(2\varphi\frac{\tau_b}{\pi}\right)\right]^{k-1}P_4(\varphi)\,d\varphi.$$

According to (2.12), the coefficient in the integral is of order Z^{-5} for large values of Z. The integral itself is of order Z^0. To find its leading term in the limit $Z\to\infty$, we take the functions F_1^k and $F_1^{k\mp1}$ entering the integrand in limiting form (2.13) and replace $(\pi/2-\varphi)^{2+2/k}$ with $(\pi/2-\varphi)^2$. Calculating the integral, we obtain

$$R_4 = \frac{2^6\cdot 5.867}{3\pi Z^5} \tag{4.10}$$

in the leading order with respect to Z.

We substitute (4.10) in (4.8), multiply the result by the additional factor N_4 (see (3.12)), and subtract it from (2.14). For the leading term in the generating function of trees with a pendant root that are constructed with double bonds, this yields the desired expression with correction,

$$F_1(\tau) = A_1(\tau_b-\tau)^{-2/k} - \frac{1}{2}k^2R_4(\tau_b-\tau)^{-1-2/k}\tau_b^{1+2/k} + \ldots. \tag{4.11}$$

Comparing the correction term in this expression with the correction term

$$\delta\tau_0\left.\frac{\partial F_1(\tau)}{\partial\tau_0}\right|_{\tau_0=\tau_b} = \delta\tau_0\left(-\frac{2}{k}\right)A_1(\tau_b-\tau)^{-1-2/k}$$

in the expansion (similar to (4.6)) of the function $F_1(\tau,\tau_0)$ with respect to the small shift $\delta\tau_0$ of the coordinate of the singular point, we find

$$\delta\tau_0 = \frac{k^3R_4\tau_b^{1+2/k}}{4A_1}.$$

Retaining the terms of the leading order with respect to $1/\sigma$ in this expression, we obtain

$$\tau_b + \delta\tau_0 = \tau_b(1+9.96\sigma^{-2}) \tag{4.12}$$

for the coordinate of the singular point of the autocorrelation function in the tree approximation with the first correction for branch intersection.

It is understood that $d\gg 1$ in asymptotic formula (4.12). However, even for $d=3$, it can already be assumed that $1/\sigma$ is small enough to write $\tau_0\approx 1.4\tau_b$. The computer simulation method was applied to the same case to derive the estimate $\tau_0\approx 1.2\tau_b$ in [4]. This result is probably underestimated because the size of the trees available for calculations is insufficient for the full manifestation of the excluded volume effect.

5. Discussion

We considered generating functions of trees on high-dimensional lattices with branch intersection taken into account and obtained some results for the coordinates of singular points with a correction of order $1/\sigma^2$ to autocorrelation function (4.12) (for trees with double bonds) and for the Eden model (4.7) (trees with single bonds). Comparison between these results and their correlation with formula (A.8) (see the appendix) for lattice configurations shows that there are three cases in which the coordinates of singular points similarly increase with decreasing d. We found no qualitative distinctions that would cast doubt on the existence of singular points of autocorrelation functions at a finite distance.

To draw the final conclusion, it remains to also include the contribution to moments (2.4) from lattice configurations with loops and multiple interaction of the same spins. However, even based on the already performed investigation, we should expect that the addition of new local corrections cannot radically change the properties of large trees specifying the position of the nearest singular points of the autocorrelation function of a high-dimensional spin system. That the existence of loops in large branching molecules does not lead to any essential changes in asymptotic properties in polymer theory [18] also supports this assumption.

There remains a known unsolved problem of this type concerning the noncommutativity of the limits $d \to \infty$ and $n \to \infty$ [11]. If a finite value of d is retained and the size of the cluster is increased, then the correction terms taken into account are no longer leading for $n > d$. In this case, the result concerning the coordinate of the singular point changes, but, as can be expected by analogy with other critical phenomena, the singularity itself must be preserved. To confirm this, we refer to experimental data. The point is that one of the consequences of the existence of the abovementioned singularities of correlation functions on the imaginary time axis is exponential high-frequency asymptotic representations of their spectra. The form of the experimentally observed spectrum "wings" turns out to be close to that of the exponential ones (see [2, 19, 20] for the corresponding analysis). Most of the experiments were performed with the nuclear magnetic resonance method for systems with anisotropic dipole–dipole interaction. The related formulas and equations become more complicated in the generalization to systems with anisotropic interaction [19–21], but the ultimate conclusions themselves do not change qualitatively.

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Appendix

We apply the suggested approach to find the coordinate of the singular point of the generating function for lattice configurations whose expansion with respect to $1/\sigma$ is well known [9, 10]. The calculations are confined to the first two terms of order σ^{-2} and σ^{-3}.

We consider the correction to (2.19) from the intersection of tree branches. Because the terms in (3.7) and (3.15) differing in the positions of the region of intersection in the square are now the same, the contribution from the square amounts to

$$P_4(x) = 5x^4\big[G_1(x)\big]^{4k+2} - 4x^5\big[G_1(x)\big]^{5k+2}. \tag{A.1}$$

We similarly find the contribution from the intersection of tree branches in the form of a loop with six components,

$$P_6(x) = 7x^6\big[G_1(x)\big]^{6k+2}. \tag{A.2}$$

If not only the trees but also the configurations with loops are considered [9], then the related term should be added to the generating function. The actual loops differ from the intersection of tree branches in the absence of free ends. Their contributions can therefore be obtained from the expressions $P_4(x)$ (see the

first term in (A.1)) and $P_6(x)$ (see (A.2)) by dividing them by $5\big[G_1(x)\big]^{\sigma+1}$ and $7\big[G_1(x)\big]^{\sigma+1}$ respectively. These contributions are not subtracted from the function $G_1(x)$ but added to it.

An analogue of Eq. (3.4) for ordinary trees is an algebraic equation whose solution for $\theta = \sigma$ is

$$L(\sigma, x, f) = \frac{f(x)}{1 - \sigma x\big[G_1(x)\big]^k}. \tag{A.3}$$

Using formulas (A.1)–(A.3), we obtain the expression

$$G_1(x) - \frac{B(x)\big[G_1(x)\big]^\sigma}{1 - \sigma x\big[G_1(x)\big]^k} + \ldots, \tag{A.4}$$

where

$$B(x) = N_4 x^5\big[G_1(x)\big]^{4k}\big[5 - 4x\big[G_1(x)\big]^k - \big[G_1(x)\big]^{-\sigma-1}\big] + N_6 x^7\big[G_1(x)\big]^{6k}\big[7 - \big[G_1(x)\big]^{\sigma-1}\big],$$

for the generating function in the case of configurations with a pendant root with inclusion of corrections for the intersection of tree branches and for the actual loops.

To find the point x_c using (A.4), we represent (A.4) in the form of an expansion (similar to (4.6)) with respect to the small shift δx_c. Indeed, by (2.20), we have

$$\frac{dG_1(x)}{dx} = \frac{\big[G_1(x)\big]^\sigma}{1 - \sigma x\big[G_1(x)\big]^k}, \tag{A.5}$$

whereas, by (2.23),

$$\frac{\partial G_1(x, x_c)}{\partial x} \approx -\frac{\partial G_1(x, x_c)}{\partial x_c} \tag{A.6}$$

in the neighborhood of the singular point. In view of (A.5) and (A.6), formula (A.4) implies

$$\delta x_c = B(x_b). \tag{A.7}$$

According to (2.22), we have

$$\big[G_1(x_b)\big]^{qk} = (x_b\sigma)^{-q}, \qquad \big[G_1(x_b)\big]^{-\sigma-1} = \left(1 - \frac{1}{\sigma}\right)^{\sigma+1} \approx \frac{1 - 3/(2\sigma)}{e}$$

at the singular point. Substituting these values and the values of N_4 and N_6 in (A.7), we finally derive the following formula including the terms of order σ^{-2} and σ^{-3}, which coincides with the corresponding result in [9]:

$$x_c = x_b\left[1 + \frac{1}{\sigma^2}\left(\frac{5}{2} - \frac{1}{2e}\right) + \frac{1}{\sigma^3}\left(7 - \frac{1}{4e}\right)\right]. \tag{A.8}$$

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