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THE EFFECT OF INHOMOGENEITY ON DIRECT CORRELATION FUNCTIONS OF A ONE–DIMENSIONAL LATTICE GAS WITH MANY–NEIGHBOUR INTERACTIONS

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The aim of this paper is to investigate the effect of a varying field on the direct correlation function (DCF) of spin chains. The problem is studied via a lattice gas with three-neighbour interactions chosen so that the long-range DCF can be obtained explicitly. The numerical calculations indicate a more rapid decay of the DCF with increasing the dispersion of the applied field. This fact permits to apply the general concept of the DCF also to inhomogeneous systems.

1. INTRODUCTION

The character of the real physical world requires to extend the general aspects of homogeneous systems to their inhomogeneous counterparts.

The degree of locality or non-locality of the free energy for Ising lattices is reflected through the range of direct correlation functions (DCF) within the inverse formulation of the profile problem (for a review see [1]). The analysis of the Ising chain with nearest-neighbour interactions shows the strictly finite range of DCF for a uniform as well as non-uniform external field [2]. According to refs. [3, 4] this fact can be explained by a special topology of the chain having articulation points, which plays a fundamental role for the case of a uniform as well as a varying field.

On the other hand, higher interactions induce long-range DCF in the presence of a uniform field [5]. The question naturally arises as to whether the dispersion of an external field influences the decay of the DCF. This question acquires a great significance. Namely the DCF of a homogeneous model decays, in general, more rapidly than its reciprocal, the spin-spin correlation function. This fact is the basis of many approximation methods in equilibrium statistical mechanics of various homogeneous models. The investigation of the above question then allows to conclude whether the concept of the DCF remains valid also for inhomogeneous models.

In this paper, we study the proposed problem via a simple one-dimensional lattice gas with three-neighbour interactions chosen in such a way that the DCF

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can be obtained explicitly using a recently developed method for solving the inverse problem [3]. Our main conclusion is that the dispersion of an external field implies a more rapid exponential decay of the DCF.

The inverse problem of the one-dimensional lattice gas with three-neighbour interactions is solved in Sec. 2. The numerical results are given in Sec. 3. The concluding remarks are presented in Sec. 4.

2. INVERSE PROBLEM FOR A ONE-DIMENSIONAL LATTICE GAS

Let us consider a lattice gas version of the Ising chain with constant three-neighbour (dimensionless) interactions J in a varying (dimensionless) field $\{H_n\}_{n=1}^N$ acting on "spins" $s_n = 0,1$ localized at sites $n = 1,2,\ldots,N$ $(N \to \infty)$. Its Hamiltonian H is defined by

$$-\beta H = \sum_{n=1}^{N-2} J s_n s_{n+1} s_{n+2} + \sum_{n=1}^{N} H_n(s_n - 1) \tag{1}$$

with β being the inverse temperature.

The equilibrium thermodynamics of the proposed model can be deduced from the statistical sum

$$Z_N(J;H_1,\ldots,H_N) = \sum_{\{s\}_N} \exp\left[\sum_{n=1}^{N-2} J s_n s_{n+1} s_{n+2} + \sum_{n=1}^{N} H_n(s_n - 1)\right]; \tag{2}$$

the spin expectation value

$$\langle s_i \rangle = \frac{S_i(J;H_1,\ldots,H_N)}{Z_N(J;H_1,\ldots,H_N)}, \tag{3a}$$

$$S_i(J;H_1\ldots,H_N) = \sum_{\{s\}_N} s_i \exp\left[\sum_{n=1}^{N-2} J s_n s_{n+1} s_{n+2} + \sum_{n=1}^{N} H_n(s_n - 1)\right]; \tag{3b}$$

the pair spin expectation

$$\langle s_i s_j \rangle = \frac{S_{ij}(J;H_1,\ldots,H_N)}{Z_N(J;H_1,\ldots,H_N)}, \tag{4a}$$

$$S_{ij}(J;H_1,\ldots,H_N) = \sum_{\{s\}_N} s_i s_j \exp\left[\sum_{n=1}^{N-2} J s_n s_{n+1} s_{n+2} + \sum_{n=1}^{N} H_n(s_n - 1)\right]; \tag{4b}$$

where $i,j = 1,\ldots,N$ and the summation proceeds over all the possible configurations of N spins. Our major interest will be in the DCF c_{ij} which is the reciprocal of the spin-spin correlation function,

$$c_{ij} = g_{ij}^{-1}, \tag{5a}$$

$$g_{ij} = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle. \tag{5b}$$

In the inverse formulation of the profile problem [1] the $\langle s_i \rangle$ are chosen as the independent controlling variables. Having the external field needed to produce a given magnetization profile the DCF can be computed in a straightforward way

$$c_{ij} = \frac{\partial H_i}{\partial \langle s_j \rangle} \left(\equiv \frac{\partial H_j}{\partial \langle s_i \rangle} \right). \tag{6}$$

In order to solve the inverse problem we will use the method presented in ref. [3]. As a first step, we will express the partition function of the considered model in terms of nonlinear recurrence relations. With this aim we eliminate consecutively spins from the chain and investigate judiciously chosen statistical quantities of the remaining fragments. Let us start with the spin at site 1. Using the identity

$$\exp(J s_1 s_2 s_3) = 1 + j s_1 s_2 s_3 \quad \text{with} \quad j = \exp(J) - 1 \tag{7}$$

for $s_1, s_2, s_3 = 0,1$ and taking in (2) the sum over s_1 we easily arrive at

$$Z_N(J;H_1,\ldots,H_N) = [h_1 + j\langle s_2 s_3\rangle_1]\, Z_{N-1}(J;H_2,\ldots,H_N), \tag{8a}$$

where $h_1 = 1+\exp(-H_1)$, $Z_{N-1}(J;H_2,\ldots,H_N)$ is the partition function of $N-1$ spins at sites $2,3,\ldots,N$ and $\langle\ \rangle_1$ denotes the ensemble average in the absence of spin at site 1. Analogously,

$$S_1(J;H_1,\ldots,H_N) = [1 + j\langle s_2 s_3\rangle_1]\, Z_{N-1}(J;H_2,\ldots,H_N), \tag{8b}$$

$$S_2(J;H_1,\ldots,H_N) = [h_1 \langle s_2\rangle_1 + j\langle s_2 s_3\rangle_1]\, Z_{N-1}(J;H_2,\ldots,H_N), \tag{8c}$$

$$S_{12}(J;H_1,\ldots,H_N) = [\langle s_2\rangle_1 + j\langle s_2 s_3\rangle_1]\, Z_{N-1}(J;H_2,\ldots,H_N) \tag{8d}$$

and so

$$\langle s_1 \rangle = \frac{1 + j\langle s_2 s_3\rangle_1}{h_1 + j\langle s_2 s_3\rangle_1}, \tag{9a}$$

$$\langle s_2 \rangle = \frac{h_1\langle s_2\rangle_1 + j\langle s_2 s_3\rangle_1}{h_1 + j\langle s_2 s_3\rangle_1}, \tag{9b}$$

$$\langle s_1 s_2 \rangle = \frac{\langle s_2\rangle_1 + j\langle s_2 s_3\rangle_1}{h_1 + j\langle s_2 s_3\rangle_1}. \tag{9c}$$

It is easy to show that $\langle s_1\rangle$, $\langle s_2\rangle$, $\langle s_1 s_2\rangle$ are related by

$$1 - \langle s_2 \rangle = h_1(\langle s_1\rangle - \langle s_1 s_2\rangle). \tag{10}$$

Proceeding in this manner for spins $2, 3, \ldots, N$ we get

$$Z_N(J; H_1, \ldots, H_N) = \prod_{n=1}^{N-2} (h_n + j \langle s_{n+1} s_{n+2} \rangle_n) h_{N-1} h_N, \tag{11}$$

where the recursion variables $\langle s_{n+1} s_{n+2} \rangle_n$ satisfy, together with $\langle s_{n+1} \rangle_n, \langle s_{n+2} \rangle_n$, the recurrence relations

$$\langle s_{n+1} \rangle_n = \frac{1 + j \langle s_{n+2} s_{n+3} \rangle_{n+1}}{h_{n+1} + j \langle s_{n+2} s_{n+3} \rangle_{n+1}}, \tag{12a}$$

$$\langle s_{n+2} \rangle_n = \frac{h_{n+1} \langle s_{n+2} \rangle_{n+1} + j \langle s_{n+2} s_{n+3} \rangle_{n+1}}{h_{n+1} + j \langle s_{n+2} s_{n+3} \rangle_{n+1}}, \tag{12b}$$

$$\langle s_{n+1} s_{n+2} \rangle_n = \frac{\langle s_{n+2} \rangle_{n+1} + j \langle s_{n+2} s_{n+3} \rangle_{n+1}}{h_{n+1} + j \langle s_{n+2} s_{n+3} \rangle_{n+1}}, \tag{12c}$$

$h_n = 1 + \exp(-H_n)$ and the elimination of the n-th spin in $\langle\,\rangle_n$ means the simultaneous elimination of all spins with indices lower than n. Eq. (10) now reads

$$1 - \langle s_{n+2} \rangle_n = h_{n+1} (\langle s_{n+1} \rangle_n - \langle s_{n+1} s_{n+2} \rangle_n). \tag{13}$$

The analogous elimination of spins starting from site N, ending at site 1, gives

$$Z_N(J; H_1, \ldots, H_N) = \prod_{n=3}^{N} (h_n + j \langle s_{n-1} s_{n-2} \rangle_n^*) h_2 h_1; \tag{14}$$

$$\langle s_{n-1} \rangle_n^* = \frac{1 + j \langle s_{n-2} s_{n-3} \rangle_{n-1}^*}{h_{n-1} + j \langle s_{n-2} s_{n-3} \rangle_{n-1}^*}, \tag{15a}$$

$$\langle s_{n-2} \rangle_n^* = \frac{h_{n-1} \langle s_{n-2} s_{n-1} \rangle^* + j \langle s_{n-2} s_{n-3} \rangle_{n-1}^*}{h_{n-1} + j \langle s_{n-2} s_{n-3} \rangle_{n-1}^*}, \tag{15b}$$

$$\langle s_{n-1} s_{n-2} \rangle_n^* = \frac{\langle s_{n-2} \rangle_{n-1}^* + j \langle s_{n-2} s_{n-3} \rangle_{n-1}^*}{h_{n-1} + j \langle s_{n-2} s_{n-3} \rangle_{n-1}^*}; \tag{15c}$$

$$1 - \langle s_{n-2} \rangle_n^* = h_{n-1} (\langle s_{n-1} \rangle_n^* + \langle s_{n-1} s_{n-2} \rangle_n^*). \tag{16}$$

Here, the elimination of the nth spin in $\langle\,\rangle_n^*$ means the simultaneous elimination of all spins with indices higher than n.

The procedure for solving the inverse problem is now straightforward. To express a specific field, say H_i, as a function of the magnetization profile we will eliminate the ith spin from the system and investigate the consequent modification of naturally chosen quantities $Z_N(J; H_1, \ldots, H_N)$, $S_i(J; H_1, \ldots, H_N)$, $S_{i+1}(J; H_1, \ldots, H_N)$, $S_{i+2}(J; H_1, \ldots, H_N)$, $S_{i-1}(J; H_1, \ldots, H_N)$, $S_{i-2}(J; H_1, \ldots, H_N)$. Using the identity (7) we are able to express each of the five magnetizations $\langle s_{i-2} \rangle$, $\langle s_{i-1} \rangle$, $\langle s_i \rangle$, $\langle s_{i+1} \rangle$, $\langle s_{i+2} \rangle$ in terms of the field acting on site i, H_i, and correlations of the four spins s_{i-2}, s_{i-1}, s_i, s_{i+1}, s_{i+2} in the absence of the ith spin. However, spins s_{i+1}, s_{i+2} are statistically independent of spins s_{i-1}, s_{i-2} in the absence of the ith spin, so we may decouple many of the above correlations, e.g. $\langle s_{i-1} s_{i+1} \rangle_i = \langle s_{i-1} \rangle_i^* \cdot \langle s_{i+1} \rangle_i$, $\langle s_{i-2} s_{i-1} s_{i+2} \rangle_i = \langle s_{i-2} s_{i-1} \rangle_i^*$, $\langle s_{i+2} \rangle_i$, etc. As a result, it is sufficient to consider only six unknows $\langle s_{i+1} \rangle_i$, $\langle s_{i+2} \rangle_i$, $\langle s_{i+1} s_{i+2} \rangle_i$; $\langle s_{i-1} \rangle_i^*$, $\langle s_{i-2} \rangle_i^*$, $\langle s_{i-1} s_{i-2} \rangle_i^*$. Eqs. (13), (16) tell us that two of them can be interchanged by field variables h_{i+1}, h_{i-1}. Consequently, we obtain a set of five equations which relate five magnetizations $\langle s_{i-2} \rangle$, $\langle s_{i-1} \rangle$, $\langle s_i \rangle$, $\langle s_{i+1} \rangle$, $\langle s_{i+2} \rangle$ to four auxiliary unknowns, say $\langle s_{i+1} \rangle_i$, $\langle s_{i+1} s_{i+2} \rangle_i$, $\langle s_{i-1} \rangle_i^*$, $\langle s_{i-1} s_{i-2} \rangle_i^*$, and three field variables h_{i-1}, h_i, h_{i+1}. The analytical derivation of the above mentioned set is simple but time consuming. We therefore write down the final result:

$$\frac{1 - \langle s_{i+1} \rangle}{1 - \langle s_i \rangle}(h_i - 1) = (1 - x_i^+)(h_i + j y_i^-), \tag{17a}$$

$$\frac{1 - \langle s_{i-1} \rangle}{1 - \langle s_i \rangle}(h_i - 1) = (1 - x_i^-)(h_i + j y_i^+), \tag{17b}$$

$$\frac{1 - \langle s_{i+2} \rangle}{1 - \langle s_i \rangle}(h_i - 1) = (x_i^+ - y_i^+)\left[j x_i^- + j^2 y_i^- + h_{i+1}(h_i + j y_i^-\right], \tag{17c}$$

$$\frac{1 - \langle s_{i-2} \rangle}{1 - \langle s_i \rangle}(h_i - 1) = (x_i^- - y_i^-)\left[j x_i^+ + j^2 y_i^+ + h_{i-1}(h_i + j y_i^+)\right], \tag{17d}$$

$$\frac{1}{1 - \langle s_i \rangle}(h_i - 1) = h_i + j(y_i^- + x_i^- x_i^+ + y_i^+) + j^2(y_i^- x_i^+ + y_i^+ x_i^-) + (1 + j) j^2 y_i^- y_i^+, \tag{17e}$$

where a simplified notation

$$x_i^+ = \langle s_{i+1} \rangle_i, \qquad x_i^- = \langle s_{i-1} \rangle_i^*; \tag{18a}$$

$$y_i^+ = \langle s_{i+1} s_{i+2} \rangle_i, \qquad y_i^- = \langle s_{i-1} s_{i-2} \rangle_i^* \tag{18b}$$

has been used.

3. NUMERICAL RESULTS

We have solved the set of Eqs. (17a–e) for 50 sites with periodical boundary conditions by the Newton algorithm for various distributions of the field. Owing to the form of (17a–e), the number of equations can be reduced to be equal to the number of sites. Indeed, if trial values of magnetizations $\langle s_i \rangle$ are given, one can find, from (17a–d), values of $x_i^\pm, y_i^\pm$. Their substitution into (17e) gives a single equation

$$f_i(\langle s_{i-2}\rangle, \langle s_{i-1}\rangle, \langle s_i\rangle, \langle s_{i+1}\rangle, \langle s_{i+2}\rangle) = 0$$

per site. The Newton algorithm needs also the Jacobi matrix $J_{ij} = \partial f_i/\partial \langle s_j\rangle$. To find values of J_{ij} for given i, one has to differentiate Eqs. (17a–d) with respect to $\langle s_{i-2}\rangle, \ldots, \langle s_{i+2}\rangle$, and to calculate, from the obtained system of equations, $\partial x_i^\pm/\partial\langle s_j\rangle, \partial y_i^\pm/\partial\langle s_j\rangle$.

Our results confirm our suggestion that the periodical boundary conditions do not influence the magnetization considerably. Thus, changing the number of sites from 40 to 45, or from 45 to 50, only magnetizations on the last/first 3-4 sites have been changed.

Having the values of $\langle s_i\rangle, x_i^\pm, y_i^\pm$, the DCF can be calculated easily. To do so, let us differentiate system (17a – e) with respect to $\langle s_j\rangle$. Then, from the first four equations, we find $\partial x_i^\pm/\partial\langle s_j\rangle, \partial y_i^\pm/\partial\langle s_j\rangle$. Their substitution into (17e) gives a simple linear equation

$$A_i \frac{\partial H_{i-1}}{\partial\langle s_j\rangle} + B_i \frac{\partial H_i}{\partial\langle s_j\rangle} + C_i \frac{\partial H_{i+1}}{\partial\langle s_j\rangle} = F(i,j) \tag{19}$$

with A_i, B_i, C_i being the functions of $x_i^\pm, y_i^\pm, h_{i-1}, h_i, h_{i+1}, \langle s_{i-2}\rangle, \ldots, \langle s_{i+2}\rangle$, and $F(i,j) \neq 0$ for $|i-j| \leqq 2$. Thus, the DCF can be found from the three-diagonal system of linear equations.

For the homogeneous case $A_i = C_i = A, B_i = B$. All our numerical results confirm that for our model $B \gg 2A$. Thus, the DCF decreases exponentially as

$$c_{ij} \sim \exp(-\lambda|i-j|) \tag{20a}$$

with

$$2\cosh\lambda = B/A. \tag{20b}$$

For the inhomogeneous case, Eq. (19) has only an exponentially decreasing (increasing) solution [6]. Thus, we have proved that the DCF has to decrease exponentially. To find parameter λ for this case, we solved the system of 50 linear Eqs. (19) and then calculated the parameters of

$$\log c_{ij} = -\lambda|i-j| + \delta.$$

The numerical results are presented graphically in Figs. 1–3.

In Fig. 1, we have drawn the plots of $\lambda(J)$ for various values of a uniform (dimensionless) field H. The plots are rather nontrivial in the ferromagnetic region ($J > 0$), where the minimum extreme of λ for certain value of J exists. It is clear that this point corresponds to the strongly correlated state of the considered

model. Its existence is caused by the divergence of λ at $J \to 0$ ($T \to \infty$; the system is completely disordered) and $J \to \infty (T \to 0$; only the ferromagnetic ground state contributes to the free energy and so there are no correlations in the system). On the other hand, in the antiferromagnetic region ($J < 0$) the infinite value of λ is attained if J approaches zero. The ground state of the system includes an infinite number of microscopic states which do not contain a cluster of three spins $s_{i-1}, s_i, s_{i+1} = 1$. Therefore, in the limit $J \to -\infty$ λ acquires a certain value λ_∞ independently of the applied field.

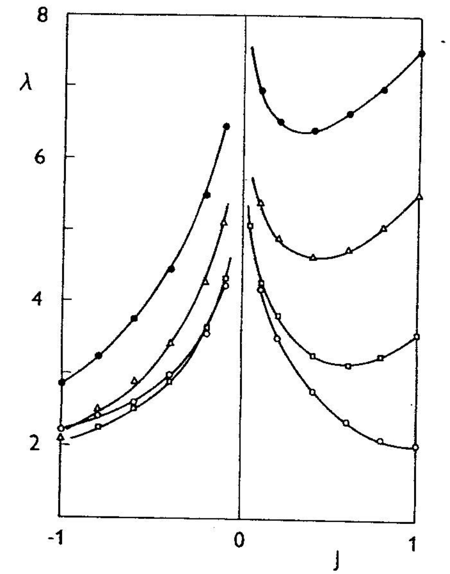

Fig. 1. The plots of $\lambda(J)$ for various values of the constant field $H = -1(\circ), 0(\square), 1(\triangle), 2(\bullet)$.

The results for the case of a varying field H_n with the mean value $\langle H\rangle$ and the dispersion σ are represented in Figs. 2, 3. The field was obtained by rescaling suitably a given sequence of random numbers generated by a generator of random numbers. In Fig. 2, we show an approximately linear decay of the DCF logarithm for $J = -1$, $\langle H\rangle = 0$ and various values of dispersion σ. It is clear that the increase of σ implies a more rapid decay of the DCF. This fact is demonstrated in Fig. 3 where the dependence of λ on σ for various values of J and $\langle H\rangle$ is plotted. A relatively large dispersion of the obtained results for high values of σ is given by the fact that the insufficient number of the considered sites does not allow to attain a correct stationary distribution of random fields. In spite of this, the tendency of lines in the (λ, σ) plane is evident.

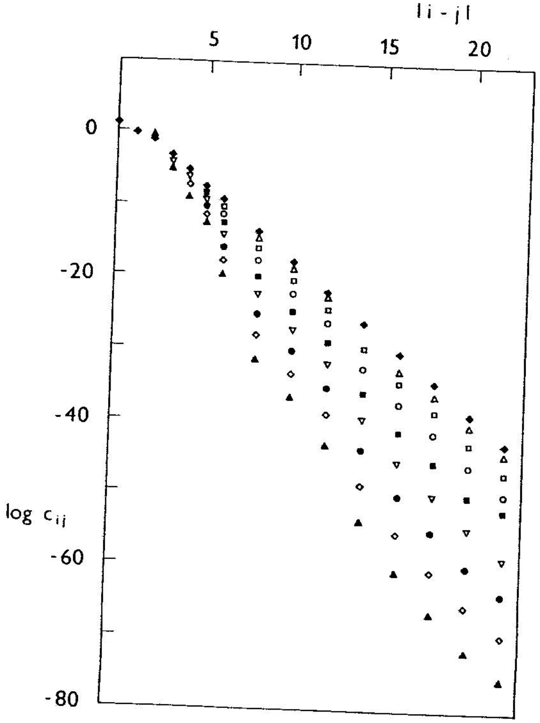

Fig. 2. The decay of the DCF for the case of antiferromagnetic three-neighbour interactions $J = -1$ and the varying field with a zero mean value and dispersion $\sigma = O$ (♦), 2 (△), 3 (□), 4 (○), 5 (■), 6 (▽), 7 (•), 8 (◊), 9 (▲).

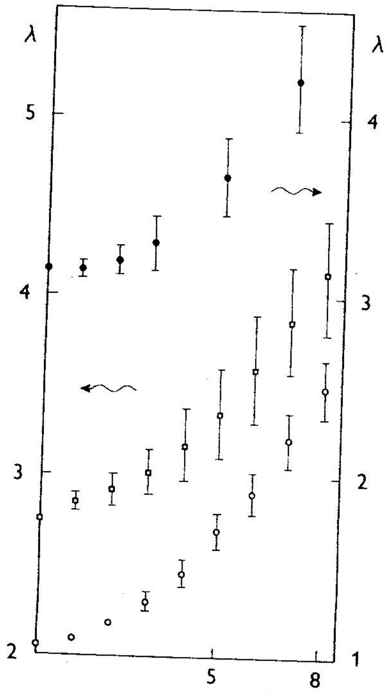

Fig. 3. The plots of $\lambda(\sigma)$ for $J = -1$, $\langle H \rangle = 0$ (o); $J = -1, \langle H \rangle = 2$ (□); $J = 0.6$, $\langle H \rangle = 0$(•).

4. CONCLUSION

In this paper, we have investigated the effect of a varying field on the decay of the long-range DCF. As a model system we have used the lattice gas defined by the Hamiltonian (1). This simple model has been studied within the recently developed method [3]. Its DCF can be obtained explicitly owing to a judicious form of the three-spin interaction leading to two constraints for introduced auxiliary quantities (13), (16). The analysis of the resulting Eqs. (17a–d) indicates a more rapid decay

of the DCF by increasing the dispersion of the applied field (see Fig. 3). This fact is clearly seen from the three-diagonal system of linear equations (19), too. This system induces the exponential decay of the DCF for a uniform field. The presence of an inhomogeneity in (19) implies also the exponential decay which is, according to [6], more rapid than the decay for the homogeneous case. We therefore conclude that the DCF concept can be applied also for the inhomogenous and random models.

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ЕФФЕКТ НЕОДНОРОДНОСТИ НА ПРЯМЫЕ КОРРЕЛАЦИОННЫЕ ФУНКЦИИ ОДНОМЕРНОЙ РЕШЕТКИ ГАЗА С МНОГОКРАТНЫМ ВЗАИМОДЕЙСТВИЕМ.

Основной целю работы является исследование влияния изменяющегося поля на прямую корреляционныю функцию (ДКФ) спиновой цепочки. Проблема изучается с применением решетки газа с тремя последующими взаимодействиями, поскольку ДКФ дальнего взаимодействия может быть получена непосредственно. Численные расчеты показывают на ускореный распад ДКФ с нарастающей дисперсией существующего поля. Это обстоятельство позволяет применить общую идею ДКФ при исследовании неоднородных систем.