

CORRELATION FUNCTIONS OF QUENCHED AND ANNEALED ISING SYSTEMS

R.R. LEVITSKII, S.I. SOROKOV, R.O. SOKOLOVSKII

*Institute for Condensed Matter Physics
of the Ukrainian National Academy of Sciences
1 Svientsitski St., UA-290011 Lviv, Ukraine*

Received March 2, 1995

Spin correlation functions (up to the 3-site one) of disordered Ising model with the nearest neighbour interaction are calculated and investigated within a two-site cluster approximation for both quenched and annealed cases. The approach yields the exact results for the one-dimensional system. The long-range interaction is taken into account in the mean field approximation.

1. Introduction

During recent years the statistical theory of disordered spin models is an object of great interest due to their various properties and applications. In this paper we will consider an alloy of Ising systems (AIS) that can describe the processes of (magnetic or ferroelectric) ordering in alloys of magnets, magnets with nonmagnetic admixtures, solid solutions of ferroelectrics etc. This model is considered usually in two limiting cases, namely the case of annealed system (equilibrium type of disorder) and the case of quenched system (nonequilibrium disorder). There is no common opinion on the question, what type of disorder is realized in partially deuterated ferroelectrics, e.g. $Cs(D_xH_{1-x})_2PO_4$, $K(D_xH_{1-x})_2PO_4$. This situation requires both annealed and quenched cases to be theoretically studied and compared with experimental data.

The exact results for both limits are known at the one-dimensional case [1]. Effect of dilution (noninteracting admixture) on the two- and three-dimensional Ising model (quenched case) have been studied by Monte-Carlo method [2,3]. AIS can also be used as a test of approximative methods of statistical mechanics. It is known that the mean field approximation (MFA) yields quite satisfactory results for the Ising model. However it is not able to reproduce some essential properties of AIS [4] (such as percolation in diluted system and some differences between the properties of annealed and quenched systems).

In spite of great attention to AIS and great advance in its investigation (see review in [5,6]) the problem of calculation of AIS's correlation functions (CFs) for the case $D \geq 2$ (within some acceptable approximation) is not solved up to now. In this paper we suggest the solution of this problem for both quenched and annealed systems generalizing the approach of [7] on disordered model. The short-range interactions are taken into account

within the two-site cluster approximation (TCA). In the appendix the long-range interactions are also taken into consideration within MFA.

2. Formulation of the problem

We shall consider an Ising mixture with the Hamiltonian $\mathcal{H}(\{S, X\})$

$$-\beta\mathcal{H}(\{S, X\}) \equiv H(\{S, X\}) = H_x(\{S\}) + H(\{X\}); \quad \beta = 1/k_B T, \quad (2.1)$$

where

$$H_x(\{S\}) = \sum_i \kappa_i S_i + \frac{1}{2} \sum_{ij} K_{ij} S_i S_j \quad (2.2)$$

describes a quasispin subsystem on the sites of a simple lattice ($i, j = 1 \dots N$) with the pair exchange interaction K_{ij} in the site dependent field κ_i . The set of spin variables $\{S_i\}$ represents a state of the spin subsystem ($S_i = \pm 1$).

The other part of the Hamiltonian

$$H(\{X\}) = \sum_i \mu_i + \frac{1}{2} \sum_{ij} V_{ij} \quad (2.3)$$

includes "nonexchange" pair interaction V_{ij} and field μ_i . Each site contains a spin of a certain sort and the sort configuration is described by the set of variables $\{X_{i\alpha}\}$ ($\alpha = 1 \dots \Omega$, Ω is a number of sorts): $X_{i\alpha} = 1$ if the site i is occupied by the spin of sort α , otherwise $X_{i\alpha} = 0$. Interactions κ_i , K_{ij} , μ_i , V_{ij} depend on the sort configuration

$$\begin{aligned} \mu_i &= \sum_{\alpha} \mu_{i\alpha} X_{i\alpha}; & V_{ij} &= \sum_{\alpha\beta} V_{i\alpha, j\beta} X_{i\alpha} X_{j\beta}; \\ \kappa_i &= \sum_{\alpha} \kappa_{i\alpha} X_{i\alpha}; & K_{ij} &= \sum_{\alpha\beta} K_{i\alpha, j\beta} X_{i\alpha} X_{j\beta}. \end{aligned} \quad (2.4)$$

It should be noted that parameters of the Hamiltonian contain inverse temperature β . We suppose the pair interactions to be short-range

$$V_{i\alpha, j\beta} = \beta V_{\alpha\beta} \pi_{ij}; \quad \beta K_{i\alpha, j\beta} = K_{\alpha\beta} \pi_{ij}; \quad \pi_{ij} = \begin{cases} 1, & \text{if } i \in \pi_j \\ 0, & \text{in opposite case} \end{cases}, \quad (2.5)$$

where π_i denotes the set of the nearest neighbours of the site i (the first coordination sphere). In an appendix we will also take into account the long-range interactions in MFA.

The model is considered at the cases of annealed system and of quenched one. At the first case an equilibrium sort configuration is realized and the system is described by the density matrix

$$\rho(\{S, X\}) = \mathcal{Z}^{-1} \exp H(\{S, X\}); \quad \mathcal{Z} = \text{Sp}_{\{S, X\}} \exp H(\{S, X\}) \quad (2.6)$$

as well as by the generating function

$$\mathcal{F}(\{\kappa, \mu\}) = \ln \mathcal{Z} = -\beta\mathcal{G}, \quad (2.7)$$

where \mathcal{G} is the grand thermodynamic potential of the system.

The generating function allows to calculate the correlation functions (CFs) of the system

$$\langle S_{i_1\alpha_1} \cdots S_{i_n\alpha_n} X_{j_1\beta_1} \cdots X_{j_l\beta_l} \rangle^c = \frac{\delta}{\delta\kappa_{i_1\alpha_1}} \cdots \frac{\delta}{\delta\kappa_{i_n\alpha_n}} \frac{\delta}{\delta\mu_{j_1\beta_1}} \cdots \frac{\delta}{\delta\mu_{j_l\beta_l}} \mathcal{F}(\{\kappa, \mu\}), \quad (2.8)$$

where $S_{i\alpha} = S_i X_{i\alpha}$, the superscript c means cumulant averaging and

$$\langle (\cdots) \rangle = \text{Sp}_{\{S, X\}} [\rho(\{S, X\})(\cdots)]. \quad (2.9)$$

The chemical potentials $\mu_{i\alpha}$ have to be found from the equations

$$\langle X_{i\alpha} \rangle = c_\alpha, \quad (2.10)$$

where c_α is a concentration of the sort α spins.

At the case of quenched type of disorder the sort configuration is fixed and independent of temperature, therefore thermodynamic averaging implies only a trace over spin degrees of freedom

$$\langle (\cdots) \rangle_H = \text{Sp}_{\{S\}} [\rho_x(\{S\})(\cdots)]; \quad \rho_x(\{S\}) = Z_x^{-1} \exp H_x(\{S\}); \quad (2.11)$$

$$Z_x = \text{Sp}_{\{S\}} \exp(H_x(\{S\})). \quad (2.12)$$

In order to obtain observable quantities one must perform also an averaging over sort configurations

$$\langle (\cdots) \rangle_x = \text{Sp}_{\{X\}} [\rho(\{X\})(\cdots)], \quad (2.13)$$

where the distribution $\rho(\{X\})$ is determined by the conditions of system's freezing. Our approximation is sensitive to the following moments of this distribution:

$$\langle X_{i\alpha} X_{j\beta} \rangle_x = w_{\alpha\beta} \quad (j \in \pi_i); \quad \langle X_{i\alpha} \rangle_x = c_\alpha \equiv \sum_{\beta} w_{\alpha\beta}. \quad (2.14)$$

Free energy of a quenched system is defined as follows

$$F = -\beta^{-1} \langle F_x \rangle_x - \beta^{-1} \langle H(\{X\}) \rangle_x; \quad \langle F_x \rangle_x = \langle \ln \text{Sp}_{\{S\}} \exp[H_x(\{S\})] \rangle_x. \quad (2.15)$$

Function $\langle F_x \rangle_x = \langle F_x \rangle_x(\{\kappa\})$ that is the cumulant generating function in this case:

$$m_{i_1\alpha_1 \cdots i_n\alpha_n}^{(n)} = \langle \langle S_{i_1\alpha_1} \cdots S_{i_n\alpha_n} \rangle^c_H \rangle_x = \frac{\delta}{\delta\kappa_{i_1\alpha_1}} \cdots \frac{\delta}{\delta\kappa_{i_n\alpha_n}} \langle F_x \rangle_x(\{\kappa\}). \quad (2.16)$$

3. Quenched case

First we carry out a cluster expansion of the generating function $\langle F_x \rangle_x$. For this purpose we write the Hamiltonian $H_x(\{S\})$ in the form

$$H_x(\{S\}) = \sum_i H_i + \sum_{(ij)} U_{ij}, \quad (3.1)$$

where

$$H_i = \bar{\kappa}_i S_i; \quad \bar{\kappa}_i = \kappa_i + \sum_{r \in \pi_i} r \bar{\varphi}_i; \quad r \bar{\varphi}_i = \sum_{\alpha} X_{i\alpha} r \bar{\varphi}_{i\alpha}; \quad (3.2)$$

$$U_{ij} = -{}_j \bar{\varphi}_i S_i - {}_i \bar{\varphi}_j S_j + K_{ij} S_i S_j. \quad (3.3)$$

We introduce here the parameters ${}_r \bar{\varphi}_i$, which play a role of the effective field acting on the spin S_i from the nearest neighbour at the site r . Summation $\sum_{(ij)}$ in (3.1) spans pairs of the nearest neighbour sites. We can write function F_x in the form

$$F_x = \sum_i F_i + \ln Q. \quad (3.4)$$

Here we use the notations

$$F_i = \ln Z_i; \quad Z_i = \text{Sp}_{S_i} \exp H_i;$$

$$Q = \langle \exp \sum_{(ij)} U_{ij} \rangle_{\rho_0}; \quad \rho_0 = \prod_i \rho_i; \quad \rho_i = Z_i^{-1} \exp(H_i). \quad (3.5)$$

The first term \mathcal{K}_1 of a cluster expansion [6,8] of $\ln Q$ has the form

$$\ln Q = \ln \langle \exp \sum_{(ij)} U_{ij} \rangle_{\rho_0} \approx \mathcal{K}_1 = \sum_{(ij)} \ln \langle \exp U_{ij} \rangle_{\rho_0} = -z \sum_i F_i + \sum_{(ij)} F_{ij}, \quad (3.6)$$

where $z = \sum_j \pi_{ij}$ is a number of the nearest neighbour sites and

$$F_{ij} = \ln Z_{ij}; \quad Z_{ij} = \text{Sp}_{S_i S_j} \exp H_{ij}; \\ H_{ij} = {}_i \bar{\kappa}_j S_i + {}_j \bar{\kappa}_i S_j + K_{ij} S_i S_j; \quad {}_r \bar{\kappa}_i = \bar{\kappa}_i - {}_r \bar{\varphi}_i. \quad (3.7)$$

So the generating function $\langle F_x \rangle_x$ restricted by the first term of the cluster expansion is obtained in the form

$$\langle F_x \rangle_x = -z' \sum_i \langle F_i \rangle_x + \sum_{(ij)} \langle F_{ij} \rangle_x \quad (z' = z - 1). \quad (3.8)$$

Parameters ${}_r \bar{\varphi}_{i\alpha}$ are found due to the minimization of the free energy

$$\frac{\partial \langle F_x \rangle_x}{\partial {}_r \bar{\varphi}_{i\alpha}} = 0. \quad (3.9)$$

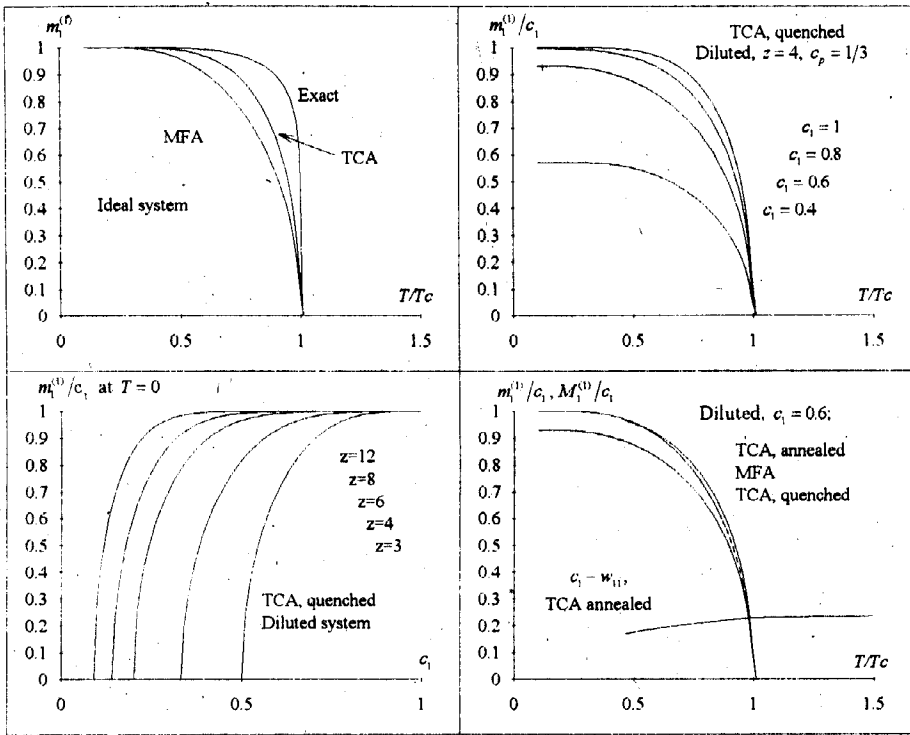


Figure 1. Order parameters of pure and dilute systems on plane square lattice ($z = 4$).

It gives the following self-consistency equations for the average value of spin $m_{i\alpha}^{(1)} = \langle \langle S_{i\alpha} \rangle \rangle_x$

$$m_{i\alpha}^{(1)} = \langle \langle S_{i\alpha} \rangle_{\rho_i} \rangle_x, \tag{3.10}$$

$$\langle \langle S_{i\alpha} \rangle_{\rho_i} \rangle_x = \langle \langle S_{i\alpha} \rangle_{\rho_{ij}} \rangle_x, \tag{3.11}$$

where $j \in \pi_i$ and

$$\rho_{ij} = \frac{\exp H_{ij}}{Z_{ij}}. \tag{3.12}$$

Relations (3.10), (3.11) can be written in the form:

$$m_{i\alpha}^{(1)} = \langle F_{i\alpha}^{(1)} \rangle_x, \tag{3.13}$$

$$\langle F_{i\alpha}^{(1)} \rangle_x = \langle F_{i\alpha,r}^{(10)} \rangle_x. \tag{3.14}$$

Here the notations

$$\langle F_{i\alpha_1 \dots \alpha_n}^{(n)} \rangle_x = \frac{\partial}{\partial \kappa_{i\alpha_1}} \dots \frac{\partial}{\partial \kappa_{i\alpha_n}} \langle F_i \rangle_x = \langle \langle S_{i\alpha_1} \dots S_{i\alpha_n} \rangle_{\rho_i}^c \rangle_x; \tag{3.15}$$

$$\begin{aligned} \langle F_{i\alpha_1 \dots \alpha_n, j\beta_1 \dots \beta_l}^{(nl)} \rangle_x &= \frac{\partial}{\partial \kappa_{i\alpha_1}} \dots \frac{\partial}{\partial \kappa_{i\alpha_n}} \frac{\partial}{\partial \kappa_{j\beta_1}} \dots \frac{\partial}{\partial \kappa_{j\beta_l}} \langle F_{ij} \rangle_x = \\ &= \langle \langle S_{i\alpha_1} \dots S_{i\alpha_n} S_{j\beta_1} \dots S_{j\beta_l} \rangle_{\rho_{ij}}^c \rangle_x \end{aligned} \tag{3.16}$$

are introduced. Below we give the explicit expressions for the quantities $\langle F_i \rangle_x$, $\langle F_{ij} \rangle_x$ and their derivatives which will be used later:

$$\begin{aligned}
 \langle F_i \rangle_x &= \sum_{\alpha} c_{\alpha} F_{i\alpha}; & F_{i\alpha} &= \ln 2 \cosh \bar{\kappa}_{i\alpha}; \\
 \langle F_{i\alpha_1 \dots \alpha_n} \rangle_x &= \delta_{\alpha_1 \alpha_2} \dots \delta_{\alpha_{n-1} \alpha_n} c_{\alpha_1} F_{i\alpha_1}^{(n)}; \\
 F_{i\alpha}^{(1)} &= \tanh \bar{\kappa}_{i\alpha}; & F_{i\alpha}^{(2)} &= 1 - \tanh^2 \bar{\kappa}_{i\alpha}; & F_{i\alpha}^{(3)} &= -2F_{i\alpha}^{(1)} F_{i\alpha}^{(2)}; \\
 \langle F_{ij} \rangle_x &= \sum_{\alpha\beta} w_{\alpha\beta} F_{i\alpha,j\beta}; & F_{i\alpha,j\beta} &= \ln 2 e^{K_{\alpha\beta}} L_{i\alpha,j\beta}; \\
 L_{i\alpha,j\beta} &= \cosh(\bar{\kappa}_{i\alpha} + \bar{\kappa}_{j\beta}) + a_{\alpha\beta} \cosh(\bar{\kappa}_{i\alpha} - \bar{\kappa}_{j\beta}); & a_{\alpha\beta} &= e^{-2K_{\alpha\beta}}; \\
 \langle F_{i\alpha_1 \dots \alpha_n, j} \rangle_x &= \delta_{\alpha_1 \alpha_2} \dots \delta_{\alpha_{n-1} \alpha_n} \sum_{\beta} w_{\alpha_1 \beta} F_{i\alpha_1, j\beta}^{(n0)}; \\
 F_{i\alpha, j\beta}^{(10)} &= (\sinh(\bar{\kappa}_{i\alpha} + \bar{\kappa}_{j\beta}) + a_{\alpha\beta} \sinh(\bar{\kappa}_{i\alpha} - \bar{\kappa}_{j\beta})) / L_{i\alpha, j\beta}; \\
 F_{i\alpha, j\beta}^{(20)} &= 1 - (F_{i\alpha, j\beta}^{(10)})^2 = (1 + a_{\alpha\beta}^2 + 2a_{\alpha\beta} \sinh(\bar{\kappa}_{i\alpha} - \bar{\kappa}_{j\beta})) / L_{i\alpha, j\beta}^2; \\
 F_{i\alpha, j\beta}^{(30)} &= -2F_{i\alpha, j\beta}^{(10)} F_{i\alpha, j\beta}^{(20)}; \\
 \langle F_{i\alpha_1 \dots \alpha_n, j\beta_1 \dots \beta_l} \rangle_x &= \delta_{\alpha_1 \alpha_2} \dots \delta_{\alpha_{n-1} \alpha_n} \delta_{\beta_1 \beta_2} \dots \delta_{\beta_{l-1} \beta_l} w_{\alpha_1 \beta_1} F_{i\alpha_1, j\beta_1}^{(nl)}; \\
 F_{i\alpha, j\beta}^{(11)} &= \frac{1 - a_{\alpha\beta}^2}{L_{i\alpha, j\beta}^2}; & F_{i\alpha, j\beta}^{(21)} &= -2F_{i\alpha, j\beta}^{(10)} F_{i\alpha, j\beta}^{(11)}. \tag{3.17}
 \end{aligned}$$

The expression (3.11) contains $Nz\Omega$ equation for the same number of variables ${}_{\tau}\bar{\varphi}_{i\alpha}$. At the case of uniform field ($\kappa_{i\alpha} \rightarrow \kappa_{\alpha}$) parameters ${}_{\tau}\bar{\varphi}_{i\alpha}$ lose their site dependence and (3.11) reduces to Ω equations for the same number of fields and we obtain a well-known result of Bethe approximation and cluster variation method for average value of spin

$$m_{\alpha}^{(1)} = c_{\alpha} \tanh \bar{\kappa}_{\alpha} = \sum_{\beta} w_{\alpha\beta} \frac{\sinh(\bar{\kappa}'_{\alpha} + \bar{\kappa}'_{\beta}) + a_{\alpha\beta} \sinh(\bar{\kappa}'_{\alpha} - \bar{\kappa}'_{\beta})}{\cosh(\bar{\kappa}'_{\alpha} + \bar{\kappa}'_{\beta}) + a_{\alpha\beta} \cosh(\bar{\kappa}'_{\alpha} - \bar{\kappa}'_{\beta})}, \tag{3.18}$$

$$\bar{\kappa}_{\alpha} = \kappa_{\alpha} + z\bar{\varphi}_{\alpha}; \quad \bar{\kappa}'_{\alpha} = \kappa_{\alpha} + z'\bar{\varphi}_{\alpha}. \tag{3.19}$$

We can obtain CFs of any order with differentiation of (3.10), (3.11) and it is an advantage of presented approach.

It follows from (3.13) that

$$m_{i\alpha, j\beta}^{(2)} = \frac{\delta m_{i\alpha}^{(1)}}{\delta \kappa_{j\beta}} = \frac{\partial \langle F_{i\alpha} \rangle_x}{\partial \bar{\kappa}_{i\gamma}} \frac{\delta \bar{\kappa}_{i\gamma}}{\delta \kappa_{j\beta}} = \langle F_{i\alpha\gamma} \rangle_x \bar{\kappa}_{i\gamma, j\beta}^{(1)}. \tag{3.20}$$

Hereafter the summation over sort indices (Greek letters) is not written explicitly so the sum over γ symbol is omitted in (3.20). We have just used the notation

$$\bar{\kappa}_{i\alpha, j\beta}^{(1)} = \frac{\delta \bar{\kappa}_{i\alpha}}{\delta \kappa_{j\beta}} = \delta_{ij} \delta_{\alpha\beta} + \sum_{\tau \in \pi_i} {}_{\tau}\bar{\varphi}_{i\alpha, j\beta}^{(1)}; \quad \bar{\varphi}_{i\alpha, j\beta}^{(1)} = \frac{\delta {}_{\tau}\bar{\varphi}_{i\alpha}}{\delta \kappa_{j\beta}} \tag{3.21}$$

(see a definition of $\bar{\kappa}_i$ (3.2)). It is convenient to write the relation (3.20) in the matrix form

$$\hat{m}_{ij}^{(2)} = \hat{F}_i^{(2)} \hat{\kappa}_{ij}^{(1)}, \quad (3.22)$$

where the matrix notation is introduced:

$$\left(\hat{m}_{ij}^{(2)}\right)_{\alpha\beta} = m_{i\alpha, j\beta}^{(2)}, \quad \left(\hat{F}_i^{(2)}\right)_{\alpha\beta} = \langle F_{i\alpha\beta}^{(2)} \rangle_x, \quad \left(\hat{\kappa}_{ij}^{(1)}\right)_{\alpha\beta} = \bar{\kappa}_{i\alpha, j\beta}^{(1)}. \quad (3.23)$$

In order to calculate the quantities ${}_r\hat{\varphi}_{i\alpha, j\beta}^{(1)}$ it is necessary to use the relation (3.14). Differentiating it with respect to $\kappa_{j\beta}$ we obtain:

$$\hat{F}_i^{(2)} \bar{\kappa}_{ij}^{(1)} = \hat{F}_{ir}^{(20)} {}_r\hat{\kappa}_{ij}^{(1)} + \hat{F}_{ir}^{(11)} {}_i\hat{\kappa}_{rj}^{(1)}, \quad (3.24)$$

where

$$\left(\hat{F}_{ir}^{(20)}\right)_{\alpha\beta} = \langle F_{i\alpha\beta, r}^{(20)} \rangle_x; \quad \left(\hat{F}_{ir}^{(11)}\right)_{\alpha\beta} = \langle F_{i\alpha, r\beta}^{(11)} \rangle_x; \quad (3.25)$$

$${}_r\hat{\kappa}_{ij}^{(1)} = \hat{\kappa}_{ij}^{(1)} - {}_r\hat{\varphi}_{ij}^{(1)}; \quad \left({}_r\hat{\varphi}_{ij}^{(1)}\right)_{\alpha\beta} = {}_r\hat{\varphi}_{i\alpha, j\beta}^{(1)}. \quad (3.26)$$

Taking into account (3.26), the equation (3.24) can be rewritten in the following form:

$$\hat{F}_{ir}^{(20)} {}_r\hat{\varphi}_{ij}^{(1)} + \hat{F}_{ir}^{(11)} {}_i\hat{\varphi}_{rj}^{(1)} = \left(\hat{F}_{ir}^{(20)} - \hat{F}_i^{(2)}\right) \hat{\kappa}_{ij}^{(1)} + \hat{F}_{ir}^{(11)} \hat{\kappa}_{rj}^{(1)}. \quad (3.27)$$

Replacing the indices $i \leftrightarrow r$ in (3.27) we get the second equation

$$\hat{F}_{ri}^{(11)} {}_r\hat{\varphi}_{ij}^{(1)} + \hat{F}_{ri}^{(20)} {}_i\hat{\varphi}_{rj}^{(1)} = \hat{F}_{ri}^{(11)} \hat{\kappa}_{ij}^{(1)} + \left(\hat{F}_{ri}^{(20)} - \hat{F}_r^{(2)}\right) \hat{\kappa}_{rj}^{(1)}, \quad (3.28)$$

which forms together with (3.27) the set of equations for the quantities ${}_r\hat{\varphi}_{ij}^{(1)}$, ${}_i\hat{\varphi}_{rj}^{(1)}$. Excluding ${}_i\hat{\varphi}_{rj}^{(1)}$ from this set and expressing the $\hat{\kappa}_{ij}^{(1)}$ via $m_{ij}^{(2)}$ (see (3.22)) we have

$${}_r\hat{\varphi}_{ij}^{(1)} = \left[\left(\hat{F}_i^{(2)}\right)^{-1} + \hat{E}_{ii}\right] \hat{m}_{ij}^{(2)} + \hat{G}_{ir} \hat{m}_{rj}^{(2)}, \quad (3.29)$$

where

$$\begin{aligned} \hat{E}_{ii} &= \left(\hat{F}_{ir}^{(11)} \left(\hat{F}_{ri}^{(20)}\right)^{-1} \hat{F}_{ri}^{(11)} - \hat{F}_{ir}^{(20)}\right)^{-1}, \\ \hat{G}_{ir} &= \left(\hat{F}_{ri}^{(20)} \left(\hat{F}_{ir}^{(11)}\right)^{-1} \hat{F}_{ir}^{(20)} - \hat{F}_{ri}^{(11)}\right)^{-1}. \end{aligned} \quad (3.30)$$

Later on we sum the relation (3.29) over $r \in \pi_i$ and take into account (3.22), (3.21). It results in the following Ornstein-Zernike-type equation for the pair CF $m_{ij}^{(2)}$

$$\hat{U}_{ii} \hat{m}_{ij}^{(2)} = \delta_{ij} + \sum_{r \in \pi_i} \hat{G}_{ir} \hat{m}_{rj}^{(2)}, \quad (3.31)$$

where

$$\hat{U}_{ii} = -z' \left(\hat{F}_i^{(2)}\right)^{-1} - \sum_{r \in \pi_i} \hat{E}_{ii}. \quad (3.32)$$

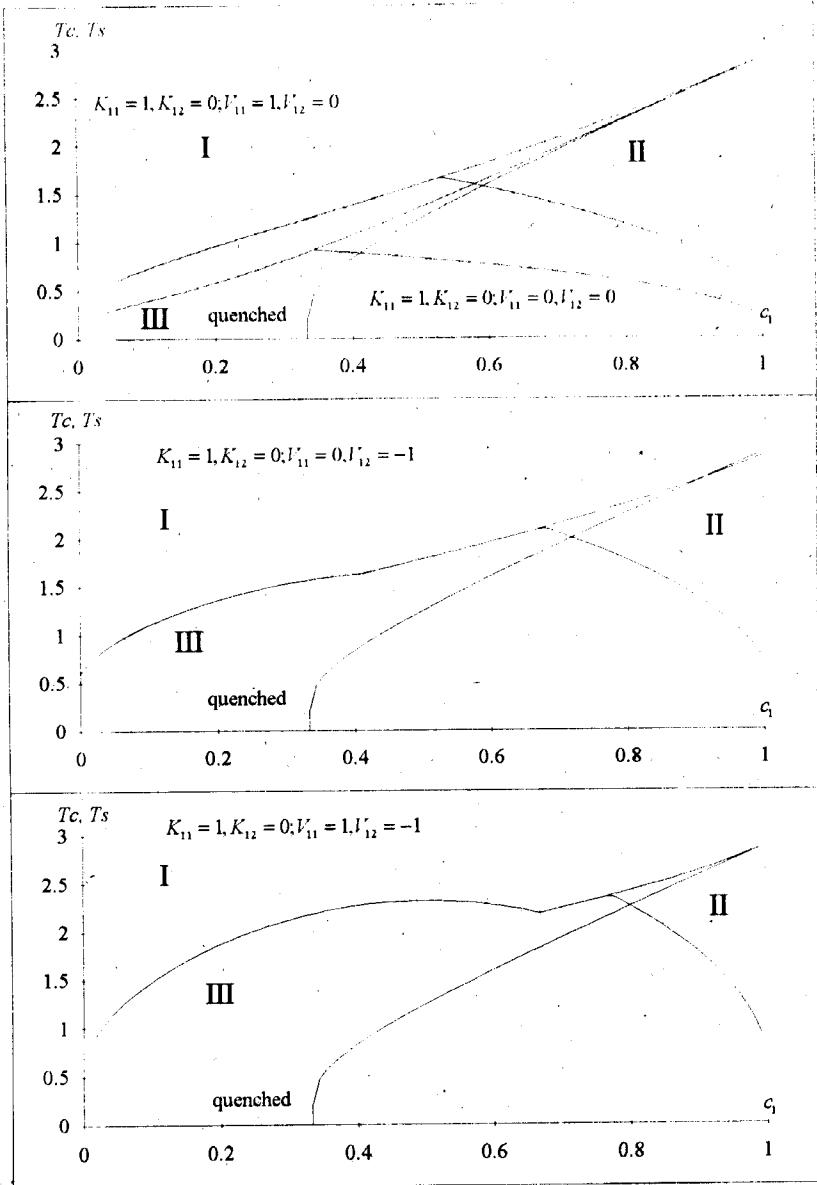


Figure 2. Phase diagrams for dilute system on plane square lattice ($z = 4$) at different "nonexchange" interactions V_{11}, V_{12} ($V_{22} = 0$). Annealed: I - paraphase, II - spin ordered phase, III - segregated alloy.

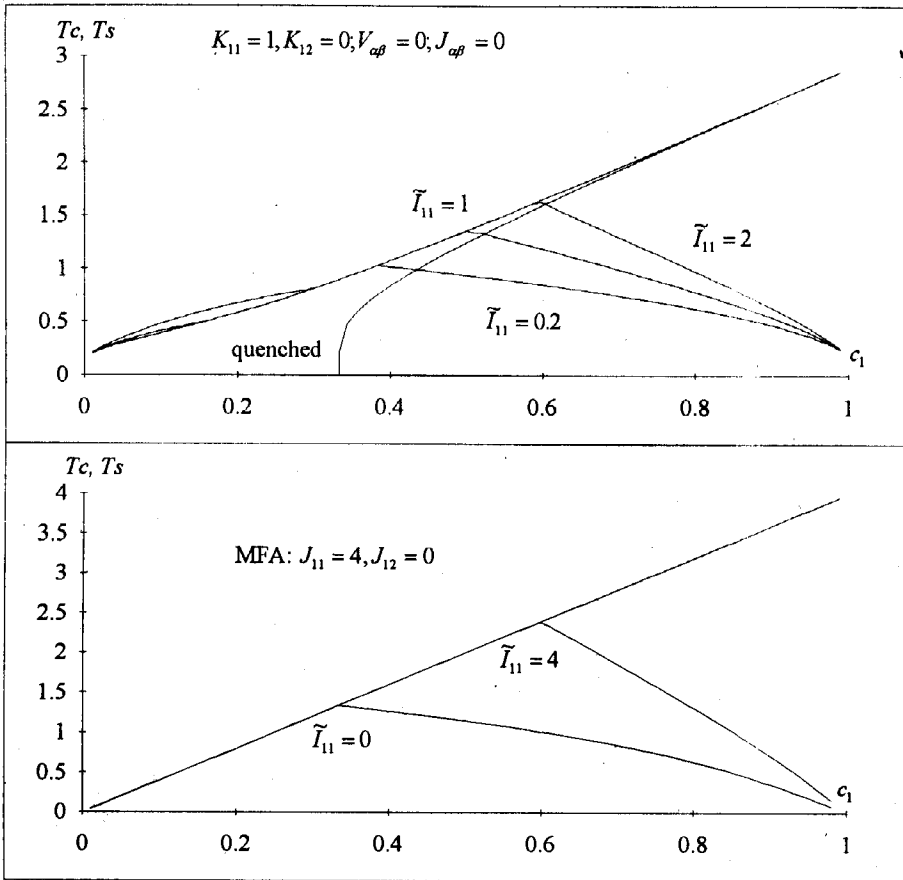


Figure 3. MFA results for the phase diagram of the system. $J_{\alpha\beta} = \sum_j J_{i\alpha,j\beta}$, $\tilde{I}_{11} = \sum_j (I_{i1,j1} - 2I_{i1,j2} + I_{i2,j2})$ (see Appendix).

In the case of uniform field the matrices \hat{F} are independent of site indices, the CF $\hat{m}_{ij}^{(2)}$ depends on the difference of the sites' 1, 2 coordinates and we can solve the equation (3.31) carrying out the Fourier transformation

$$\hat{m}_{ij}^{(2)} = \hat{m}^{(2)}(\vec{r}_j - \vec{r}_i) = \frac{1}{V_e(2\pi)^D} \int d\vec{q} e^{-i\vec{q}(\vec{r}_j - \vec{r}_i)} \hat{m}^{(2)}(\vec{q}), \quad (3.33)$$

V_e is a volume of the elementary cell, D being the dimension of the lattice (space). The solution has the form

$$\begin{aligned} (\hat{m}^{(2)}(\vec{q}))^{-1} = & -z'(\hat{F}^{(2)})^{-1} + z(\hat{F}^{(20)} + \hat{F}^{(11)})^{-1} + \\ & + (\pi(\vec{0}) - \pi(\vec{q})) \left(\hat{F}^{(20)} (\hat{F}^{(11)})^{-1} \hat{F}^{(20)} - \hat{F}^{(11)} \right)^{-1}, \end{aligned} \quad (3.34)$$

where

$$\pi(\vec{q}) = \sum_{j \in \pi_i} e^{i\vec{q}(\vec{r}_j - \vec{r}_i)}; \quad \pi(\vec{0}) = z. \quad (3.35)$$

For the hypercubic lattices one has

$$\pi(\vec{q}) = 2 \sum_{l=1}^D \cos(\vec{q}l a), \quad (3.36)$$

where a is the lattice spacing.

The expression (3.34) in the limit $c_1 = 1$ yields the TCA result for the ideal (one-sort) system [7]. Taking $\vec{q} = 0$ in (3.34) one gets the earlier result [4,6]. The known exact formula for the one-dimensional system in zero external field [1] also follows from (3.34).

We will obtain the expression for the 3-site CF $m_{1\alpha,2\beta,3\gamma}^{(3)}$ differentiating equation (3.31) which can be written in the form

$$U_{1\alpha,1\delta} m_{1\delta,2\beta}^{(2)} = \delta_{12} \delta_{\alpha\beta} + \sum_{r \in \pi_1} G_{1\alpha,r\delta} m_{r\delta,2\beta}^{(2)} \quad (3.37)$$

(here free site indices are denoted with numbers and summation over repeated sort indices is implied). The differentiation with respect to $\kappa_{3\gamma}$ yields

$$\dot{U}_{1\alpha,1\delta,3\gamma} m_{1\delta,2\beta}^{(2)} + U_{1\alpha,1\delta} m_{1\delta,2\beta,3\gamma}^{(3)} = \sum_{r \in \pi_1} \left(\dot{G}_{1\alpha,r\delta,3\gamma} m_{r\delta,2\beta}^{(2)} + G_{1\alpha,r\delta} m_{r\delta,2\beta,3\gamma}^{(3)} \right), \quad (3.38)$$

where the point denotes the derivatives of corresponding quantities:

$$\begin{aligned} \dot{U}_{1\alpha,1\delta,3\gamma} &= \frac{\delta U_{1\alpha,1\delta}}{\delta \kappa_{3\gamma}} \equiv \begin{array}{c} 1\alpha \quad \triangle \quad 1\delta \\ \dot{U} \\ 3\gamma \end{array}, \\ \dot{G}_{1\alpha,r\delta,3\gamma} &= \frac{\delta G_{1\alpha,r\delta}}{\delta \kappa_{3\gamma}} \equiv \begin{array}{c} 1\alpha \quad \triangle \quad r\delta \\ \dot{G} \\ 3\gamma \end{array}, \\ m_{1\alpha,2\beta,3\gamma}^{(3)} &= \frac{\delta m_{1\alpha,2\beta}^{(2)}}{\delta \kappa_{3\gamma}} \equiv \begin{array}{c} 1\alpha \quad \triangle \quad 2\beta \\ m^{(3)} \\ 3\gamma \end{array}. \end{aligned} \quad (3.39)$$

In (3.39) the threepoles are introduced which allows us to write (3.38) in more convenient form:

$$\begin{aligned} & \begin{array}{c} 1 \quad \triangle \quad 1 \\ \dot{U} \\ 3 \end{array} \hat{m}_{12}^{(2)} + \dot{U}_{11} \begin{array}{c} 1 \quad \triangle \quad 2 \\ m^{(3)} \\ 3 \end{array} = \\ &= \sum_{r \in \pi_1} \left(\begin{array}{c} 1 \quad \triangle \quad r \\ \dot{G} \\ 3 \end{array} \hat{m}_{r2}^{(2)} + \hat{G}_{1r} \begin{array}{c} 1 \quad \triangle \quad 2 \\ m^{(3)} \\ 3 \end{array} \right). \end{aligned} \quad (3.40)$$

It should be noted that equality of site indices in threepoles and matrices implies also the symmetry with respect to corresponding sort indices, *i.e.*

$$\begin{array}{c} 1\gamma \\ \triangle \\ 3\epsilon \end{array} \dot{U} = \begin{array}{c} 1\delta \\ \triangle \\ 3\epsilon \end{array} \dot{U} \quad (3.41)$$

Differentiating expressions (3.30) and (3.32) we find

$$\begin{array}{c} 1 \\ \triangle \\ 3 \end{array} \dot{U} = z' \begin{array}{c} (\hat{F}_1^{(2)})^{-1} \\ 1 \\ \triangle \\ 3 \end{array} \dot{F}^{(2)} \begin{array}{c} (\hat{F}_1^{(2)})^{-1} \\ 1 \\ \triangle \\ 3 \end{array} + \\
 + \sum_{r \in \pi_1} \hat{E}_{11} \left(\begin{array}{c} 1 \\ \triangle \\ 3 \end{array} \dot{F}^{(11)} \begin{array}{c} (\hat{F}_{r1}^{(20)})^{-1} \\ r \\ \triangle \\ 3 \end{array} \hat{F}_{r1}^{(11)} - \right. \\
 \left. \hat{F}_{1r}^{(11)} \begin{array}{c} (\hat{F}_{r1}^{(20)})^{-1} \\ r \\ \triangle \\ 3 \end{array} \dot{F}^{(20)} \begin{array}{c} (\hat{F}_{r1}^{(20)})^{-1} \\ r \\ \triangle \\ 3 \end{array} \hat{F}_{r1}^{(11)} \right. \\
 \left. + \begin{array}{c} \hat{F}_{1r}^{(11)} \begin{array}{c} (\hat{F}_{r1}^{(20)})^{-1} \\ r \\ \triangle \\ 3 \end{array} \dot{F}^{(11)} - \begin{array}{c} 1 \\ \triangle \\ 3 \end{array} \dot{F}^{(20)} \begin{array}{c} 1 \\ \triangle \\ 3 \end{array} \right) \hat{E}_{11} \quad (3.42)$$

When obtaining the formula (3.42) the identities of the following type are used:

$$\frac{\delta (\hat{F}_1^{(2)})^{-1}}{\delta \kappa_{3\gamma}} = - (\hat{F}_1^{(2)})^{-1} \left(\frac{\delta \hat{F}_1^{(2)}}{\delta \kappa_{3\gamma}} \right) (\hat{F}_1^{(2)})^{-1} \quad (3.43)$$

They can be obtained for any matrix \hat{A} by means of differentiation of the identity $\hat{A}\hat{A}^{-1} = 1$.

Now we shall obtain the expressions for the threepoles which have appeared in (3.42)

$$\frac{\delta (\hat{F}_1^{(2)})_{\alpha\beta}}{\delta \kappa_{3\gamma}} = \frac{\delta (F_{1\alpha\beta})_x}{\delta \kappa_{3\gamma}} = \langle F_{1\alpha\beta\delta}^{(3)} \rangle_x \hat{\kappa}_{1\delta,3\gamma}^{(1)} \quad (3.44)$$

In the diagram form it can be represented as

$$\begin{array}{c} 1 \\ \triangle \\ 3 \end{array} \dot{F}^{(2)} = \begin{array}{c} 1 \\ \triangle \\ 1 \hat{\kappa}_{13}^{(1)} \end{array} F^{(3)} \quad (3.45)$$

The other threepoles we find in the same way:

$$\begin{array}{c} r \\ \triangle \\ 3 \end{array} \dot{F}^{(20)} = \begin{array}{c} r \\ \triangle \\ r \hat{\kappa}_{r3}^{(1)} \end{array} F^{(30)} + \begin{array}{c} r \\ \triangle \\ 1 \hat{\kappa}_{13}^{(1)} \end{array} F^{(21)}, \quad (3.46)$$

$$\begin{array}{c} 1 \\ \triangle \\ \hat{F}^{(11)} \\ 3 \end{array} = \begin{array}{c} 1 \\ \triangle \\ F^{(21)} \\ 1 \quad r \hat{\kappa}_{13}^{(1)} \end{array} + \begin{array}{c} 1 \\ \triangle \\ F^{(21)} \\ r \quad 1 \hat{\kappa}_{r3}^{(1)} \end{array}, \quad (3.47)$$

where

$$\begin{array}{c} 1\alpha \\ \triangle \\ F^{(30)} \\ 1\gamma \\ 1\beta \end{array} = \langle F_{1\alpha\beta\gamma,r}^{(30)} \rangle_x = \langle \langle S_{1\alpha} S_{1\beta} S_{1\gamma} \rangle_{\rho_{1r}}^c \rangle_x, \\
 \begin{array}{c} r\alpha \\ \triangle \\ F^{(21)} \\ 1\gamma \\ r\beta \end{array} = \langle F_{r\alpha\beta,1\gamma}^{(21)} \rangle_x = \langle \langle S_{r\alpha} S_{r\beta} S_{1\gamma} \rangle_{\rho_{1r}}^c \rangle_x, \\
 \begin{array}{c} 1\alpha \\ \triangle \\ F^{(21)} \\ 1\gamma \\ r\beta \end{array} = \langle F_{1\alpha\gamma,r\beta}^{(21)} \rangle_x = \langle \langle S_{1\alpha} S_{1\gamma} S_{r\beta} \rangle_{\rho_{1r}}^c \rangle_x, \\
 \begin{array}{c} 1\alpha \\ \triangle \\ F^{(12)} \\ r\gamma \\ r\beta \end{array} = \langle F_{1\alpha,r\beta\gamma}^{(12)} \rangle_x = \langle \langle S_{1\alpha} S_{r\beta} S_{r\gamma} \rangle_{\rho_{1r}}^c \rangle_x. \quad (3.48)$$

The quantity $r \hat{\kappa}_{13}^{(1)}$ which appears in (3.46) follows from (3.26), (3.29) and can be expressed as

$$r \hat{\kappa}_{13}^{(1)} = \hat{\kappa}_{13}^{(1)} - r \hat{\varphi}_{13}^{(1)} = -\hat{E}_{11} \hat{m}_{13}^{(2)} - \hat{G}_{1r} \hat{m}_{r3}^{(2)}. \quad (3.49)$$

Using (3.45)-(3.46) in (3.42) and taking into account (3.49), (3.22) we get the expression for the threepole \hat{U} involving only the quantities calculated above, i.e. the matrices and threepoles F and the pair CF $\hat{m}_{ij}^{(2)}$. The same procedure is used to calculate the threepole \hat{G} . Using the obtained expressions in (3.40) we get the equation for the 3-site CF:

$$\begin{array}{c} \hat{U}_{11} \\ \triangle \\ m^{(3)} \\ 3 \end{array} = \sum_{r \in \pi_1} \left(\begin{array}{c} 1 \\ \triangle \\ A \\ 1 \hat{m}_{13}^{(2)} \end{array} + \begin{array}{c} 1 \\ \triangle \\ B \\ r \hat{m}_{r3}^{(2)} \end{array} + \begin{array}{c} 1 \\ \triangle \\ C \\ 1 \hat{m}_{13}^{(2)} \end{array} + \begin{array}{c} 1 \\ \triangle \\ D \\ r \hat{m}_{r3}^{(2)} \end{array} \right) + \sum_{r \in \pi_1} \hat{G}_{1r} \begin{array}{c} \triangle \\ m^{(3)} \\ 3 \end{array}, \quad (3.50)$$

where

$$\begin{array}{c} 1 \\ \triangle \\ A \\ 1 \end{array} = \frac{z'}{z} (\hat{F}_1^{(2)})^{-1} \begin{array}{c} 1 \\ \triangle \\ F^{(3)} \\ 1 \end{array} (\hat{F}_1^{(2)})^{-1} - \dots$$

$$\begin{aligned}
 & - \left(\hat{G}_{1r} \begin{array}{c} \nearrow \\ F^{(30)} \\ \searrow \\ \hat{G}_{r1} \end{array} + \hat{G}_{1r} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{G}_{r1} \end{array} + \right. \\
 & \left. \hat{E}_{11} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{G}_{r1} \end{array} + \hat{G}_{1r} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{G}_{r1} \end{array} \right) - \\
 & - \left\{ \hat{E}_{11} \begin{array}{c} \nearrow \\ F^{(30)} \\ \searrow \\ \hat{E}_{11} \end{array} + \hat{E}_{11} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{G}_{r1} \end{array} + \right. \\
 & \left. \hat{G}_{1r} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{E}_{11} \end{array} + \hat{E}_{11} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{E}_{11} \end{array} \right\}, \tag{3.51}
 \end{aligned}$$

$$\begin{aligned}
 \begin{array}{c} \nearrow \\ B \\ \searrow \\ \hat{r} \end{array} & = - \left(\hat{G}_{1r} \begin{array}{c} \nearrow \\ F^{(30)} \\ \searrow \\ \hat{E}_{rr} \end{array} + \hat{G}_{1r} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{G}_{r1} \end{array} + \right. \\
 & \left. \hat{E}_{11} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{E}_{rr} \end{array} + \hat{G}_{1r} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{E}_{11} \end{array} \right) - t.i., \tag{3.52}
 \end{aligned}$$

$$\begin{aligned}
 \begin{array}{c} \nearrow \\ C \\ \searrow \\ \hat{1} \end{array} & = - \left(\hat{G}_{1r} \begin{array}{c} \nearrow \\ F^{(30)} \\ \searrow \\ \hat{E}_{rr} \end{array} + \hat{G}_{1r} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{E}_{rr} \end{array} + \right. \\
 & \left. \hat{E}_{11} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{E}_{rr} \end{array} + \hat{G}_{1r} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{G}_{r1} \end{array} \right) - t.i., \tag{3.53}
 \end{aligned}$$

$$\begin{aligned}
 \begin{array}{c} \nearrow \\ D \\ \searrow \\ \hat{r} \end{array} & = - \left(\hat{G}_{1r} \begin{array}{c} \nearrow \\ F^{(30)} \\ \searrow \\ \hat{E}_{rr} \end{array} + \hat{G}_{1r} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{E}_{rr} \end{array} + \right. \\
 & \left. \hat{E}_{11} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{E}_{rr} \end{array} + \hat{G}_{1r} \begin{array}{c} \nearrow \\ F^{(21)} \\ \searrow \\ \hat{G}_{r1} \end{array} \right) - t.i. \tag{3.54}
 \end{aligned}$$

In (3.51)-(3.54) "t.i." means twin to the previous (in parentheses) item, i.e. item where the matrix substitution $\hat{E} \leftrightarrow \hat{G}$ has been carried out. The last (in braces) item of (3.51) is an example of t.i. to the previous (in parentheses) one.

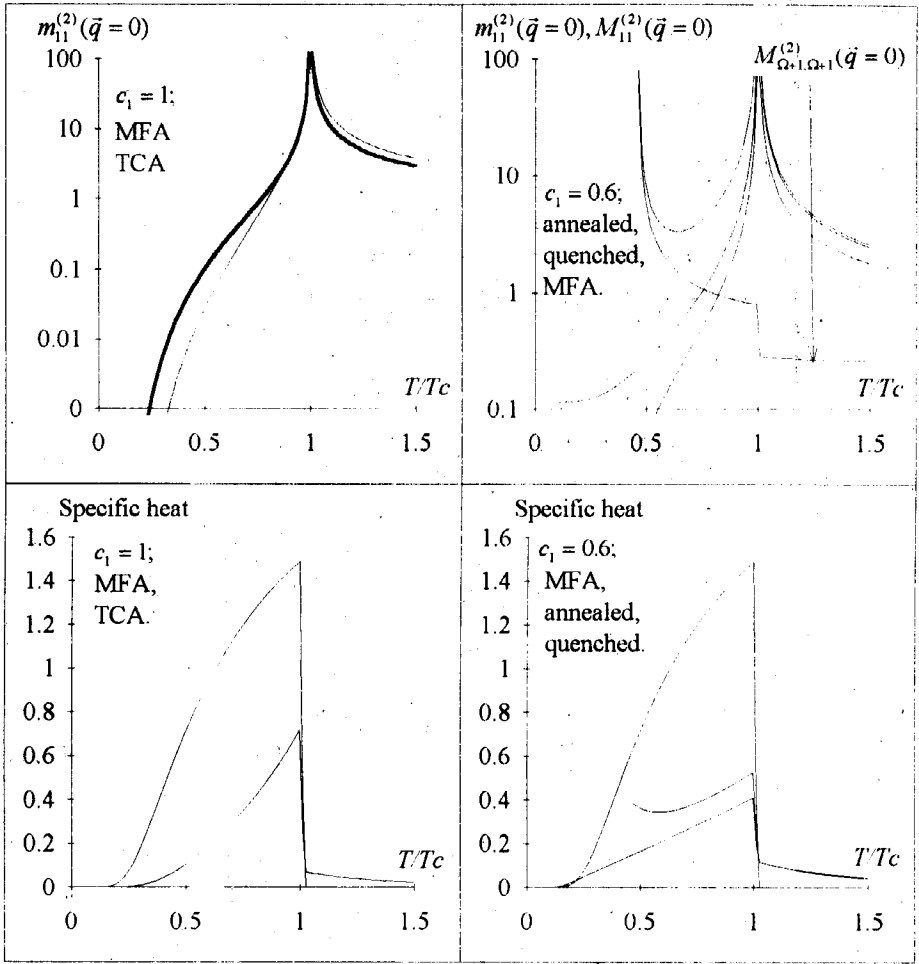


Figure 4. Temperature dependencies of spin-spin and sort-sort CFs' $\bar{q} = 0$ Fourier-transforms and of specific heat (in units of k_B) of pure and dilute ($c_1 = 0.6$) systems on plane square lattice ($z = 4$).

Assuming uniform field and performing the Fourier transformation

$$\begin{array}{c} i \\ \triangle \\ m^{(3)} \\ k \end{array} = \begin{array}{c} \triangle \\ m^{(3)} \end{array} (\vec{r}_j - \vec{r}_i, \vec{r}_k - \vec{r}_i) = \tag{3.55}$$

$$\frac{1}{V_e(2\pi)^D} \int_{V_e} d\vec{q}_1 e^{-i\vec{q}_1(\vec{r}_j - \vec{r}_i)} \frac{1}{V_e(2\pi)^D} \int_{V_e} d\vec{q}_2 e^{-i\vec{q}_2(\vec{r}_k - \vec{r}_i)} \begin{array}{c} \triangle \\ m^{(3)} \end{array} (\vec{q}_1, \vec{q}_2)$$

we can obtain from (3.50) the following expression for the 3-site CF

$$\begin{aligned}
 \triangle_{m^{(3)}}(\vec{q}_1, \vec{q}_2) &= \hat{m}^{(2)}(\vec{q}_1 + \vec{q}_2) \left(z \triangle_A + \right. \\
 &\pi(\vec{q}_1) \triangle_B + \pi(\vec{q}_2) \triangle_C + \\
 &\left. \pi(\vec{q}_1 + \vec{q}_2) \triangle_D \right) \begin{pmatrix} \hat{m}^{(2)}(\vec{q}_1) \\ \hat{m}^{(2)}(\vec{q}_2) \end{pmatrix}, \tag{3.56}
 \end{aligned}$$

where the equality which follows from (3.31)

$$\hat{U} - \pi(\vec{q}_1 + \vec{q}_2)\hat{G} = \left(\hat{m}^{(2)}(\vec{q}_1 + \vec{q}_2) \right)^{-1} \tag{3.57}$$

has been taken into account.

4. Annealed case

In this case we shall introduce into Hamiltonian additional variation parameters $\bar{\psi}$. The quantity ${}_r\bar{\psi}_{i\alpha}$ plays the role of effective field acting on the spin of sort α in the site i from its neighbour (of any sort) in the site r . $H(\{S, X\})$ takes the form

$$H(\{S, X\}) = \sum_i H_i + \sum_{(ij)} W_{ij}, \tag{4.1}$$

where

$$\begin{aligned}
 H_i &= \bar{\kappa}_i S_i + \bar{\mu}_i; \quad \bar{\mu}_i = \mu_i + \sum_{r \in \pi_i} {}_r\bar{\psi}_i; \quad {}_r\bar{\psi}_i = \sum_{\alpha} X_{i\alpha} {}_r\bar{\psi}_{i\alpha} \\
 W_{ij} &= - {}_j\bar{\varphi}_i S_i - {}_i\bar{\varphi}_j S_j + K_{ij} S_i S_j - {}_j\bar{\psi}_i - {}_i\bar{\psi}_j + V_{ij}. \tag{4.2}
 \end{aligned}$$

Further, the technique of the previous section leads to the generating function being (within TCA) of the following form:

$$\mathcal{F}(\{\kappa, \mu\}) = -z' \sum_i \mathcal{F}_i + \sum_{(ij)} \mathcal{F}_{ij}, \tag{4.3}$$

where

$$\mathcal{F}_{ij} = \ln \mathcal{Z}_{ij}; \quad \mathcal{Z}_{ij} = \text{Sp}_{S_i S_j} e^{H_{ij}}; \tag{4.4}$$

$$\begin{aligned}
 H_{ij} &= {}_j\bar{\kappa}_i S_i + {}_i\bar{\kappa}_j S_j + K_{ij} S_i S_j + \\
 &+ {}_j\bar{\mu}_i + {}_i\bar{\mu}_j + V_{ij}; \tag{4.5}
 \end{aligned}$$

$${}_j\bar{\mu}_i = \bar{\mu}_i - {}_j\bar{\psi}_i = \mu_i + \sum_{r \in \pi_i, r \neq j} {}_r\bar{\psi}_i. \tag{4.6}$$

The conditions

$$\frac{\partial \mathcal{F}}{\partial {}_r\bar{\varphi}_{i\alpha}} = 0; \quad \frac{\partial \mathcal{F}}{\partial {}_r\bar{\psi}_{i\alpha}} = 0 \quad (4.7)$$

lead to

$$\langle S_{i\alpha} \rangle = \langle S_{i\alpha} \rangle_{\rho_i} = \langle S_{i\alpha} \rangle_{\rho_{ij}}, \quad (4.8)$$

$$\langle X_{i\alpha} \rangle = \langle X_{i\alpha} \rangle_{\rho_i} = \langle X_{i\alpha} \rangle_{\rho_{ij}}, \quad (4.9)$$

where

$$\rho_i = \mathcal{Z}_i^{-1} \exp H_i; \quad \rho_{ij} = \mathcal{Z}_{ij}^{-1} \exp H_{ij}; \quad j \in \pi_i, \quad (4.10)$$

i.e. again equality of the one-site and intracluster unary CFs is implied. We note that equations (4.9) like the ones for the chemical potential (2.10) are not independent due to the identity

$$\sum_{\alpha} \langle X_{i\alpha} \rangle = 1. \quad (4.11)$$

Therefore the number of independent fields ${}_r\bar{\psi}_{i\alpha}$ and chemical potentials $\mu_{i\alpha}$ decreases. We put

$${}_r\bar{\psi}_{i\Omega} \equiv 0; \quad \mu_{i\Omega} \equiv 0. \quad (4.12)$$

In order to shorten following formulae let us introduce a notation $\mathbf{S} = \{S, X\}$, *i.e.*

$$\mathbf{S}_{i\alpha} = \begin{cases} S_{i\alpha}, & \text{if } \alpha \leq \Omega \\ X_{i\alpha-\Omega}, & \text{if } \alpha > \Omega \end{cases},$$

and $\boldsymbol{\kappa} = \{\kappa, \mu\}$, $\varphi = \{\varphi, \psi\}$,

$$M_{i_1\alpha_1 \dots i_n\alpha_n}^{(n)} = \langle \mathbf{S}_{i_1\alpha_1} \dots \mathbf{S}_{i_n\alpha_n} \rangle^c = \frac{\delta}{\delta \kappa_{i_1\alpha_1}} \dots \frac{\delta}{\delta \kappa_{i_n\alpha_n}} \mathcal{F}(\{\boldsymbol{\kappa}\}) \quad (4.13)$$

With this new notations (4.8) and (4.9) can be written as

$$M_{i\alpha}^{(1)} = \langle \mathbf{S}_{i\alpha} \rangle_{\rho_i} = \langle \mathbf{S}_{i\alpha} \rangle_{\rho_{ij}}, \quad (4.14)$$

The same technique as for quenched case yields a result for a pair CF in the same form:

$$\begin{aligned} (\hat{M}^{(2)}(\bar{q}))^{-1} &= (1-z) (\hat{\mathcal{F}}^{(2)})^{-1} + z (\hat{\mathcal{F}}^{(20)} + \hat{\mathcal{F}}^{(11)})^{-1} + \\ &+ (\pi(\bar{0}) - \pi(\bar{q})) (\hat{\mathcal{F}}^{(20)} (\hat{\mathcal{F}}^{(11)})^{-1} \hat{\mathcal{F}}^{(20)} - \hat{\mathcal{F}}^{(11)})^{-1} \end{aligned} \quad (4.15)$$

where

$$(\hat{M}_{ij}^{(2)})_{\alpha\beta} = \frac{\delta^2 \mathcal{F}}{\delta \kappa_{i\alpha} \delta \kappa_{j\beta}} = \langle \mathbf{S}_{i\alpha} \mathbf{S}_{j\beta} \rangle^c = \begin{pmatrix} \langle S_i S_j \rangle^c & \langle S_i X_j \rangle^c \\ \langle X_i S_j \rangle^c & \langle X_i X_j \rangle^c \end{pmatrix}; \quad (4.16)$$

$$(\hat{\mathcal{F}}^{(2)})_{\alpha\beta} = \langle \mathbf{S}_{i\alpha} \mathbf{S}_{i\beta} \rangle_{\rho_i}^c; \quad (\hat{\mathcal{F}}^{(20)})_{\alpha\beta} = \langle \mathbf{S}_{i\alpha} \mathbf{S}_{i\beta} \rangle_{\rho_{ij}}^c; \quad (\hat{\mathcal{F}}^{(11)})_{\alpha\beta} = \langle \mathbf{S}_{i\alpha} \mathbf{S}_{j\beta} \rangle_{\rho_{ij}}^c. \quad (4.17)$$

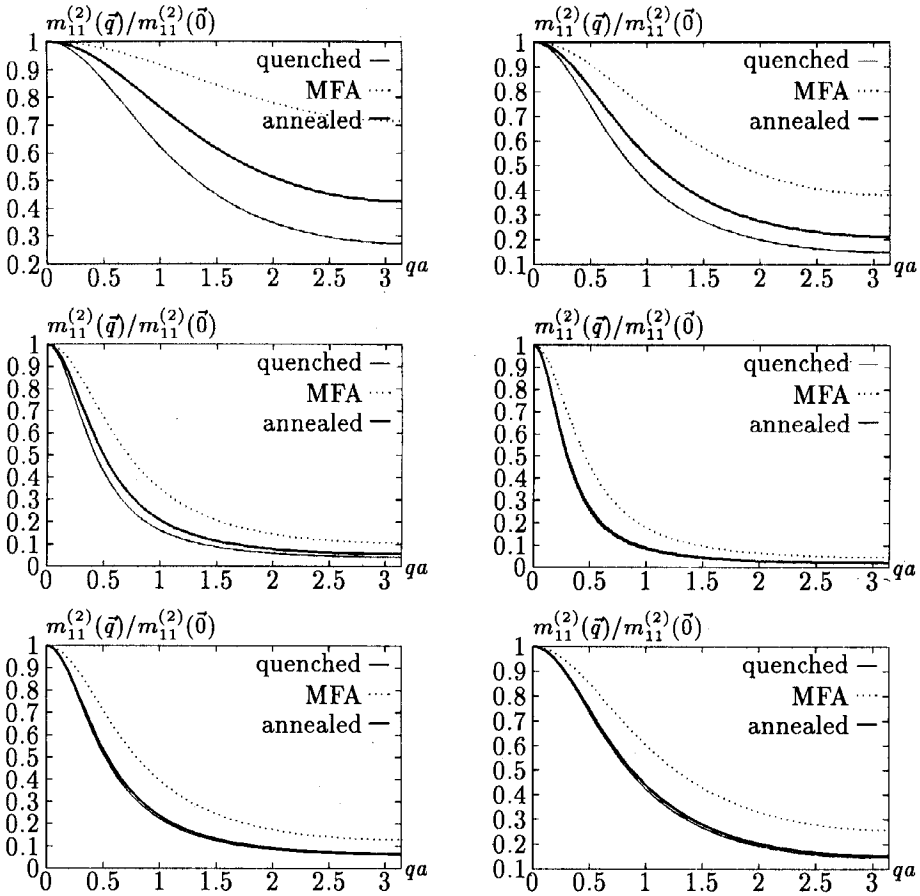


Figure 5. \vec{q} -dependence of the diluted system CFs. $c_1 = 0.6$, $V_{\alpha\beta} = 0$. $T/T_c = 0.5, 0.7, 0.9, 1.1, 1.3, 1.7$.

In equation (4.15) the sort indices lay in the restricted interval $\alpha = 1 \dots 2\Omega - 1$ due to (4.11), (4.12); and the matrices (4.17) have the dimension $(2\Omega - 1) \times (2\Omega - 1)$. The exact result [1] for the one-dimensional system ($z = 2$) is a partial case of the formula (4.17).

The relation (4.14) is equivalent to

$$\text{Sp}_{S_j, X_j} \rho_{ij} = \rho_i, \tag{4.18}$$

and it yields

$$\mathcal{F}_{ij}^{(n0)} = \mathcal{F}_i^{(n)}. \tag{4.19}$$

Therefore (4.15) can be written more simple form

$$\hat{M}^{(2)}(\vec{q}) = \hat{\mathcal{F}}^{(2)} (1 - f^2)^{-1} (1 + z' f^2 - \pi(\vec{q})f); \quad f = (\mathcal{F}^{(2)})^{-1} \mathcal{F}^{(11)}. \tag{4.20}$$

An expression for the 3-site CFs also remains the same form as in the quenched case

$$\begin{aligned}
 \triangle_{M^{(3)}}(\vec{q}_1, \vec{q}_2) &= \hat{M}^{(2)}(\vec{q}_1 + \vec{q}_2) \left(z \triangle_A + \right. \\
 &\pi(\vec{q}_1) \triangle_B + \pi(\vec{q}_2) \triangle_C + \\
 &\left. \pi(\vec{q}_1 + \vec{q}_2) \triangle_D \right) \begin{pmatrix} \hat{M}^{(2)}(\vec{q}_1) \\ \hat{M}^{(2)}(\vec{q}_2) \end{pmatrix}, \quad (4.21)
 \end{aligned}$$

with A, B, C, D given by (3.51)-(3.54) and intracluster CFs

$$\begin{aligned}
 \triangle_{\mathcal{F}^{(30)}} &= \frac{\partial^3 \mathcal{F}}{\partial \kappa_{i\alpha} \partial \kappa_{i\beta} \partial \kappa_{i\gamma}} = \langle \mathbf{S}_{i\alpha} \mathbf{S}_{i\beta} \mathbf{S}_{i\gamma} \rangle_{\rho_{ij}}^c, \\
 \triangle_{\mathcal{F}^{(21)}} &= \frac{\partial^3 \mathcal{F}}{\partial \kappa_{j\alpha} \partial \kappa_{j\beta} \partial \kappa_{i\gamma}} = \langle \mathbf{S}_{j\alpha} \mathbf{S}_{j\beta} \mathbf{S}_{i\gamma} \rangle_{\rho_{ij}}^c, \\
 \triangle_{\mathcal{F}^{(21)}} &= \frac{\partial^3 \mathcal{F}}{\partial \kappa_{i\alpha} \partial \kappa_{i\beta} \partial \kappa_{j\gamma}} = \langle \mathbf{S}_{i\alpha} \mathbf{S}_{i\beta} \mathbf{S}_{j\gamma} \rangle_{\rho_{ij}}^c, \\
 \triangle_{\mathcal{F}^{(12)}} &= \frac{\partial^3 \mathcal{F}}{\partial \kappa_{i\alpha} \partial \kappa_{j\beta} \partial \kappa_{j\gamma}} = \langle \mathbf{S}_{i\alpha} \mathbf{S}_{j\beta} \mathbf{S}_{j\gamma} \rangle_{\rho_{ij}}^c. \quad (4.22)
 \end{aligned}$$

5. Discussion

The great fluctuations of quantities under discussion make the results of "effective field" theories (like TCA and MFA) worse. Thus for the present model a great difference in interactions (e.g., $K_{\alpha\beta} = K\delta_{1\alpha}$ (sort 1 is diluted by noninteracting impurities)) is expected to worsen the quality of TCA results whereas great z , when interaction $K_{i\alpha, j\beta}$ couples many sites, improves these results. Taking into account that TCA gives exact results for the one-dimensional system ($z = 2$), the diluted system on plane square lattice seems to be the most difficult test for TCA, which can discover all its shortcomings. That is why below we concentrate our attention at this case.

Now let us consider a numerical investigation of the obtained results. In the quenched case we assume for simplicity $w_{\alpha\beta} = c_\alpha c_\beta$ (complete chaos: $\langle X_{i\alpha} X_{j\beta} \rangle_x = \langle X_{i\alpha} \rangle_x \langle X_{j\beta} \rangle_x$). The figures 2, 3 show model's phase diagrams of two-sort system for different parameters of the Hamiltonian. Curie temperature T_c and temperature of alloy spinodal segregation T_s are found from

the condition $M_{\alpha\beta}^{(2)}(\vec{q} = 0, T) \rightarrow \infty$. Apart from a complicated form of the TCA phase diagrams 2 with respect to those of MFA 3 one can also remark the rule, that great values of the quantities $\tilde{K} = K_{11} + K_{22} - 2K_{12}$, $\tilde{J} = J_{11} + J_{22} - 2J_{12}$ enhance both segregation and spin alignment, whereas great $V_{11} + V_{22} - 2V_{12}$, $I_{11} + I_{22} - 2I_{12}$ enhance segregation and therefore enhance spin alignment, if $\tilde{K} > 0$, $\tilde{J} > 0$, and suppress alignment, if $\tilde{K} < 0$, $\tilde{J} < 0$.

Temperature dependence of order parameters $m_1^{(1)}/c_1$ or $M_1^{(1)}/c_1$ of pure and dilute systems are shown in the fig. 1. TCA and MFA results are compared. The known exact result for the pure system on the plane square lattice is also depicted. For quenched system within TCA the quantity $\sigma^{(1)} = m_1^{(1)}/c_1$ stays less than 1 even at $T = 0$ and vanishes at $c_1 < c_p = \frac{1}{z-1}$ (below percolation point). This contradicts to MFA result $\sigma^{(1)} = 1$ at $T = 0$ for all c_1 . Moreover, within MFA $\sigma^{(1)}$ and $\sigma^{(2)} = J_{11}m_{11}^{(2)}(\vec{q})/(c_1T)$ depend on temperature, concentration and interaction strength only via T/T_c^{MFA} ($T_c^{MFA} = c_1J_{11}/k_B$): $\sigma^{(1)} = \sigma^{(1)}(T/T_c^{MFA})$, $\sigma^{(2)} = \sigma^{(2)}(\vec{q}, T/T_c^{MFA})$. In TCA this takes place for the case $w_{11} = c_1$ only (all interacting spins constitute one infinite cluster).

One can see in the figure 6 that within TCA pair CF of the quenched diluted system $m_{11}^{(2)}(\vec{q})$ is not zero at $T = 0$ and it yields infinite rise of the susceptibility at zero temperature $\chi(\vec{q}) \xrightarrow{T \rightarrow 0} \infty$ ($\chi(\vec{q}) \sim m_{11}^{(2)}(\vec{q})/T$) whereas MFA gives $\chi(\vec{q}) \rightarrow 0$ similarly to the case of the pure system. The TCA behavior of $\chi(\vec{q})$ and $\sigma^{(1)}$ can be attributed to interacting spins out of the infinite cluster of interacting spins (finite size cluster effect [9]). Indeed, one can find that susceptibility of the isolated spins, which are always present in diluted system, diverges at $T = 0$. Finite size cluster effects are observed also in other approximations (e.g., $\chi(\vec{0})$ of the quenched diluted system in the effective field approximation of Kaneyoshi et.al. [9]). Figure 5 shows, that significant differences between annealed and quenched CFs appear at low temperatures.

The ref. [10], where the pair CF of the pure system in paraphase within TCA was obtained, reports that $\chi(\vec{q})$ has a maximum as a function of T above T_c for a fixed \vec{q} greater than \vec{q}_0 . We do not find any maximum for $\chi(\vec{q})$, but instead we notice a maximum of $m_{11}^{(2)}(\vec{q})$ for all $\pi(\vec{q}) \in \left[0, \frac{2zz'}{z'^2+1}\right]$ in the pure and diluted systems. It should be noted that MFA does not find any maximum for $m_{11}^{(2)}(\vec{q})$.

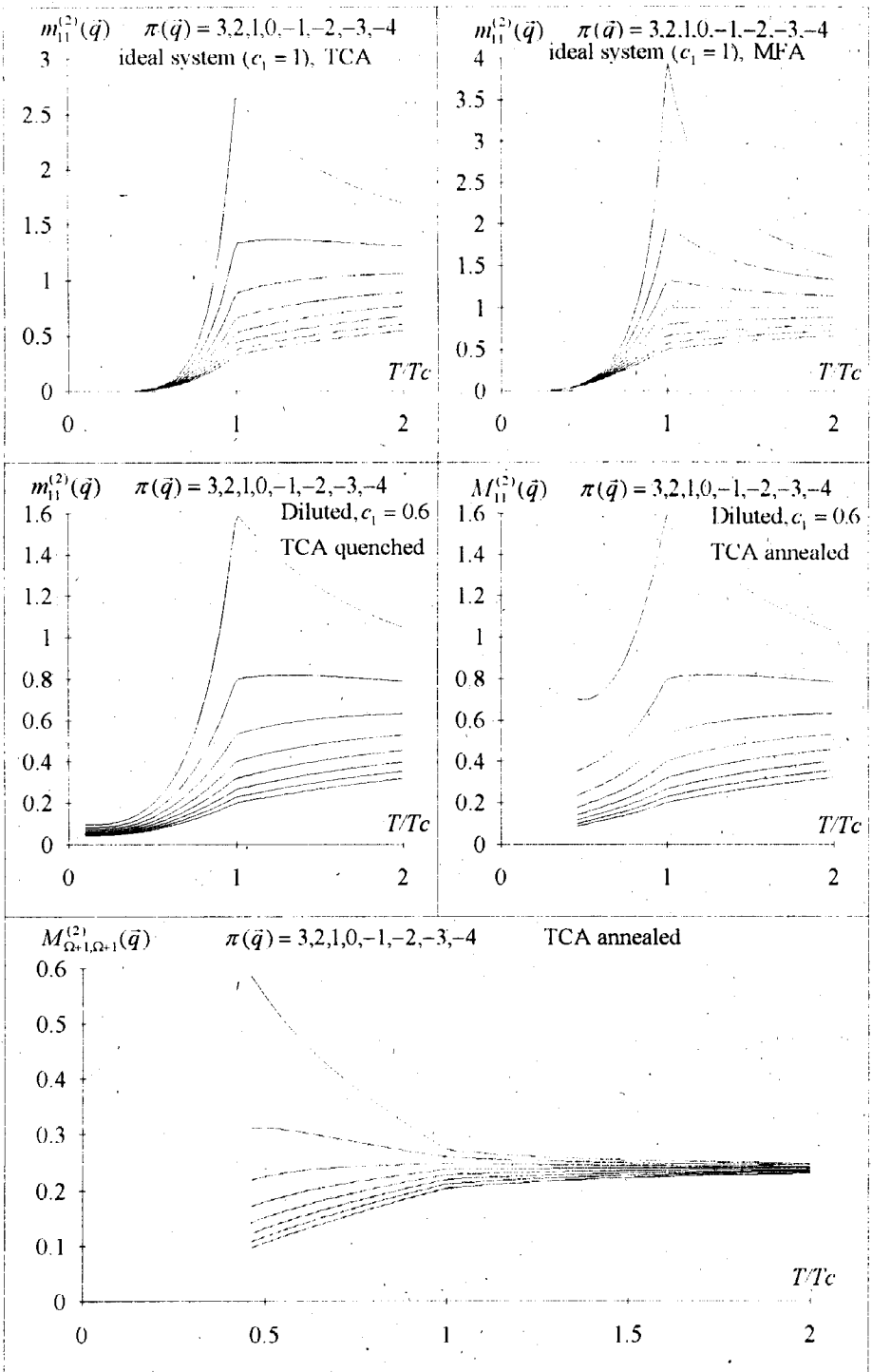


Figure 6. CFs of the ideal ($c_1 = 1$) and diluted ($c_1 = 0.6$) systems.

References

- [1] B. Ja. Balagurov, V. G. Vaks, R. O. Zajtsev. Statistics of one-dimensional model of solid solution. // Fiz. Tver. Tela, 1974, vol. 16, No 8, p. 2302-2309. (In Russian).
- [2] W. Y. Ching, D. L. Huber. Monte-Carlo studies of the critical behavior of site-diluted two-dimensional Ising models //Phys. Rev. B, 1976, vol. 13, No 7, p. 2962-2964.
- [3] E. Stoll, T. Schneider. Ising ferromagnet with quenched impurities //J. Phys. A, 1976, vol. 9, No 7, p. L67-L70.
- [4] V. G. Vaks, N. E. Zein. On the theory of phase transitions in solid solution. // J. Exp. Teor. Fiz., 1974, vol. 67, No 9, p. 1082-1100. (In Russian).
- [5] H. Sato, A. Arrott. Remarks on magnetically dilute systems. // J. Phys. Chem. Solids, 1959, vol. 10, p. 19-34.
- [6] R. R. Levitskii, S. I. Sorokov, R. O. Sokolovskii. Thermodynamics and relaxational dynamics of disordered Ising model. // Lviv, 1993, 43p. (Preprint / Ukr.Acad.Sci. Inst.Theor.Phys.; IFKS-93-17U). (In Ukrainian).
- [7] I. R. Yukhnovskii, R. R. Levytskii, S. I. Sorokov. Thermodynamics and distribution functions of Ising model. Two-site cluster approximation. // Kiev, 1986, 33p. (Preprint / Acad. Sci. Ukr.SSR. Inst.Theor.Phys.; ITP-86-142R). (In Russian).
- [8] R. Kubo. Generalized cumulant expansion method. //J. Phys. Soc. Japan, 1962, vol. 17, No 7, p. 1100-1120.
- [9] T. Kaneyoshi, I. Tamura and R. Honmura. Diluted Ising ferromagnet: Its physical properties. // Phys.Rev.B, 1984, vol. 29, p. 2769-2776.
- [10] S. Haylin, H. Sompolinsky. Cluster approximation for q-dependent correlations in magnetic and ferroelectric systems. // Phys. Rev. B, 1982, vol. 25, No 9, p. 5828-5835.

Appendix

Here we calculate the thermodynamic potential and CFs of the system with long-range interaction. Let the Hamiltonian be

$$\begin{aligned}
 {}^L H(\{S\}) &= \sum_{i\alpha} \Gamma_{i\alpha} S_{i\alpha} + \frac{1}{2} \sum_{i\alpha, j\beta} K_{i\alpha, j\beta} S_{i\alpha} S_{j\beta} + \\
 &+ \sum_{i\alpha} \nu_{i\alpha} X_{i\alpha} + \frac{1}{2} \sum_{i\alpha, j\beta} V_{i\alpha, j\beta} X_{i\alpha} X_{j\beta} + \Delta^L H, \quad (A1)
 \end{aligned}$$

$$\Delta^L H = \frac{1}{2} \sum_{i\alpha, j\beta} J_{i\alpha, j\beta} S_{i\alpha} S_{j\beta} + \frac{1}{2} \sum_{i\alpha, j\beta} I_{i\alpha, j\beta} X_{i\alpha} X_{j\beta}, \quad (A2)$$

where the interactions $J_{i\alpha, j\beta}$, $I_{i\alpha, j\beta}$ are not restricted by the nearest neighbour sites. Consider first the quenched case. Within MFA the (A2) is taken in the following form

$$\Delta^L H_{MFA} = \sum_{i\alpha, j\beta} \mathbf{J}_{i\alpha, j\beta} {}^L m_{i\alpha}^{(1)} \mathbf{S}_{j\beta} - \frac{1}{2} \sum_{i\alpha, j\beta} \mathbf{J}_{i\alpha, j\beta} {}^L m_{i\alpha}^{(1)} {}^L m_{j\beta}^{(1)}, \quad (A3)$$

where ${}^L m_{i\alpha}^{(1)} = \langle \langle \mathbf{S}_{i\alpha} \rangle_{LH} \rangle_x$ is the one-site CF of the system, $\mathbf{J}_{i\alpha, j\beta} = \begin{pmatrix} \hat{J}_{ij} & 0 \\ 0 & \hat{I}_{ij} \end{pmatrix}$. The generating function ${}^L \langle F_x \rangle_x(\{\Gamma\})$ of the

system can be expressed through the generating function $\langle F_x \rangle_x(\{\kappa\})$ of the reference system (2.1).

$$L\langle F_x \rangle_x(\{\Gamma\}) = \langle F_x \rangle_x(\{\kappa\}) - \frac{1}{2} \sum_{i\alpha, j\beta} J_{i\alpha, j\beta} L m_{i\alpha}^{(1)} L m_{j\beta}^{(1)}, \quad (\text{A4})$$

where

$$\kappa_{i\alpha} = \Gamma_{i\alpha} + \lambda_{i\alpha}; \quad \lambda_{i\alpha} = \sum_{j\beta} J_{i\alpha, j\beta} L m_{j\beta}^{(1)}. \quad (\text{A5})$$

Here $\lambda_{i\alpha}$ is the mean field caused by the long-range interaction. Taking into account the relation

$$\frac{\delta}{\delta \Gamma_{i\alpha}} = \sum_{j\beta} \frac{\delta \kappa_{j\beta}}{\delta \Gamma_{i\alpha}} \frac{\delta}{\delta \kappa_{j\beta}} = \sum_{j\beta} \left(\delta_{i\alpha, j\beta} + \sum_{k\gamma} J_{j\beta, k\gamma} L m_{k\gamma, i\alpha}^{(2)} \right) \frac{\delta}{\delta \kappa_{j\beta}} \quad (\text{A6})$$

the CFs of the system

$$L m_{i_1 \alpha_1 \dots i_n \alpha_n}^{(n)} = \frac{\delta}{\delta \Gamma_{i_1 \alpha_1}} \dots \frac{\delta}{\delta \Gamma_{i_n \alpha_n}} L F(\{\Gamma\}) \quad (\text{A7})$$

are found to be

$$L m_{i\alpha}^{(1)} = m_{i\alpha}^{(1)}, \quad (\text{A8})$$

$$L m_{i\alpha, j\beta}^{(2)} = m_{i\alpha, k\gamma}^{(2)} \left(\delta_{k\gamma, j\beta} + J_{k\gamma, l\delta} L m_{l\delta, j\beta}^{(2)} \right), \quad (\text{A9})$$

$$\begin{aligned} L m_{i\alpha, j\beta, k\gamma}^{(3)} &= m_{i\alpha, l\delta}^{(2)} J_{l\delta, n\eta} m_{n\eta, j\beta, k\gamma}^{(3)} + \\ &+ m_{i\alpha, l\delta, m\epsilon}^{(3)} \left(\delta_{l\delta, j\beta} + J_{l\delta, n\eta} L m_{n\eta, j\beta}^{(2)} \right) \times \\ &\times \left(\delta_{m\epsilon, k\gamma} + J_{m\epsilon, o\lambda} L m_{o\lambda, k\gamma}^{(2)} \right), \end{aligned} \quad (\text{A10})$$

where $m^{(1)}$, $m^{(2)}$, $m^{(3)}$ are CFs of the reference system (2.1) in molecular field (A5). We note that in (A9), (A10) the sum over repeated sort and site indices is implied. Fourier transformation (3.33), (3.55) allows us to write (A9), (A10) in the form

$$L m_{\alpha\beta}^{(2)}(\vec{q}) = m_{\alpha\gamma}^{(2)}(\vec{q}) \left(\delta_{\gamma\beta} + J_{\gamma\delta}(\vec{q}) L m_{\delta\beta}^{(2)}(\vec{q}) \right), \quad (\text{A11})$$

$$\begin{aligned} L m_{\alpha\beta\gamma}^{(3)}(\vec{q}_1, \vec{q}_2) &= m_{\alpha\delta}^{(2)}(\vec{q}_1 + \vec{q}_2) J_{\delta\eta}(\vec{q}_1 + \vec{q}_2) m_{\eta\beta\gamma}^{(3)}(\vec{q}_1 + \vec{q}_2) + \\ &+ m_{\alpha\delta\epsilon}^{(3)}(\vec{q}_1, \vec{q}_2) \left(\delta_{\delta\beta} + J_{\delta\eta}(\vec{q}_1) L m^{(2)}(\vec{q}_1) \right) \times \\ &\times \left(\delta_{\epsilon\gamma} + J_{\epsilon\lambda}(\vec{q}_2) L m_{\lambda\gamma}^{(2)}(\vec{q}_2) \right). \end{aligned} \quad (\text{A12})$$

The solutions of equations (A11), (A12) read

$$L \hat{m}^{(2)}(\vec{q}) = \left(1 - \hat{m}^{(2)}(\vec{q}) \hat{J}(\vec{q}) \right)^{-1} \hat{m}^{(2)}(\vec{q}), \quad (\text{A13})$$

$$\triangleleft_{Lm^{(3)}}(\vec{q}_1, \vec{q}_2) = \left(1 - \hat{m}^{(2)}(\vec{q})\hat{J}(\vec{q})\right)^{-1} \triangleleft_{m^{(3)}}(\vec{q}_1, \vec{q}_2) \left(1 - \hat{J}(\vec{q})\hat{m}^{(2)}(\vec{q})\right)^{-1} \cdot \left(1 - \hat{J}(\vec{q})\hat{m}^{(2)}(\vec{q})\right)^{-1} \quad (A14)$$

In (A14) the equality

$$1 + \hat{J}(\vec{q})L\hat{m}^{(2)}(\vec{q}) = \left(1 - \hat{J}(\vec{q})\hat{m}^{(2)}(\vec{q})\right)^{-1}, \quad (A15)$$

which follows from (A13) is used.

In the case of annealed system the same scheme leads to similar relations.

$$L\mathcal{F}(\{\Gamma\}) = \mathcal{F}(\{\kappa\}) - \frac{1}{2} \sum_{i\alpha, j\beta} \mathbf{J}_{i\alpha, j\beta} L M_{i\alpha}^{(1)} L M_{j\beta}^{(1)}, \quad (A16)$$

$$L M_{i\alpha}^{(1)} = M_{i\alpha}^{(1)}, \quad (A17)$$

where $\Gamma = \{\Gamma, \nu\}$,

$$\kappa_{i\alpha} = \Gamma_{i\alpha} + \sum_{j\beta} \mathbf{J}_{i\alpha, j\beta} L M_{j\beta}^{(1)}, \quad (A18)$$

and sums over sort indices run within interval $1 \dots 2\Omega$. Taking into account $\langle X_{i\Omega} \rangle \equiv 1 - \sum_{\alpha=1}^{\Omega-1} \langle X_{i\alpha} \rangle$, (A16) can be rewritten in the form

$$L\mathcal{F}(\{\Gamma\}) = \mathcal{F}(\{\kappa\}) - \frac{1}{2} \sum_{i\alpha, j\beta} \tilde{\mathbf{J}}_{i\alpha, j\beta} L M_{i\alpha}^{(1)} L M_{j\beta}^{(1)}, \quad (A19)$$

where $1 \leq \alpha, \beta \leq 2\Omega - 1$ and $\hat{\mathbf{J}}_{ij} = \begin{pmatrix} \hat{J}_{ij} & 0 \\ 0 & \hat{I} \end{pmatrix}$ is a matrix of $(2\Omega - 1) \times (2\Omega - 1)$ size with $(\Omega - 1) \times (\Omega - 1)$ submatrix $(\hat{I}_{ij})_{\alpha\beta} = I_{i\alpha, j\beta} - I_{i\alpha, j\Omega} - I_{i\Omega, j\beta} + I_{i\Omega, j\Omega}$. For the two-sort system ($\Omega = 2$) we have

$$\hat{\mathbf{J}}_{ij} = \begin{pmatrix} J_{i1, j1} & J_{i1, j2} & 0 \\ J_{i2, j1} & J_{i2, j2} & 0 \\ 0 & 0 & I_{i1, j1} - 2I_{i1, j2} + I_{i2, j2} \end{pmatrix}.$$

Making use of the identity $\langle X_{i\alpha} X_{j\Omega} \rangle^c \equiv - \sum_{\beta=1}^{\Omega-1} \langle X_{i\alpha} X_{j\beta} \rangle^c$ one obtains the higher CFs in the form

$$L\hat{M}^{(2)}(\vec{q}) = \left(1 - \hat{M}^{(2)}(\vec{q})\hat{\mathbf{J}}(\vec{q})\right)^{-1} \hat{M}^{(2)}(\vec{q}), \quad (A20)$$

$$\triangleleft_{LM^{(3)}}(\vec{q}_1, \vec{q}_2) = \left(1 - \hat{M}^{(2)}(\vec{q})\hat{\mathbf{J}}(\vec{q})\right)^{-1} \triangleleft_{M^{(3)}}(\vec{q}_1, \vec{q}_2) \left(1 - \hat{\mathbf{J}}(\vec{q})\hat{M}^{(2)}(\vec{q})\right)^{-1} \cdot \left(1 - \hat{\mathbf{J}}(\vec{q})\hat{M}^{(2)}(\vec{q})\right)^{-1} \quad (A21)$$

КОРЕЛЯЦІЙНІ ФУНКЦІЇ ІЗІНГІВСЬКИХ СИСТЕМ З РІВНОВАЖНИМ І НЕРІВНОВАЖНИМ ТИПАМИ СОРТОВОГО ХАОСУ

Р.Р. Левицький, С.І. Сороков, Р.О. Соколовський

У наближенні двочастинкового кластера по короткодійючих взаємодіях з врахуванням далекодійючих взаємодій у наближенні середнього поля розраховано і досліджено спінові корелятори (до тернарного) моделі Ізінга з рівноважним і нерівноважним типами безладу. У одновимірному випадку одержані результати співпадають з точними.