

ІНСТИТУТ
ФІЗИКИ
КОНДЕНСОВАНИХ
СИСТЕМ

ICMP-96-26E

S.I.Sorokov, R.R.Levitskii, T.M.Verkholyak

INVESTIGATION OF
THE ANNEALED DISORDERED ISING SYSTEMS
WITHIN TWO-TAIL APPROXIMATION

УДК: 537.226

РАС: 61.26Dk, 63.75.+z

Дослідження неупорядкованих відпалених ізінгівських систем в наближенні двохвосток

С.І.Сороков, Р.Р.Левицький, Т.М.Верхоляк

Анотація. В даній роботі запропоновано підхід для дослідження двохкомпонентних ізінгівських систем з далекосяжною взаємодією. Розглянуті можливі застосування до металічних та магнітних сплавів. Отримані також числові результати для термодинамічних властивостей цих моделей. Проведено порівняння числових результатів отриманих в наближенні молекулярного поля, гаусового поля та двохвосток.

Investigation of the annealed disordered Ising systems within two-tail approximation

S.I.Sorokov, R.R.Levitskii, T.M.Verkholyak

Abstract. In the present paper an approach for investigation of the disordered two-component Ising systems with long range interaction has been suggested. Possible applications to metallic and magnetic alloys and lattice gas are considered. We have also obtained numerical results for thermodynamical properties of these models. The comparison of numerical results obtained within mean field, gaussian field and two-tail approximations are carried out.

Подается до Журнал фізичних досліджень
Submitted to Journal of physical studies

1. Introduction

The present paper is devoted to the investigation of a binary annealed disordered magnet on the basis of Ising model. This model and its simpler versions are often used in the study of metallic alloys [1–3], magnetic alloys [4,5], ferroelectric solutions, in particular, the ferroelectrics with hydrogen bonds [6].

Let us point out several works concerning the magnetic alloys. In the work [4], V.G.Vaks and N.E.Zein obtained phase diagrams for the model of the binary magnetic alloy with non-magnetic impurities within two particle cluster approximation at $T > T_m$ (T_m is the temperature of the magnetic ordering). It was noted that in mean field approximation (MFA) in contrast to cluster approximation the magnetic subsystem does not influence the phase diagram. Later by means of MFA T.Kawasaki [5] investigated the influence of the magnetic subsystem on the properties of the atomic subsystem and v.v. at $T < T_m$. In the work [6] a detailed investigation of this model within two-site cluster approximation were performed. There was found the influence of the spin subsystem on binodal (coexistence temperature T_b) and spinodal (spontaneous separation temperature T_s) temperatures of the system in a spin ordering phase. Here the difference between quenched and annealed types of disorder has been investigated and correlation functions have been calculated.

The non-magnetic version of the model is often applied to the study of real binary alloys [1–3]. Using the pseudopotential theory for defining of intersite interaction Z.Gurskii and Yu.Khokhlov tried to explain the properties of Ca-Ba and K-Cs alloys [2]. For the thermodynamical averaging they used the collective variables method with a non-selfconsistent equation for unknown chemical potential.

This work has been directed to the study of a disordered model with long range interaction or short range one in a case of large z (z is the number of nearest neighbours). At first we consider the Hamiltonian of M -component Ising model and study the model within mean field approximation (MFA), Gaussian field approximation (GFA) and two-tail approximation (TTA). But for the sake of simplicity all approximations are formulated for the case $M = 2$.

2. Description of the model

Let us consider M -component system with site disorder on Bravais lattice with the following Hamiltonian:

$$-\beta H = \mathcal{H} = \mathcal{H}_x + \mathcal{H}_s, \quad (2.1)$$

where

$$\mathcal{H}_x = \sum_{\alpha=1}^M \sum_{i=1}^N \varepsilon_{\alpha} x_{i\alpha} + \frac{1}{2} \sum_{\alpha,\beta=1}^M \sum_{i,j=1}^N V_{\alpha\beta}(i-j) x_{i\alpha} x_{j\beta}, \quad (2.2)$$

$$\mathcal{H}_s = \sum_{\alpha=1}^M \sum_{i=1}^N \Gamma_{\alpha} x_{i\alpha} S_{i\alpha} + \frac{1}{2} \sum_{\alpha,\beta=1}^M \sum_{i,j=1}^N \mathcal{I}_{\alpha\beta}(i-j) x_{i\alpha} S_{i\alpha} x_{j\beta} S_{j\beta}. \quad (2.3)$$

All parameters of the Hamiltonian (2.1) contain the factor $(-\beta)$. The Hamiltonian \mathcal{H}_x corresponds to the disordered ionic subsystem. Here $\varepsilon_{\alpha} = \vartheta_{\alpha} + \mu_{\alpha}$, $\mu_{\alpha} = -\beta \mu_{\alpha}^R$ is the dimensionless chemical potential of α -type ions, ϑ_{α} is related to the difference between alloy component ion characteristics; $V_{\alpha\beta}(i-j) = V_{\alpha\beta}(R_{ij})$ is the potential of effective ionic interaction; $x_{i\alpha} = 1$, if the site is occupied by the ion of type α and 0 otherwise. The Hamiltonian \mathcal{H}_s corresponds to the system of N Ising spins ($S_{i\alpha} = S_{i\alpha}^z$) situated on the ions with external field energy $h_{\alpha} = (\mu_{\alpha} \mathbf{h})$ and exchange interaction $\mathcal{I}_{\alpha\beta}(i-j) = \mathcal{I}_{\alpha\beta}(R_{ij})$.

In the present paper we confine ourselves by the case of binary alloy ($M = 2$). It should be noted that suggested approximations below can be applied to magnetic alloys with arbitrary number of sorts. It is convenient to use the spin variables instead of x_{i1}, x_{i2} ($\alpha = 1, 2$)

$$x_{i\alpha} = \frac{1 - (-1)^{\alpha} S_{i0}}{2}; \quad S_{i0} = x_{i1} - x_{i2}. \quad (2.4)$$

Now the Hamiltonian (2.1) can be written as follows

$$\mathcal{H}_{xs} = E(\varepsilon) + \mathcal{H}_{\Theta}(\Gamma), \quad (2.5)$$

$$\mathcal{H}_{\Theta}(\Gamma) = \sum_{\sigma=0,1,2} \sum_{i=1}^N \Gamma_{\sigma} \Theta_{i,\sigma} + \frac{1}{2} \sum_{\sigma,\sigma'} \sum_{i,j=1}^N \mathcal{I}_{\sigma,\sigma'}(R_{ij}) \Theta_{i\sigma} \Theta_{j\sigma}.$$

Here we use the following notations

$$\begin{aligned} \Gamma &= \begin{pmatrix} \Gamma_0 \\ h_1 \\ h_2 \end{pmatrix}, \quad \Theta_i = \begin{pmatrix} S_{i0} \\ x_{i1} S_{i1} \\ x_{i2} S_{i2} \end{pmatrix}, \\ \hat{\mathcal{I}}(R) &= \begin{pmatrix} \mathcal{I}(R) & 0 & 0 \\ 0 & \mathcal{I}_{11}(R) & \mathcal{I}_{12}(R) \\ 0 & \mathcal{I}_{12}(R) & \mathcal{I}_{22}(R) \end{pmatrix}, \\ \frac{1}{N} E &= \frac{1}{2}(\varepsilon_1 + \varepsilon_2) + \frac{1}{8}(V_{11} + V_{22} + 2V_{12}), \\ \Gamma_0 &= \frac{1}{2}(\varepsilon_1 - \varepsilon_2) + \frac{1}{4}(V_{11} - V_{22}) \quad (V_{\alpha,\beta} = V_{\alpha,\beta}(q \rightarrow 0)), \\ 4\mathcal{I}(R) &= V_{11}(R) + V_{22}(R) - 2V_{12}(R). \end{aligned} \quad (2.6)$$

The Hamiltonian $\mathcal{H}_\Theta(\mathbf{\Gamma})$ describes the three-sort spin system. The thermodynamical potential (TP) of system (2.1) has the following form ($\mathbf{h} = (h_1, h_2)$)

$$\Omega(\varepsilon, \mathbf{h}) = -\beta^{-1} \ln \text{Sp}_{\{s,x\}} e^{\mathcal{H}(x,s)} = E(\varepsilon) + \Omega_\Theta(\mathbf{\Gamma}). \quad (2.7)$$

Here $\Omega_\Theta(\mathbf{\Gamma})$ is the TP for the Hamiltonian $\mathcal{H}_\Theta(\mathbf{\Gamma})$. The correlation functions (CFs) of an arbitrary order can be obtained on the basis of the relations

$$\Omega_\Theta^{(l)}(i_1 \delta_1, \dots, i_l \delta_l) = \langle \Theta_{i_1 \delta_1} \cdots \Theta_{i_l \delta_l} \rangle^c = \frac{\delta}{\delta \Gamma_{i_1 \delta_1}} \cdots \frac{\delta}{\delta \Gamma_{i_l \delta_l}} [-\beta \Omega_\Theta(\mathbf{\Gamma})]. \quad (2.8)$$

Here we have replaced the uniform fields Γ_α with nonuniform ones $\Gamma_{i\alpha}$. The TP (2.7) is a function of temperature (T) and chemical potentials (μ_1, μ_2). Transition to concentration variables c_α instead of μ_α can be performed by the Legendre transformation

$$\frac{1}{N} F(\mathbf{c}, \mathbf{h}) = \frac{1}{N} \Omega(\varepsilon, \mathbf{h}) - \sum_{\alpha=1,2} \mu_\alpha^R c_\alpha. \quad (2.9)$$

Here $F(\mathbf{c}, \mathbf{h})$ is a free energy of system (2.1) and chemical potentials are defined by ($m_0 = \langle S_{i0} \rangle$)

$$c_\alpha = \frac{N_\alpha}{N} = \frac{\delta}{\delta \varepsilon_\alpha} [-\beta \Omega(\varepsilon, h)] = \frac{1 - (-1)^\alpha m_0}{2}. \quad (2.10)$$

The system (2.10) gives only one independent equation for $\mu_1 - \mu_2$ or Γ_0 , because $\sum_\alpha c_\alpha = 1$. Here we consider the system which undergoes both the separation phase transition and magnetic phase at temperature T_m . Therefore, the expression for $\langle S_{i0} \rangle$ can contain the magnetic moments $m_1 = \langle S_{i1} \rangle$ and $m_2 = \langle S_{i2} \rangle$ as well. The equations for them we will obtain proceeding from (2.8):

$$m_1 = \frac{\delta}{\delta \Gamma_1} \cdot \frac{1}{N} [-\beta \Omega_\Theta(\mathbf{\Gamma})], \quad m_2 = \frac{\delta}{\delta \Gamma_2} \cdot \frac{1}{N} [-\beta \Omega_\Theta(\mathbf{\Gamma})]. \quad (2.11)$$

The system of equations (2.10), (2.11) gives the values for Γ_0 , m_1 , m_2 as function of temperature T and concentration $c = c_1$. The spontaneous separation transition occurs at T_s (spinodal temperature) which is found as divergence temperature of CF ($\langle S_{i0} S_{j0} \rangle^c$) $_{\mathbf{q}=0}$. The coexistence temperature T_b (binodal temperature) of both phases A and B is calculated from the following system

$$\begin{cases} \Omega(\varepsilon(m_0), \mathbf{h}, T_b) /_{m_0=m_{0A}} = \Omega(\varepsilon(m_0), \mathbf{h}, T_b) /_{m_0=m_{0B}} \\ \Gamma_0(m_{0A}, \mathbf{h}, T_b) = \Gamma_0(m_{0B}, \mathbf{h}, T_b) \end{cases} \quad (2.12)$$

The system (2.12) gives the dependences $m_{0A}(T_b)$, $m_{0B}(T_b)$ and it is solved jointly with system (2.10), (2.11).

Although for the system (2.12) exact solution has not been found, one can make some conclusions about the symmetry of phase diagrams. In case $\mathcal{I}_{11} = \mathcal{I}_{22}$ and $\Gamma_1 = \Gamma_2$ the thermodynamical potential

$$\Omega_\Theta(\Gamma_0, \mathbf{h}) = -\beta^{-1} \ln \text{Sp} \exp \left[\sum_{i=1}^N \Gamma_0(x_{i1} - x_{i2}) + \frac{1}{2} \sum_{i,j=1}^N \mathcal{I}(i-j)(x_{i1} - x_{i2})(x_{j1} - x_{j2}) + \mathcal{H}_s \right] = \Omega_\Theta(-\Gamma_0, \mathbf{h})$$

will be even function of Γ_0 (because trace over x_{i1} and x_{i2} becomes equivalent). Similarly, it can be proved that

$$\begin{aligned} m_0(\Gamma_0) &= \langle x_{i1} - x_{i2} \rangle = \\ &= \frac{\text{Sp}(x_{i1} - x_{i2}) e^{\sum \Gamma_0(x_{i1} - x_{i2}) + \frac{1}{2} \sum \mathcal{I}(i-j)(x_{i1} - x_{i2})(x_{j1} - x_{j2}) + \mathcal{H}_s}}{\text{Sp} e^{\sum \Gamma_0(x_{i1} - x_{i2}) + \frac{1}{2} \sum \mathcal{I}(i-j)(x_{i1} - x_{i2})(x_{j1} - x_{j2}) + \mathcal{H}_s}} = \\ &= \frac{\text{Sp}(x_{i2} - x_{i1}) e^{\sum (-\Gamma_0)(x_{i1} - x_{i2}) + \frac{1}{2} \sum \mathcal{I}(i-j)(x_{i1} - x_{i2})(x_{j1} - x_{j2}) + \mathcal{H}_s}}{\text{Sp} e^{\sum \Gamma_0(x_{i1} - x_{i2}) + \frac{1}{2} \sum \mathcal{I}(i-j)(x_{i1} - x_{i2})(x_{j1} - x_{j2}) + \mathcal{H}_s}} \\ &= \langle x_{i2} - x_{i1} \rangle = -m_0(-\Gamma_0) \end{aligned}$$

is odd function of Γ_0 , where $\Gamma_0 \sim (\mu_1 - \mu_2)$ and determined by the formula (2.6). This means that Ω_Θ is even function relatively variable m_0 and first equation of the system (2.12) has following solution $m_{0B} = -m_{0A}$. Then second equation for m_0 can be rewritten as following: $\Gamma_0(m_{0A}, \mathbf{h}, T_b) = 0$. Therefore, phase diagram is symmetrical relatively variables m_0 or permutation of components' concentration c_1 and c_2 .

The spinodal temperature also is symmetrical function of $m_0 = c_1 - c_2$ in case $\mathcal{I}_{11} = \mathcal{I}_{22}$ and $\Gamma_1 = \Gamma_2$. Spinodal decay takes place if the CF ($\langle S_{i0} S_{j0} \rangle^c$) $_{\mathbf{q}=0}$ diverges. It means that the system becomes unstable against the infinitesimal fluctuation of concentration: $\frac{\partial^2 F}{\partial m_0^2} = 0$. Since $\frac{\partial F}{\partial m_0} = \Gamma_0$, the last condition may be rewritten as $\frac{\partial \Gamma_0}{\partial m_0} = 0$. Γ_0 is odd function of m_0 , then $\frac{\partial \Gamma_0}{\partial m_0}$ will be even function of m_0 . This means if for a certain temperature T_s the equation $\frac{\partial \Gamma_0}{\partial m_0} = 0$ has solution m_0 , the solution $-m_0$ also exists and spinodal temperature T_s is an even function relatively m_0 .

Further for calculation of TP and CFs of system with Hamiltonian $\mathcal{H}_\Theta(\mathbf{\Gamma})$ we will use the expansion over $1/z$ and the results of ref. [7].

Now the TP $\Omega_{\Theta}(\Gamma)$ can be written as follows ($\mathcal{I}_{\alpha\beta} = \mathcal{I}_{\alpha\beta}(\mathbf{q} \rightarrow 0)$, $V = V(\mathbf{q} \rightarrow 0)$)

$$-\frac{\beta}{N}\Omega_{\Theta}(\Gamma) = -\frac{1}{2} \sum_{\delta, \delta'=0,1,2} \mathcal{I}_{\delta\delta'} m_{\delta} m_{\delta'} + f(\mathbf{a}), \quad (2.13)$$

$$f(\mathbf{a}) = \langle F^{(0)}(\mathbf{a} + \boldsymbol{\sigma}) \rangle - \frac{1}{2} \sum_{\delta, \delta'=0,1,2} \lambda_{\delta\delta'}^{(2)} \langle F_{\delta\delta'}^{(2)}(\mathbf{a} + \boldsymbol{\sigma}) \rangle - \frac{1}{2N} \sum_q \ln \det [1 - \hat{\mathcal{I}}(q) \langle \hat{F}_{\delta\delta'}^{(2)}(\mathbf{a} + \boldsymbol{\sigma}) \rangle]. \quad (2.14)$$

Here irreducible part $f(\mathbf{a})$ of $\Omega_{\Theta}(\Gamma)$ is written with the accuracy up to one-loop diagrams (two-tail diagrams approximation (TTA)).

We use the following notations from ref. [7] for averages of arbitrary function $y(\mathbf{a} + \boldsymbol{\sigma})$ over fluctuating fields $\boldsymbol{\sigma}$ with Gaussian distribution function $\rho_2(\boldsymbol{\sigma})$:

$$\langle y(\mathbf{a} + \boldsymbol{\sigma}) \rangle = \int d\sigma_0 d\sigma_1 d\sigma_2 \rho_2(\boldsymbol{\sigma}) y(\mathbf{a} + \boldsymbol{\sigma}), \quad (2.15)$$

$$\rho_2(\boldsymbol{\sigma}) = [\det 2\pi \hat{\lambda}^{(2)}]^{-1/2} \exp\left\{-\frac{1}{2} \sum_{\delta, \delta'} [\hat{\lambda}^{(2)}]_{\delta\delta'}^{-1} \sigma_{\delta} \sigma_{\delta'}\right\},$$

$$\mathbf{a}_0 = \Gamma_0 + \mathcal{I}m_0, \quad \mathbf{a}_{\alpha} = h_{\alpha} + \sum_{\beta} \mathcal{I}_{\alpha\beta} m_{\beta} \quad (\alpha, \beta = 1, 2),$$

where $[\hat{\lambda}^{(2)}]^{-1}$ is the inverse matrix to $\hat{\lambda}^{(2)}$. In (2.15) we use the following notations for functions on $\mathbf{x} = (x_0, x_1, x_2)$

$$F^{(0)}(\mathbf{x}) = \ln Z(\mathbf{x}) = \ln\{e^{x_0} Z_1(x_1) + e^{-x_0} Z_2(x_2)\};$$

$$F_{\delta}^{(1)}(\mathbf{x}) = \frac{\delta}{\delta x_{\delta}} F^{(0)}(\mathbf{x}); \quad F_{\delta\delta'}^{(2)}(\mathbf{x}) = \frac{\delta}{\delta x_{\delta'}} \cdot \frac{\delta}{\delta x_{\delta}} F^{(0)}(\mathbf{x}); \quad (2.16)$$

$$Z_{\alpha}(x_{\alpha}) = Sp_{s_{\alpha}} e^{x_{\alpha} s_{\alpha}} \xrightarrow{s_{\alpha}=\pm 1} 2 \cosh x_{\alpha};$$

$$\mathcal{F}_{\alpha}^{(0)}(x_{\alpha}) = \ln Z_{\alpha}(x_{\alpha}); \quad \mathcal{F}_{\alpha}^{(l)}(x_{\alpha}) = \frac{\delta^l}{\delta x_{\alpha}^l} \mathcal{F}_{\alpha}^{(0)}(x_{\alpha}).$$

From stationarity conditions with respect to nine variables m_0, m_{α} , $\lambda_{00}^{(2)}, \lambda_{0\alpha}^{(2)} = \lambda_{\alpha 0}^{(2)}, \lambda_{\alpha\beta}^{(2)}$ we find the system of nine equations for nine unknown $\Gamma_0, m_{\alpha}, \lambda_{00}^{(2)}, \lambda_{0\alpha}^{(2)} = \lambda_{\alpha 0}^{(2)}, \lambda_{\alpha\beta}^{(2)}$

$$2c - 1 = m_0 = \langle F_0^{(1)}(\mathbf{a} + \boldsymbol{\sigma}) \rangle, \quad m_{\alpha} = \langle F_{\alpha}^{(1)}(\mathbf{a} + \boldsymbol{\sigma}) \rangle, \quad (2.17)$$

$$\lambda_{\delta\delta'}^{(2)} = \left(\frac{1}{2N} \sum_q [\hat{1} - \hat{\mathcal{I}}(q) \langle F^{(2)}(\mathbf{a} + \boldsymbol{\sigma}) \rangle]^{-1} \hat{\mathcal{I}}(q) \right)_{\delta\delta'}. \quad (2.18)$$

In the works of Onyszkiewicz at all [8] GFA was suggested. It can be obtained expanding $\ln \det [\hat{1} - \hat{\mathcal{I}}(q) \langle \hat{F}_{\delta\delta'}^{(2)}(\mathbf{a} + \boldsymbol{\sigma}) \rangle]$ in (2.14) and $\left(\frac{1}{2N} \sum_q [\hat{1} - \hat{\mathcal{I}}(q) \langle \hat{F}^{(2)}(\mathbf{a} + \boldsymbol{\sigma}) \rangle]^{-1} \hat{\mathcal{I}}(q) \right)_{\delta\delta'}$ in (2.18) in $\mathcal{I}(q)$ up to the terms of second order. In the result :

$$f(\mathbf{a}) = \langle F^{(0)}(\mathbf{a} + \boldsymbol{\sigma}) \rangle - \frac{1}{2} \sum_{\delta, \delta'=0,1,2} \lambda_{\delta\delta'}^{(2)} \langle F_{\delta\delta'}^{(2)}(\mathbf{a} + \boldsymbol{\sigma}) \rangle - \frac{1}{2N} \sum_{\delta, \delta_1, \delta_2=0,1,2} \langle F_{\delta_1\delta'}^{(2)}(\mathbf{a} + \boldsymbol{\sigma}) \rangle \langle F_{\delta_2\delta}^{(2)}(\mathbf{a} + \boldsymbol{\sigma}) \rangle \sum_q \mathcal{I}_{\delta\delta_1}(q) \mathcal{I}_{\delta'\delta_2}(q), \quad (2.19)$$

$$\lambda_{\delta\delta'}^{(2)} = \frac{1}{2N} \sum_{\delta_1, \delta_2=0,1,2} \langle F_{\delta_1\delta_2}^{(2)}(\mathbf{a} + \boldsymbol{\sigma}) \rangle \sum_q \mathcal{I}_{\delta\delta_1}(q) \mathcal{I}_{\delta_2\delta'}(q). \quad (2.20)$$

In contrast to GFA and TTA MFA permits to get analytical results for thermodynamical functions and transition temperatures in case of non-magnetic alloys. This approximation one can obtain neglecting fluctuation of molecular field m_{δ} . The expression for TP is

$$-\frac{\beta}{N}\Omega_{\Theta}(\Gamma) = -\frac{1}{2} \sum_{\delta, \delta'=0,1,2} \mathcal{I}_{\delta\delta'} m_{\delta} m_{\delta'} + F^{(0)}(\mathbf{a}). \quad (2.21)$$

The equation for chemical potential and order parameters is determined by the relations (2.10), (2.11). In MFA one can obtain:

$$2c_1 - 1 = m_0 = F_0^{(1)}(\mathbf{a}) = [e^{a_0} Z_1(a_1) - e^{-a_0} Z_2(a_2)] Z(\mathbf{a})^{-1}, \quad (2.22)$$

$$m_{\alpha} = F_{\alpha}^{(1)}(\mathbf{a}) = e^{(-1)^{\alpha+1} a_0} Z_{\alpha}^{(1)}(a_{\alpha}) Z(\mathbf{a})^{-1}. \quad (2.23)$$

The equation for m_0 can be transformed to two dependent equations for the components' concentration c_{α} (see 2.10):

$$c_{\alpha} = e^{(-1)^{\alpha+1} a_0} Z_{\alpha}(a_{\alpha}) Z(\mathbf{a})^{-1}. \quad (2.24)$$

From (2.23), (2.24) it follows

$$m_{\alpha} = c_{\alpha} \mathcal{F}_{\alpha}^{(1)}(a_{\alpha}). \quad (2.25)$$

The equation (2.22) for unknown difference of chemical potential can be solved analytically

$$\Gamma_0 = -\mathcal{I}m_0 + \frac{1}{2} \ln \frac{1 + m_0}{1 - m_0} \frac{Z_2(a_2)}{Z_1(a_1)}. \quad (2.26)$$

Using (2.9) one can obtain following result for the free energy:

$$\begin{aligned} \frac{1}{N}F(\mathbf{c}, \mathbf{h}) &= \sum_{\alpha=1,2} c_{\alpha} \vartheta_{\alpha} + \ln 2 + \frac{1}{8}(V_{11} + V_{22} + 2V_{12}) \\ &+ \frac{1}{4}(V_{22} - V_{11})m_0 + \frac{1}{2}\mathcal{I}m_0^2 - \frac{1}{2}\ln(1 - m_0^2) - \frac{m_0}{2}\ln\frac{1 + m_0}{1 - m_0} \\ &- \frac{1}{2}\sum_{\alpha,\beta=1,2} \mathcal{I}_{\alpha,\beta}m_{\alpha}m_{\beta} - \frac{m_0}{2}\ln\frac{Z_2(\mathfrak{a}_2)}{Z_1(\mathfrak{a}_1)} + \frac{1}{2}\ln Z_1(\mathfrak{a}_1)Z_2(\mathfrak{a}_2). \end{aligned} \quad (2.27)$$

The system (2.12) in a case $\mathcal{I}_{11} = \mathcal{I}_{22}$ and $\Gamma_1 = \Gamma_2$ can be solved analytically with the following result:

$$T_b = \frac{-2\mathcal{I}m_0}{\ln\frac{1-m_0}{1+m_0}\frac{Z_2(\mathfrak{a}_2)}{Z_1(\mathfrak{a}_1)}}. \quad (2.28)$$

However, \mathfrak{a}_1 and \mathfrak{a}_2 is to find from equations (2.11). The expression for spinodal temperature can be found exactly only for non-magnetic case:

$$T_s = \mathcal{I}(1 - m_0^2) = 4\mathcal{I}c_1c_2. \quad (2.29)$$

The pair CFs we obtain on the basis of the relation (2.8) (the details see in [7]) and this procedure leads to expression for matrix of CF $\hat{\Omega}_{\Theta}^{(2)}(\mathbf{q}) = \{\Omega_{\Theta,\delta_1\delta_2}^{(2)}(\mathbf{q})\}$

$$\begin{aligned} \hat{\Omega}_{\Theta}^{(2)}(\mathbf{q}) &= [\hat{1} - \hat{f}^{(2)}(q)\hat{\mathcal{I}}(q)]^{-1} \hat{f}^{(2)}(q), \\ f_{\delta_1\delta_2}^{(2)}(\mathbf{q}) &= \left(\frac{\delta}{\delta\mathfrak{a}_{i_1\delta_1}} \cdot \frac{\delta}{\delta\mathfrak{a}_{i_2\delta_2}} f(\{\mathfrak{a}\}) /_{\mathfrak{a}_i=\mathfrak{a}} \right) (\mathbf{q}), \\ \left(\langle x_{i_1} x_{j_1} \rangle^c \right)_{(\mathbf{q})} &= \frac{1}{4}\Omega_{\Theta,00}^{(2)}(\mathbf{q}), \quad \left(\langle x_{i_1} x_{j_{\alpha}} s_{j_{\alpha}} \rangle^c \right)_{(\mathbf{q})} = \frac{1}{2}\Omega_{\Theta,0\alpha}^{(2)}(\mathbf{q}). \end{aligned} \quad (2.30)$$

Here $f_{\delta_1\delta_2}^{(2)}(\mathbf{q})$ is the irreducible part of CF $\hat{\Omega}_{\Theta}^{(2)}(q)$ with respect to interaction $\hat{\mathcal{I}}(\mathbf{q})$. It is obtained by double differentiation of irreducible part $f(\mathfrak{a})$ with respect to nonuniform fields $\mathfrak{a}_{i_1\delta_1}, \mathfrak{a}_{i_2\delta_2}$. Within TTA at $T \geq T_m$ $\hat{f}^{(2)}$ is independent of \mathbf{q} and has form

$$f_{\delta_1\delta_2}^{(2)}(\mathbf{q}) = \langle F_{\delta_1\delta_2}^{(2)}(\mathfrak{a} + \boldsymbol{\sigma}) \rangle \xrightarrow{MFA} F_{\delta_1\delta_2}^{(2)}(\mathfrak{a}), \quad (2.31)$$

$$\left. \begin{aligned} F_{00}^{(2)}(\mathfrak{a}) &\equiv 4c_1c_2; F_{\alpha 0}^{(2)} = -(-1)^{\alpha}m_{\alpha}2c_{\alpha} \\ F_{\alpha\beta}^{(2)}(\mathfrak{a}) &= c_{\alpha}\frac{Z_{\alpha}^{(2)}(\mathfrak{a}_{\alpha})}{Z(\mathfrak{a})}\delta_{\alpha,\beta} - c_{\alpha}c_{\beta}m_{\alpha}m_{\beta}. \end{aligned} \right\} MFA \quad (2.32)$$

From matrix expression for $\hat{\Omega}_{\Theta}^{(2)}(q)$ (2.30) it can be found

$$\begin{aligned} \Omega_{\Theta,00}^{(2)}(\mathbf{q}) &= [1 - \Phi_{00}(\mathbf{q})V(\mathbf{q})]^{-1}\Phi_{00}(\mathbf{q}), \\ \Omega_{\Theta}^{(2)ss}(\mathbf{q}) &= [1 - \hat{\Phi}^s(\mathbf{q})\mathcal{I}^s(\mathbf{q})]^{-1}\hat{\Phi}^s(\mathbf{q}), \end{aligned} \quad (2.33)$$

$$\begin{aligned} \Phi_{00}(\mathbf{q}) &= f_{00}^{(2)}(\mathbf{q}) + \sum_{\alpha_1\alpha_2} f_{0\alpha_1}^{(2)}(\mathbf{q}) \left(\hat{\mathcal{I}}^s(\mathbf{q})[1 - \hat{f}^s(\mathbf{q})\hat{\mathcal{I}}^s(\mathbf{q})]^{-1} \right)_{\alpha_1\alpha_2} f_{\alpha_2 0}^{(2)}(\mathbf{q}), \\ \Phi_{\alpha\alpha'}^s(\mathbf{q}) &= f_{\alpha\alpha'}^{(2)}(\mathbf{q}) + f_{\alpha 0}^{(2)}(\mathbf{q})V(\mathbf{q})[1 - f_{00}(\mathbf{q})]^{-1}f_{0\alpha'}^{(2)}(\mathbf{q}), \end{aligned}$$

$$\hat{f}^s(\mathbf{q}) = \{f_{\alpha\beta}^{(2)}(\mathbf{q})\}, \quad \mathcal{I}^s(\mathbf{q}) = \{\mathcal{I}_{\alpha\beta}(\mathbf{q})\}. \quad (2.34)$$

At the temperature of second order phase transition the CFs of system diverge at certain values \mathbf{q}^* (we consider here only case $\mathbf{q}^* = 0$).

In the case $T > T_m$ the $f_{0\alpha}^{(2)}(\mathbf{q}) \equiv 0$ and $\Phi_{00}(\mathbf{q}) = f_{00}^{(2)}(\mathbf{q})$, $\Phi_{\alpha\alpha'}^s(\mathbf{q}) = f_{\alpha\alpha'}^{(2)}(\mathbf{q})$. Within MFA from first expression we obtain the T_s (the influence of magnetic subsystem is absent) and from the second one the equation for T_m (T_m is the temperature of magnetic transition)

$$\begin{aligned} T_s &= 4c_1c_2\mathcal{I}(0), \\ 2T_m &= c_1T_{11} + CT_{22} - \{(c_1T_{11} - c_1T_{22})^2 + 4c_1c_2T_{12}^2\}^{1/2}, \end{aligned} \quad (2.35)$$

$$T_{\alpha\beta} = \mathcal{I}_{\alpha\beta}\sqrt{\mathcal{F}_{\alpha}^{(2)}\mathcal{F}_{\beta}^{(2)}}. \quad (2.36)$$

3. Results of numerical investigation

The Hamiltonian (2.1) corresponds to the most generalized model of M -component magnet. There is no possibility at present to obtain any analytical solutions in this case. Therefore, in this section we represent some numerical results performed for particular cases of one-component Ising model, binary alloys and lattice gas. Here the numerical calculations become simpler.

3.1. Ising model

The case of Ising model will correspond to $M = 1$. The ionic part of the Hamiltonian becomes constant and does not influence on the thermodynamical and correlation functions of the system:

$$\mathcal{H} = \sum_{i=1}^N \Gamma_1 S_{i1} + \frac{1}{2} \sum_{i,j=1}^N \mathcal{I}_{11} S_{i1} S_{j1} + const \quad (3.1)$$

For calculation of free energy, magnetization, two-tail we can use formulae (2.13)-(2.20) and put $\alpha, \beta = 1$. In this case we have to solve system of only two equations for order parameter m_1 and fluctuating parameter $\lambda_{11}^{(2)}$. Therefore, one can write the following expression for generating function in the framework of two-tail approximation (2.13)-(2.18) that corresponds to free energy in the case of Ising model:

$$-\frac{\beta}{N}F(\Gamma) = -\frac{1}{2}\mathcal{I}_{11}m_1^2 + \langle F^{(0)}(\mathfrak{x}_1 + \sigma_1) \rangle - \frac{1}{2}\lambda_{11}^{(2)}\langle F_{11}^{(2)}(\mathfrak{x}_1 + \sigma_1) \rangle - \frac{1}{2N}\sum_q \ln[1 - \mathcal{I}_{11}(q)\langle F_{11}^{(2)}(\mathfrak{x}_1 + \sigma_1) \rangle]. \quad (3.2)$$

The equations for order parameters m_1 and two-tail $\lambda_{11}^{(2)}$ follow from the equations (2.17)-(2.18) :

$$m_1 = \langle F_1^{(1)}\{\mathfrak{x}_1 + \sigma_1\} \rangle, \quad (3.3)$$

$$\lambda_{11}^{(2)} = \frac{1}{2N}\sum_q \frac{\mathcal{I}_{11}(q)}{1 - \mathcal{I}_{11}(q)\langle F_{11}^{(2)}\{\mathfrak{x}_1 + \sigma_1\} \rangle}. \quad (3.4)$$

Here the averaging is performed with distribution function :

$$\rho_2\{\sigma\} = \int \frac{d\zeta}{2\pi} e^{i\zeta\sigma} e^{-\frac{1}{2}\zeta^2\lambda_{11}^{(2)}} = \frac{1}{\sqrt{2\pi\lambda_{11}^{(2)}}} e^{-\frac{\sigma^2}{2\lambda_{11}^{(2)}}}. \quad (3.5)$$

GFA gives the following results for the free energy and equation for two-tail $\lambda_{11}^{(2)}$ (see (2.19), (2.20)):

$$-\frac{\beta}{N}F(\Gamma) = -\frac{1}{2}\mathcal{I}_{11}m_1^2 + \langle F^{(0)}(\mathfrak{x}_1 + \sigma_1) \rangle - \frac{1}{2}\lambda_{11}^{(2)}\langle F_{11}^{(2)}(\mathfrak{x}_1 + \sigma_1) \rangle + \frac{1}{4}\langle F_{11}^{(2)}(\mathfrak{x}_1 + \sigma_1) \rangle \left[\langle F_{11}^{(2)}(\mathfrak{x}_1 + \sigma_1) \rangle \frac{1}{N}\sum_q \mathcal{I}_{11}^2(q) - 2\lambda_{11}^{(2)} \right], \quad (3.6)$$

$$m_1 = \langle F^{(1)}\{\mathfrak{x}_1 + \sigma_1\} \rangle_{\rho_2}, \quad (3.7)$$

$$\lambda_{11}^{(2)} = \langle F_{11}^{(2)}\{\mathfrak{x}_1 + \sigma_1\} \rangle_{\rho_2} \frac{1}{N}\sum_q \mathcal{I}_{11}^2(q). \quad (3.8)$$

Neglecting the fluctuation term $-\frac{1}{2}\sum_{ij} \mathcal{I}_{ij} \Delta S_i \Delta S_j$ in the Hamiltonian we

get the MFA approximation. This concerns the case $\lambda_{11}^{(2)} = 0$, $-\beta F(\Gamma)/N = -\frac{1}{2}\mathcal{I}_{11}m_1^2 + F^{(0)}\{\mathfrak{x}_1\}$ and $m_1 = F^{(1)}\{\mathfrak{x}_1\}$.

The numerical calculations were performed for the model with nearest neighbours interaction :

$$\mathcal{I}_{11}(q) = I \sum_{\alpha=1}^3 \cos q\alpha. \quad (3.9)$$

The results of this investigation can be seen in Fig.1, 2. In Fig.1 the free energy of the system as a function of order parameter for various temperatures is depicted. It is known, that we get first order phase transition in the framework of two-tail approximation. This can be seen in Fig.1. The curve for $T/\mathcal{I}(0) = 0.72$ has two minima with equal energy. Although the GFA is more rough than two-tail approximation, it gives us a second order phase transition at $T/\mathcal{I}(0) = 0.86$. The results of temperature dependences of magnetization in different approximation are plotted in Fig.2.

The obtained results show that the two-tail approximation predicts a non-physical behaviour in the close vicinity of the critical temperature. This may lead to the non-controlled errors by investigation of binary alloys and lattice gas. Therefore, for these systems we shall restrict only GFA and compare results with MFA.

3.2. Binary alloy

The Hamiltonian of the non-magnetic binary alloy follows from (2.1) if we put $\mathcal{I}_{11}(i-j) = \mathcal{I}_{12}(i-j) = \mathcal{I}_{22}(i-j) = 0, \Gamma_{i1} = \Gamma_{i2} = 0$:

$$\mathcal{H} = \mathcal{H}_x = \sum_{\alpha=1}^2 \sum_{i=1}^N \varepsilon_{\alpha} x_{i\alpha} + \frac{1}{2} \sum_{\alpha,\beta=1}^2 \sum_{i,j=1}^N V_{\alpha\beta}(i-j) x_{i\alpha} x_{j\beta}. \quad (3.10)$$

The MFA and GFA may be easily reformulated for this case using formulae of previous section. Our numerical calculations concern the system with nearest neighbours interaction. As may be proved in section 2 the critical temperatures of binodal and spinodal decay depends only on $\mathcal{I} = V_{11} + V_{22} - 2V_{12}$ and are symmetrical relatively substitution c_2 instead of c_1 . This can be seen in Fig. 4, where binodal and spinodal temperatures as a function of c_1 are depicted. The comparison of GFA and MFA approximation results show that GFA approximation is essentially better than MFA in the vicinity of $c_1 = 0.5$. When $c_1 \rightarrow 0$ or $c_1 \rightarrow 1$, the difference disappears. It should be noticed that two-tail approximation will give non-physical results namely in the vicinity of $c_1 = 0.5$.

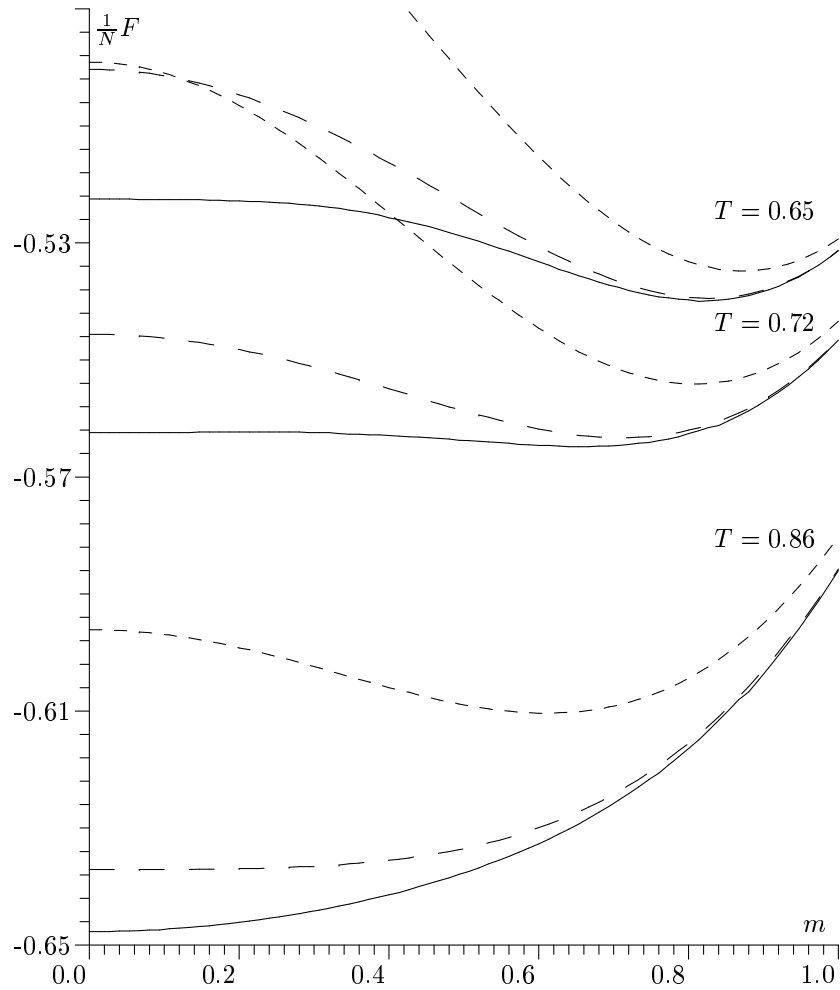


Figure 1: The free energy $\frac{1}{N}F$ as a function of magnetization m for various temperature (solid curves - two-tail approximation, long dashed curves - GFA, short dashed curves - MFA)

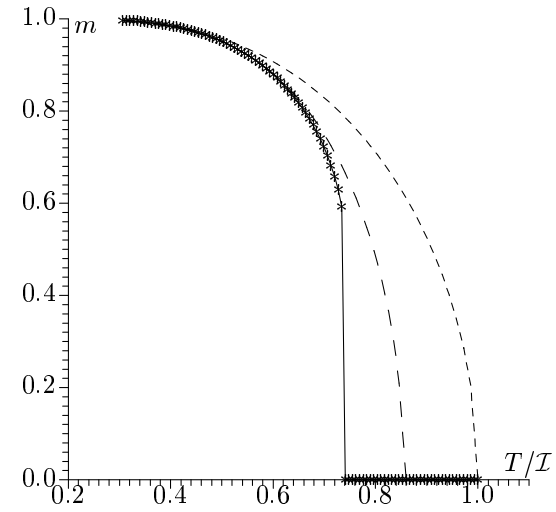


Figure 2: The magnetization m as a function of temperature T (solid curve - two-tail approximation, long dashed curve - GFA, short dashed curve - MFA)

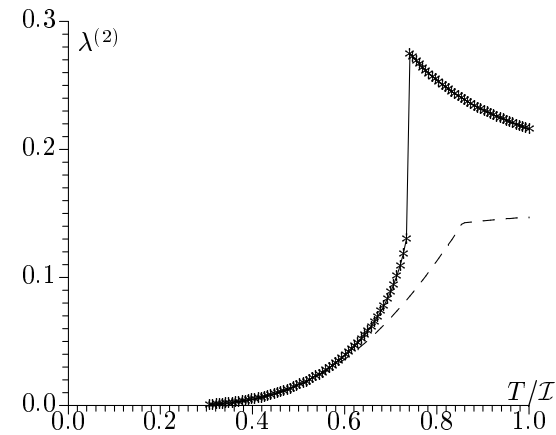


Figure 3: The two tail λ as a function of temperature T (solid curve - two-tail approximation, dashed curve - GFA)

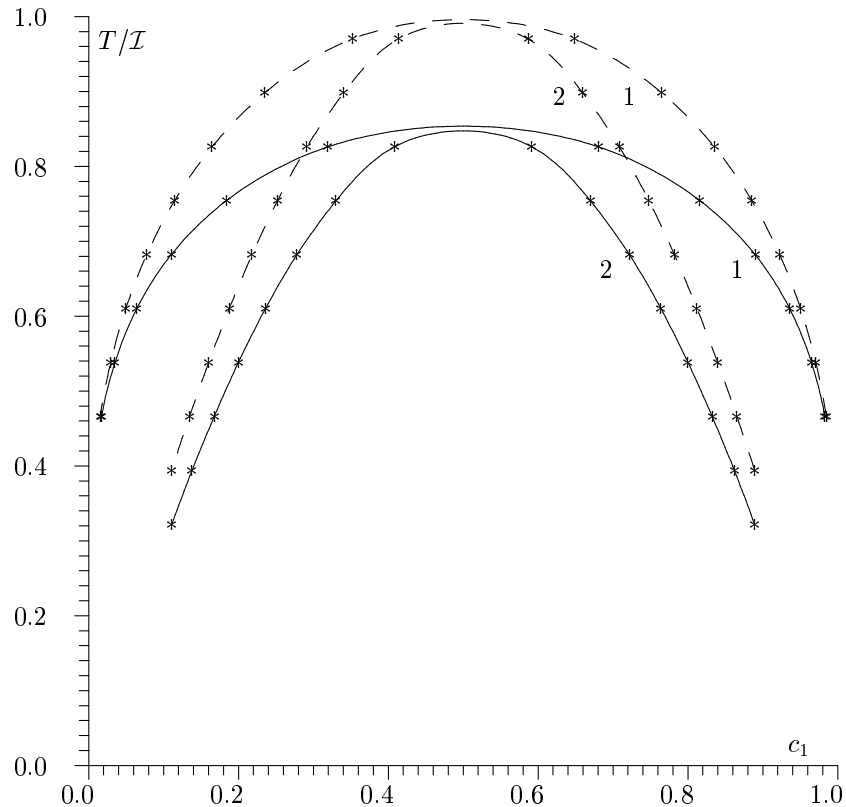


Figure 4: Phase diagrams for the model (3.9): 1- correspond to the binodal temperature, 2- spinodal temperature (solid line - GFA, dashed line - MFA)

3.3. Lattice gas

We shall get the Hamiltonian of the non-magnetic lattice gas, if we put $V_{12}(i-j) = V_{22}(i-j) = 0$ in case of binary alloy:

$$\mathcal{H} = \sum_{i=1}^N \mu x_i + \frac{1}{2} \sum_{i,j=1}^N V(i-j)x_i x_j. \quad (3.11)$$

Indeed, the Hamiltonian (3.11) may describe the gas. Let us consider the system in volume \mathcal{V} and divide volume on $N = \mathcal{V}$ equal cubic cells. We will use the condition that more than one particle can not be situated in one site. Therefore, we get a rough model of a gas with repulsion between particles on short distance and model interaction for long distance.

Here we neglect the kinetic energy of the particles. But being taken into account it leads only to the renormalization of the chemical potential

$$\mu \rightarrow \mu + \frac{3}{2} \ln(2\pi h^{-2} m k T), \quad (3.12)$$

where m - particle's mass.

Similarly to (2.5), the Hamiltonian (3.13) can be transformed to

$$\mathcal{H} = E(\mu) + \sum_{i=1}^N \Gamma_0 S_{i0} + \frac{1}{2} \sum_{i,j=1}^N \mathcal{I}(i-j) S_{i0} S_{j0}, \quad (3.13)$$

where $E(\mu) = \frac{1}{2}\mu + \frac{1}{8}V$, $\Gamma_0 = \frac{1}{2}\mu + \frac{1}{4}V$, $4\mathcal{I}(i-j) = V(i-j)$.

It is known from thermodynamics, that thermodynamical potential of the system $\Omega(\mu, T) = -p\mathcal{V}$, where p is pressure and \mathcal{V} is volume of the system. The average of x_i that equal $n = 1/v$, plays the role of gas density. The state equation can be written in the following form

$$p\mathcal{V} = \Omega(\mu(n), T) \text{ or } p = \frac{1}{\mathcal{V}} \Omega(\mu(n), T). \quad (3.14)$$

In MFA the state equation can be obtained in the analytical form. The expression for TP follows from (2.21) and has the following form:

$$\frac{1}{N} \Omega(\mu, T) = \frac{1}{2}\mu + \frac{1}{2}V - \frac{1}{2}\mathcal{I}m_0^2 + \ln 2 \cosh(\Gamma_0 + \mathcal{I}m_0), \quad (3.15)$$

where $\Gamma_0(m_0) = -\beta\mathcal{I}m_0 + \frac{1}{2} \ln \frac{1+m_0}{1-m_0}$, $\mu = 2\Gamma_0 - \frac{1}{2}\mathcal{I}$. If we take into account that $m_0 = 2n - 1$, we can obtain state equation in variables p , n , T :

$$\frac{p}{T} = -\beta a n^2 + \Phi(n), \quad (3.16)$$

where $\Phi(n) = \ln \frac{1}{1-n}$. It should be noted that for van der Waals state equation $\Phi(n) = \frac{n}{1-bn}$.

We have also obtained isotherms in GFA. Since the Hamiltonian of the lattice gas is identical to the Hamiltonian of the binary alloy with $V_{12}(i-j) = V_{22}(i-j) = 0$, we can use all approximation formulated in the previous subsection to its investigation.

In the Fig.5 the isotherms for the lattice gas with nearest neighbours interaction are depicted. The dashed curve corresponds to the MFA and solid curve for the GFA. It can be seen that values of the pressure p and binodal and spinodal temperature of the system obtained within GFA are smaller than those obtained within MFA.

4. Conclusions

In this paper we have considered the M -component Ising model with site disorder. Several approximation for this model have been formulated here. Namely, we have obtained the expressions for the thermodynamical potential, free energy and pair correlation functions within TTA, GFA and MFA.

The numerical calculations were performed for some simpler models: one-component Ising model, non-magnetic binary alloy and lattice gas. For example, we have chosen the nearest neighbours interaction. For the one-component Ising model we calculated the free energy as a function of the magnetization, temperature dependences of the magnetization $m(T)$ and the two-tail $\lambda^{(2)}$ (fluctuating parameter) within TTA, GFA, MFA. For non-magnetic binary alloy we obtained phase diagrams (binodal and spinodal curves) within GFA and MFA. For lattice gas the isotherms and coexistence curves are depicted.

This work was supported in part by the International Soros Science Education Program (ISSEP) through grant No. PSU062015.

References

- [1] Yukhnovskii I.R., Gurskii Z.A. Quantum-Statistical Theory of Disordered Systems.- Kiev: Naukova Dumka, 1991 (in Russian).
- [2] Z.Gurskii and Yu.Khokhlov, *J.Phys s.: Cond.Mat.*, **6** (1994),p.8711-8724.
- [3] Khachatryan A.G., Theory of Structural Transformations in Solids. New York: Wiley 1983.

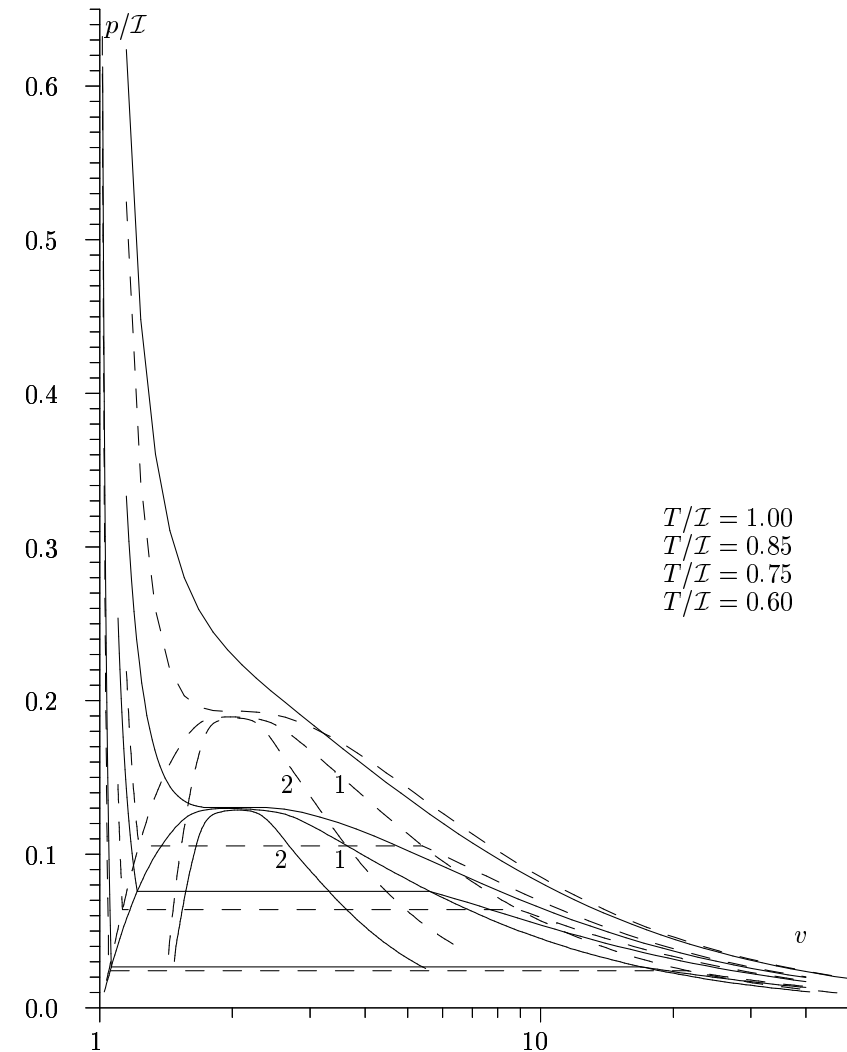


Figure 5: The $p - V$ diagram for the lattice gas by various temperature (solid curves - two-tail GFA, dashed curves - MFA; 1 - binodal, 2 - spinodal)

-
- [4] V.G.Vaks, N.E.Zein, *J.Exp.Theor.Fiz.*, **67** (1974), p.1082-1100 (in Russian).
 - [5] T.Kawasaki, *Progr.Theor.Phys.*, **58** (1977), p.1357-1366
 - [6] R.R.Levitskii, S.I.Sorokov, R.O.Sokolovskii, *Cond.Mat.Phys.*, **5** (1995), p.81-104.
 - [7] Yukhnovskii I.R., Levitskii R.R., Sorokov S.I., Derzhko O.V., *Bul. Ac. Sci. USSR, Ser. Fiz.*, **55** (1991), p.481.
 - [8] Z.Onyszkiewicz, A.Wierzbicki, *Pysica B*, **151** (1988), p.462-474.
-

Препринти Інституту фізики конденсованих систем НАН України розповсюджуються серед наукових та інформаційних установ. Вони також доступні по електронній комп'ютерній мережі на WWW-сервері інституту за адресою <http://www.icmp.lviv.ua/>

The preprints of the Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine are distributed to scientific and informational institutions. They also are available by computer network from Institute's WWW server (<http://www.icmp.lviv.ua/>)

Сергій Іванович Сороков
Роман Романович Левицький
Тарас Михайлович Верхоляк

ДОСЛІДЖЕННЯ НЕВПОРЯДКОВАНИХ ВІДПАЛЕНИХ ІЗІНГІВСЬКИХ
СИСТЕМ В НАБЛИЖЕННІ ДВОХВОСТОК

Роботу отримано 23 грудня 1996 р.

Затверджено до друку Вченою радою ІФКС НАН України

Рекомендовано до друку семінаром відділу теорії модельних
спінових систем

Виготовлено при ІФКС НАН України

© Усі права застережені