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PHASE TRANSITIONS IN PSEUDOSPIN-ELECTRON MODEL
WITH DIRECT INTERACTION BETWEEN PSEUDOSPINS

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Фазові переходи в псевдоспін-електронній моделі з прямою взаємодією між псевдоспінами

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Анотація. Проведено аналіз термодинамічних властивостей псевдоспін-електронної моделі у випадку відсутності електронного переносу з включенням прямої взаємодії між псевдоспінами сегнетоелектричного типу. У наближенні середнього поля досліджуються умови рівноваги в режимах $\mu = const$ та $n = const$. Показано, що взаємодія з електронами приводить при фіксованому значенні μ до можливості фазового переходу першого роду при зміні температури з стрибкоподібною зміною $\langle S^z \rangle$. В режимі $n = const$ має місце нестабільність щодо розділення фаз в широкому інтервалі значень параметра асиметрії h .

Phase transitions in pseudospin-electron model with direct interaction between pseudospins

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Abstract. The analysis of thermodynamic properties of the pseudospin-electron model in the case of zero electron transfer with the inclusion of the direct pseudospin-pseudospin interaction of ferroelectric type is performed. The equilibrium conditions in the regimes $\mu = const$ and $n = const$ are investigated in the mean field approximation. It is shown that the interaction with electrons leads at the fixed μ value to the possibility of the first order phase transition at the change of temperature with a jump-like behaviour of $\langle S^z \rangle$. In the regime $n = const$ there takes place an instability with respect to phase separation in the wide range of asymmetry parameter h values.

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1. Introduction

Pseudospin-electron model (so called Muller model [1]) is the one of theoretical models which were proposed in connection with the investigation of characteristic features of electron spectrum and lattice dynamics in high temperature superconductors. In this model strong Hubbard-type electron correlations are taken into account. Pseudospin formalism is used for the description of locally anharmonic lattice vibrations (in case of $YBa_2Cu_3O_7$ - crystals it corresponds to the vibrational states of apex oxygen ions O_4 , which move in the double-minimum potential wells). The analogous pseudospin-electron model has been applied recently to the crystals $(MA_2X)Y_2$ ($M = Pt, Pd$; $X = Cl, Br, I$; $A =$ ligand molecule; Y counter anion) with A-H-Y hydrogen bonds with the purpose to describe the effects caused by proton-electron interaction [2].

Hamiltonian of the model has the following form

$$H = \sum_i H_i + \sum_{ij\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} - \frac{1}{2} \sum_{ij} J_{ij} S_i^z S_j^z \quad (1)$$

$$H_i = U n_{i\uparrow} n_{i\downarrow} - \mu \sum_{\sigma} n_{i\sigma} + g \sum_{\sigma} n_{i\sigma} S_i^z + \Omega S_i^x - h S_i^z, \quad (2)$$

where in the single site part in addition to Hubbard correlation U there are terms that describe tunneling splitting and asymmetry of local anharmonic potential (longitudinal field h). Hamiltonian (1) also contains terms, which describe electron transfer t_{ij} and direct interaction between pseudospins J_{ij} . The energy is accounted from the level of chemical potential.

Using the model for the description of anharmonic subsystem of oxygen ions in crystals $YBa_2Cu_3O_7$ (or similar systems) the following values of parameters can be taken as characteristic for the system: $U = 4 \dots 11eV$; $g = 2 \dots 6eV$; $t = 0.1 \dots 0.06eV$; $\Omega = 0 \dots 0.05eV$ [3]. In this case the perturbation theory can not be applied for the interaction gnS^z as well as Hubbard correlation Unn . It is reasonable to include these interactions in zero order Hamiltonian. In this role the single site Hamiltonian (2) can be taken. Its eigenfunctions are built of the vectors $|n_{i\uparrow}, n_{i\downarrow}, S_i^z\rangle$, which form the full basis of states of the unit cell:

$$\begin{aligned} |1\rangle &= \left|0, 0, \frac{1}{2}\right\rangle & |\hat{1}\rangle &= \left|0, 0, -\frac{1}{2}\right\rangle \\ |2\rangle &= \left|1, 1, \frac{1}{2}\right\rangle & |\hat{2}\rangle &= \left|1, 1, -\frac{1}{2}\right\rangle \\ |3\rangle &= \left|0, 1, \frac{1}{2}\right\rangle & |\hat{3}\rangle &= \left|0, 1, -\frac{1}{2}\right\rangle \\ |4\rangle &= \left|1, 0, \frac{1}{2}\right\rangle & |\hat{4}\rangle &= \left|1, 0, -\frac{1}{2}\right\rangle \end{aligned} \quad (3)$$

The tunneling mixes states $|r\rangle$ and $|\hat{r}\rangle$. Because of this final eigenfunctions are linear combinations of corresponding pairs of vectors (3) [4].

The main attention at the investigation of this model has been paid to examination of electron states, effective electron-electron interaction, to the elucidation of additional possibilities of occurrence of superconducting pair correlations. A series of works has been carried out in which the pseudospin $\langle SS \rangle$ and charge $\langle nn \rangle$ correlation functions as well as so-called transverse dielectric susceptibility were calculated. It has been shown with the use of the generalized random phase approximation (GRPA) [5,6], that there exists a possibility of divergences of these functions at some values of temperature. This effect was interpreted as a manifestation of dielectric instability or ferroelectric type anomaly. The tendency to the spatially modulated charge and pseudospin ordering at certain model parameter values was found out.

This work is devoted to the study of thermodynamics of the pseudospin-electron model. The case of zero electron transfer ($t_{ij} = 0$) and zero frequency of tunneling splitting ($\Omega = 0$) is considered. The direct interaction between pseudospins is taken into account. It is supposed to be a long-ranged ($J_{ij} \sim J/N$) that allows to use the mean field approximation. The similar problem was studied earlier for two-sublattice model [7], but the obtained results were only partial and didn't cover all the possibilities.

In this approximation, the Hamiltonian of the model has the following form

$$\begin{aligned} H &= \sum_i \tilde{H}_i + \frac{N}{2} J \eta^2; \\ \tilde{H}_i &= -\mu \sum_{\sigma} n_{i\sigma} + U n_{i\uparrow} n_{i\downarrow} + g \sum_{\sigma} n_{i\sigma} S_i^z - (h + J\eta) S_i^z \end{aligned} \quad (4)$$

The interaction J_{ij} is taken as the ferroelectric type one ($J(\vec{q})$ has maximum value at $\vec{q} = 0$; $J(0) \equiv J > 0$); the order parameter $\eta = \langle S_i^z \rangle$ does not depend on the unit cell index.

We investigate the possible states and phases of the system as well as the transitions between them at the change of temperature and model parameters values.

2. Mean field approximation; $\Omega = 0$.

If the tunneling splitting is not taken into account ($\Omega = 0$) single site Hamiltonian \tilde{H}_i on the basis (3) is diagonal. Its eigenvalues for this case

are:

$$\begin{aligned}\lambda_{1,\bar{1}} &= \mp H; \\ \lambda_{2,\bar{2}} &= -2\mu + U \pm g \mp H; \\ \lambda_{3,\bar{3}} &= \lambda_{4,\bar{4}} = -\mu \pm \frac{g}{2} \mp H,\end{aligned}\quad (5)$$

where

$$H = \frac{h}{2} + \frac{J\eta}{2}. \quad (6)$$

Thermodynamic potential of the model, calculated per one lattice site is equal to

$$\begin{aligned}\frac{\Omega}{N} &= -\theta \ln Z_i + \frac{1}{2} J\eta^2 \\ Z_i &= 2 \left[ch\beta H + e^{-\beta(U-2\mu)} ch\beta(H-g) + 2e^{\beta\mu} ch\beta \left(H - \frac{g}{2} \right) \right]\end{aligned}\quad (7)$$

For investigation of equilibrium conditions we will separate two regimes: $\mu = const$ and $n = const$. The equilibrium for the first regime is defined by the minimum of thermodynamical potential:

$$\left(\frac{\partial \Omega}{\partial \eta} \right)_{T,\mu,h} = 0 \quad (8)$$

The equation for the order parameter is obtained from is condition:

$$\eta = \frac{1}{2Z_i} \left[\sum_{p=1}^4 e^{-\beta\lambda_p} - \sum_{p=\bar{1}}^{\bar{4}} e^{-\beta\lambda_p} \right], \quad (9)$$

or in an explicit form

$$\eta = \frac{1}{2} \frac{sh\beta H + e^{-\beta(U-2\mu)} sh\beta(H-g) + 2e^{\beta\mu} sh\beta \left(H - \frac{g}{2} \right)}{ch\beta H + e^{-\beta(U-2\mu)} ch\beta(H-g) + 2e^{\beta\mu} ch\beta \left(H - \frac{g}{2} \right)} \quad (10)$$

The same equation can be derived using thermodynamical relation:

$$\left(\frac{\partial \Omega}{\partial h} \right)_{T,\mu} = -\eta \quad (11)$$

The average number of electrons for this regime is determined as follows:

$$-\frac{1}{N} \left(\frac{\partial \Omega}{\partial \mu} \right)_{T,h} = \left\langle \frac{1}{N} \sum_i n_i \right\rangle \equiv n, \quad (12)$$

namely

$$n = \frac{4}{Z_i} \left[e^{-\beta(U-2\mu)} ch\beta(H-g) + e^{\beta\mu} ch\beta \left(H - \frac{g}{2} \right) \right] \quad (13)$$

The equilibrium condition for the regime $n=const$ is determined by the minimum of free energy $F = \Omega + \mu N$. The equation

$$\left(\frac{\partial F}{\partial \eta} \right)_{T,n,h} = 0 \quad (14)$$

and expression (13) form a set of equations for the parameter and chemical potential. Using (13) it is easy to show that the equation which goes from (14) is the same as the given above using condition (8).

The equation (13) is solvable for the chemical potential. When the notations

$$y = e^{\beta\mu}; a = \frac{ch\beta \left(H - \frac{g}{2} \right)}{ch\beta(H-g)}; b = \frac{ch\beta H}{ch\beta(H-g)}, \quad (15)$$

are introduced the following equation for the variable y is obtained:

$$(2-n)e^{-\beta U} y^2 + 2a(1-n)y - nb = 0 \quad (16)$$

The solution of this equation is

$$y = \frac{-a(1-n) + \sqrt{a^2(1-n) + (2-n)e^{-\beta U} nb}}{(2-n)e^{-\beta U}} \quad (17)$$

(the physical meaning has the root $y > 0$).

After the eliminating of the chemical potential, the equation for the order parameter transforms to the following form:

$$\begin{aligned}\eta &= \frac{1}{2} \left(\frac{n}{2} - \frac{\delta}{2} \right) th\beta(H-g) + \frac{1}{2} \delta th\beta \left(H - \frac{g}{2} \right) + \\ &+ \frac{1}{2} \left(\frac{2-n}{2} - \frac{\delta}{2} \right) th\beta H,\end{aligned}\quad (18)$$

where

$$\delta = \frac{(2-n)ay}{b+ay} = \frac{\sqrt{(1-n)^2 + n(2-n)e^{-\beta U} \frac{b}{a^2}} - 1}{e^{-\beta U} \frac{b}{a^2} - 1}, \quad (19)$$

and the $\frac{b}{a^2}$ ratio, is given by the expression

$$\frac{b}{a^2} = \frac{ch\beta g + ch\beta(2H-g)}{1 + ch\beta(2H-g)} \quad (20)$$

The equations (10) and (18) determine the values of η parameter, which correspond to the extrema of thermodynamical potential Ω and free energy F respectively. From the set of all possible roots of it is necessary to take into consideration only those which provide the minimum values of Ω or F .

The equation (18) possesses the symmetry as to the transformations

$$\begin{aligned} n &\rightarrow 2 - n; H \rightarrow g - H; \eta \rightarrow -\eta \\ (h &\rightarrow 2g - h) \end{aligned} \quad (21)$$

This transformation leads to replacements:

$$b \rightarrow \frac{1}{b}, a \rightarrow \frac{a}{b}, \frac{b}{a^2} \rightarrow \frac{b}{a^2}, \delta \rightarrow \delta. \quad (22)$$

With a substitution $y \rightarrow e^{\beta U} y^{-1} (\mu \rightarrow U - \mu)$, the equation (13) for the chemical potential remains the same as well as the equation (10).

The symmetry (21)-(22) allows to study the problem for the $n = \text{const}$ within the interval $0 \leq n \leq 1$. The extension to the interval $1 \leq n \leq 2$ is performed by means of the above-mentioned transformations.

3. The equation of state $\eta = \eta(h)$ and phase diagrams at $T = 0$ (regime $n = \text{const}$).

The equation for the parameter η , obtained in regime of fixed number of electrons, can be solved analytically in the limit $T = 0$. The quantity

$$e^{-\beta U} \frac{b}{a^2} \equiv \varphi, \quad (23)$$

which is presented in the expression for the parameter, has a form of a ratio of an algebraic sums of exponents like $\exp[(\beta \dots)]$. At $T \rightarrow 0$

$$\varphi \rightarrow \begin{cases} \infty, & \eta^* < \eta < \bar{\eta}^* & (a) \\ 0, & \eta < \eta^*; \eta > \bar{\eta}^* & (b) \end{cases} \quad (24)$$

where

$$\eta^* = \frac{U - h}{J}; \bar{\eta}^* = \frac{2g - U - h}{J} \quad (25)$$

(it is clear that if $U > g$, the case (a) can't be realized). Respectively,

$$\delta \rightarrow \begin{cases} \frac{\sqrt{n(2-n)}}{\sqrt{\delta}} \rightarrow 0 \\ 1 - \sqrt{(1-n)^2} = \begin{cases} n, & 0 \leq n \leq 1 \\ 2 - n, & 1 \leq n \leq 2 \end{cases} \end{cases} \quad (26)$$

In a consequence, the equation (18) can be written in the following form

$$\eta = \begin{cases} n\theta(h-g+J\eta) + (1-n)\theta(h+J\eta) - \frac{1}{2} & \varphi = 0, 0 \leq n \leq 1 \\ (n-1)\theta(h-2g+J\eta) + (2-n)\theta(h-g+J\eta) - \frac{1}{2}; & \varphi = 0, 1 \leq n \leq 2 \end{cases} \quad (27)$$

$$\eta = \frac{n}{2}\theta(h-2g+J\eta) + \left(1 - \frac{n}{2}\right)\theta(h+J\eta) - \frac{1}{2}; \quad \varphi = \infty \quad (28)$$

The solution of this equation is determined by the intersection of $f(\eta) = \eta$ line with a stairs-like function that corresponds to the right part of the equation.

Typical example of $\eta(h)$ dependence is shown in Fig. 1, which corresponds to the n value in the interval $0 \leq n \leq 1$. At some regions of values of h , where $\eta(h)$ function possesses S-like behaviour and has three or more values, the first order phase transitions with the jumps of parameter take place at the change of h . Phases $\eta = -\frac{1}{2}$ (phase 1), $\eta = \frac{1}{2} - n$ (phase 2), $\eta = \frac{1}{2} - \frac{n}{2}$ (phase 3), $\eta = \frac{1}{2}$ (phase 4) exist between phase transition points and outside of them. At the change of parameter values the regions, where metastable phases exist, can overlap, the disappearing of some phase transitions takes place and therefore some intermediate phases can not be realized. In case $1 \leq n \leq 2$ the dependence of $\eta(h)$ is generally similar. The phase 3 and phase 2' at $\eta = \frac{3}{2} - n$, which now appears instead of phase 2, may play the role of intermediate phases.

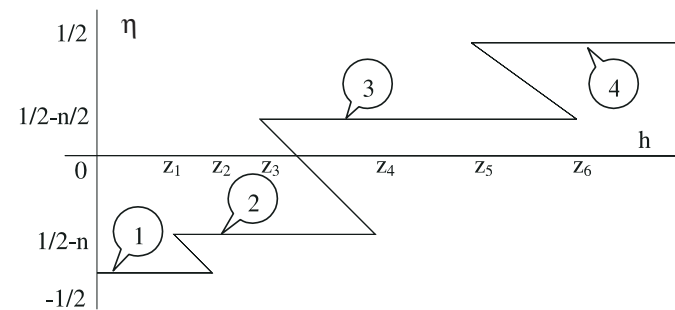


Figure 1. The dependence of η parameter on h field at $T = 0$ (in the case $g > \frac{J}{2}; \frac{J}{2} - \frac{nJ}{4} < U < g - \frac{nJ}{4}; 0 < n < 1$)

In order to clarify the conditions of appearing of any phases, we will study the the localization of a minimum values of the free energy

function. Using the relation

$$\left(\frac{\partial F}{\partial h}\right)_{T,n} = -\eta, \quad (29)$$

we have

$$F = \int_{h_0}^h (-\eta) dh. \quad (30)$$

That defines the function F up to a constant. In correspondence with notations presented in Fig.1,

$$\begin{aligned} F_1(h) &= \frac{1}{2}(h - h_0), & (h \leq z_2) \\ \bar{F}_1(h) &= \bar{F}_1(z_2) + \frac{1}{2J}(h^2 - z_2^2), & (z_1 \leq h \leq z_2) \\ F_2(h) &= \bar{F}_1(z_1) + \left(-\frac{1}{2} + n\right)(h - z_1), & (z_1 \leq h \leq z_4) \\ \bar{F}_2(h) &= \bar{F}_2(z_4) + \frac{1}{2J}(h^2 - z_4^2) - \frac{U}{J}(h - z_4), & (z_3 \leq h \leq z_4) \\ F_3(h) &= \bar{F}_2(z_3) + \left(-\frac{1}{2} + \frac{n}{2}\right)(h - z_3), & (z_3 \leq h \leq z_6) \\ \bar{F}_3(h) &= \bar{F}_3(z_6) + \frac{1}{2J}(h^2 - z_6^2) + \frac{U-2g}{J}(h - z_6), & (z_5 \leq h \leq z_6) \\ F_4(h) &= \bar{F}_3(z_5) - \frac{1}{2}(h - z_5), & (z_5 \leq h) \end{aligned} \quad (31)$$

Here

$$\begin{aligned} z_1 &= -\frac{J}{2} + nJ & z_4 &= U - \frac{J}{2} + nJ \\ z_2 &= \frac{J}{2} & z_5 &= 2g - U - \frac{J}{2} \\ z_3 &= U - \frac{J}{2} + \frac{nJ}{2} & z_6 &= 2g - U - \frac{J}{2} + \frac{nJ}{2} \end{aligned} \quad (32)$$

The states with the lowest value of free energy are thermodynamically stable. The states described by $\bar{1}, \bar{2}, \bar{3}$ -curves are unstable. The intersections of F_1, F_2, F_3, F_4 - lines determine the points of the first order phase transition between relevant phases. Some of these phase transitions will not be realized, if the relevant points of crossing lie above some other F_k -line.

Similar analysis one can do for the case $1 \leq n \leq 2$. In fact this can be done through the substitution $n \rightarrow 2 - n$, $\eta \rightarrow -\eta$, $h \rightarrow 2g - h$ with respect of the mentioned above symmetry of the model.

The values of field $h = h_{ik}$, at which the mentioned above phase transitions $i \leftrightarrow k$ occur, are the following:

$$\begin{aligned} h_{12} &= \frac{nJ}{2}; & h_{23} &= U - \frac{J}{2} + \frac{3n}{4}J; \\ h_{34} &= 2g - U - \frac{J}{2} + \frac{Jn}{4}; & h_{13} &= \frac{nJ}{4} + \frac{n}{2-n}U; \\ h_{24} &= g - \frac{1-n}{2}J; & h_{14} &= ng \end{aligned} \quad (33)$$

at $0 \leq n \leq 1$, and

$$\begin{aligned} h_{12} &= g - \frac{1-n}{2}J; & h_{23} &= 2g - U - J + \frac{3n}{4}J; \\ h_{13} &= U + \frac{Jn}{4}; & h_{12} &= 2g - \frac{J}{2} + \frac{Jn}{4} - \frac{2-n}{n}U; \\ h_{2'4} &= 2g - J + \frac{Jn}{2}J; & h_{14} &= ng \end{aligned} \quad (34)$$

at $1 \leq n \leq 2$.

Phase diagrams (U, h) that correspond to some values of n are presented on Fig.2. The areas of existence of phases $1 \dots 4$ at $T = 0$ are shown. They have qualitatively different appearance in the cases $g > \frac{J}{2}$, $\frac{J}{4} < g < \frac{J}{2}$ and $g < \frac{J}{4}$. For the limit $U \rightarrow \infty$ (i.e. when the state with two electrons at a single site is prohibited) the transitions $1 \rightarrow 2 \rightarrow 4$ (if $g > \frac{J}{2}$, $n < 1$) or $1 \rightarrow 2' \rightarrow 4$ (if $g > \frac{J}{2}$, $n > 1$), or $1 \rightarrow 4$ (if $g < \frac{J}{2}$) take place. If $U \rightarrow 0$, the transitions $1 \rightarrow 3 \rightarrow 4$ (if $g > \frac{J}{4}$), or $1 \rightarrow 4$ (if $g < \frac{J}{4}$) take place.

Phase diagrams (n, h) can be built on the basis of diagrams (U, h) and formulas (33), (34). These diagrams are presented in Fig.3. Their appearance depends on the values of U and g constants. In addition they show the possibility of transformation of phases at the change of electron concentration n . More detailedly this issue will be discussed below.

4. Instability with respect to phase separation.

It is known that the dependence of concentration of particles on chemical potential is one of the factors that determine thermodynamical equilibrium of the system. The state with homogenous distribution of particles is unstable at $\left(\frac{\partial n}{\partial \mu}\right)_T < 0$, and the phase separation into the regions with different concentrations takes place. To investigate this possibility in our case, we will study the dependence $\mu(n)$, described by the equation (13), more attentively. In the limit $T \rightarrow 0$ there is a possibility to do this analytically.

According to formula (17) in this case we have:

$$y = \begin{cases} \frac{a\varphi}{e^{-\beta U}} \frac{\sqrt{n(2-n)}}{2-n} \frac{1}{\sqrt{\varphi}}; & \varphi \rightarrow \infty \\ \frac{a\varphi}{e^{-\beta U}} \frac{n}{2(1-n)}; & \varphi \rightarrow 0, n < 1 \\ \frac{a\varphi}{e^{-\beta U}} \frac{1}{\sqrt{\varphi}}; & \varphi \rightarrow 0, n = 1 \end{cases} \quad (35)$$

(at $0 \leq n \leq 1$). This expression allows to get the limit value of $\mu = \theta \ln y$ for the each of mentioned above phases, taking into account conditions

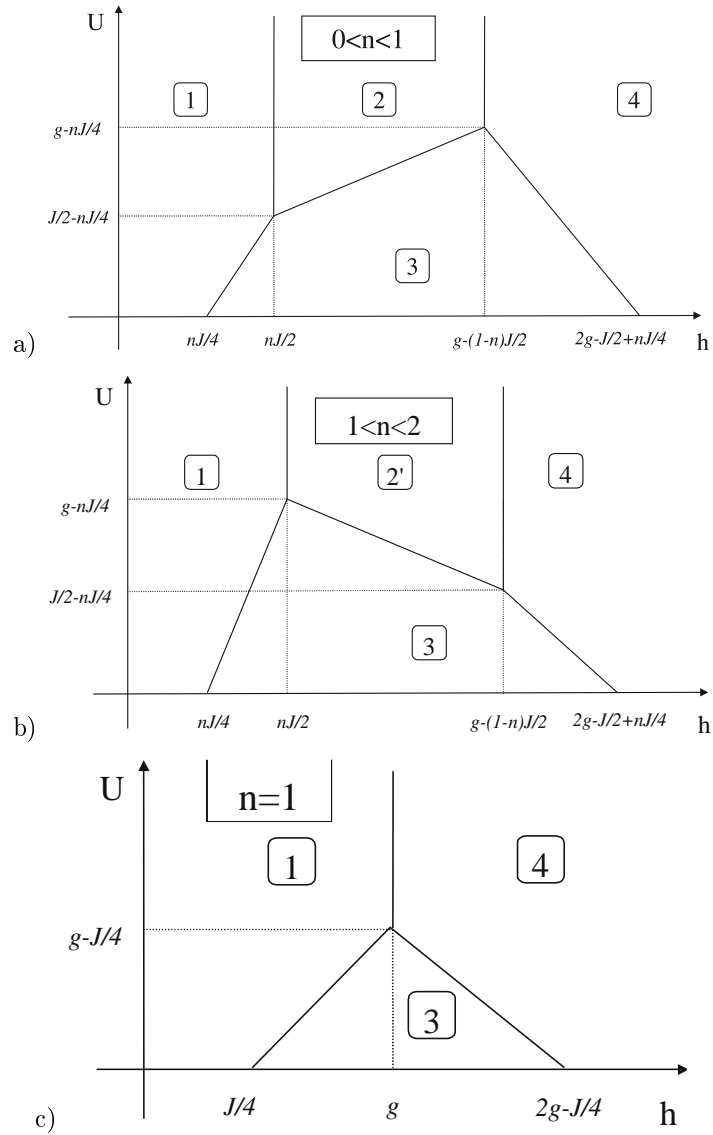


Figure 2. (U, h) -phase diagrams at $T=0$ (regime $n=\text{const}$). a), b) $g > \frac{J}{2}$, c) $\frac{J}{4} < g < \frac{J}{2}$

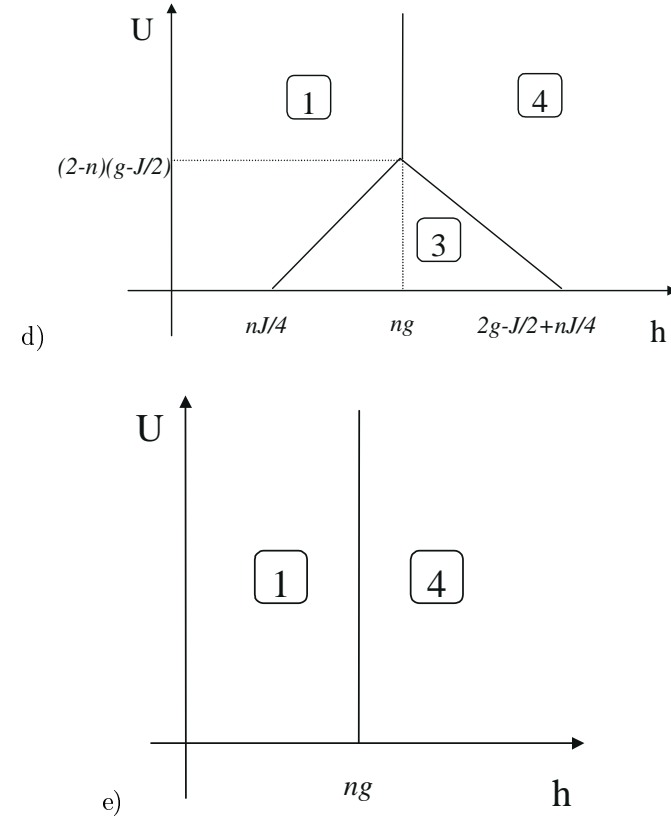


Figure 2. d) $\frac{J}{4} < g < \frac{J}{2}$, $0 \leq n < 1$, $1 < n \leq 2$, e) $g < \frac{J}{4}$

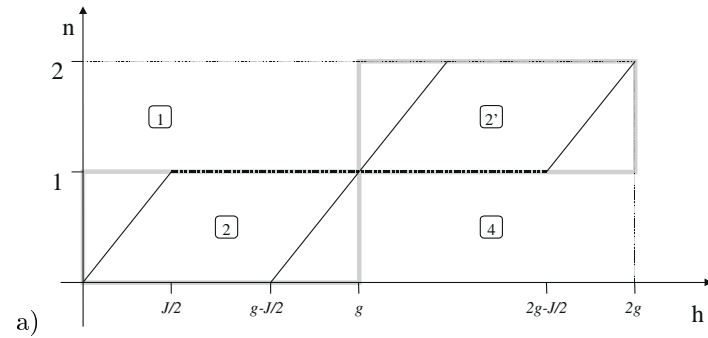
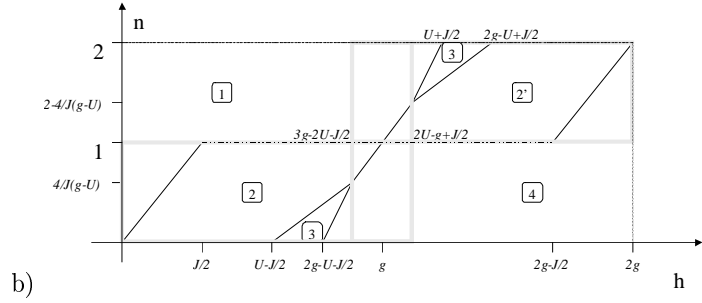
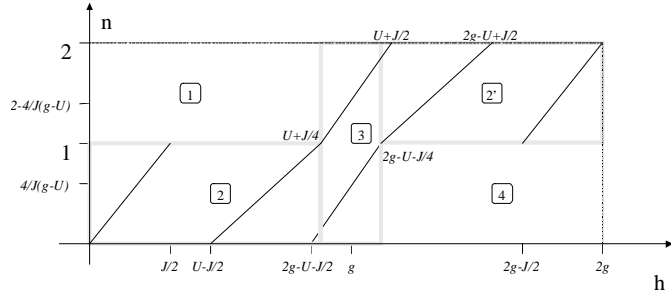


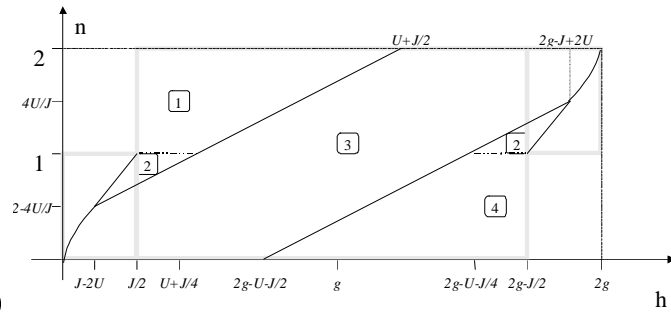
Figure 3. (n, h) - phase diagrams at $T = 0$; a) $U > g$;



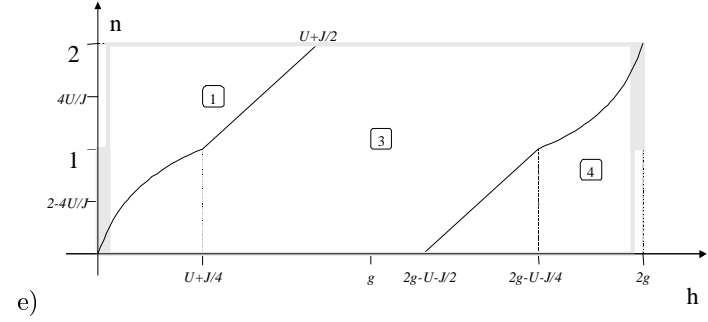
b)



c)



d)

Figure 3. b) $g - \frac{J}{4} < U < g$; c) $\frac{U}{2} < U < g - \frac{J}{4}$; d) $\frac{J}{4} < U < \frac{J}{2}$;

e)

Figure 3. e) $U < \frac{J}{4}$

(24), by separating the main exponents in expressions for a and φ at different relations between the values of parameters of the model. Let's take as an example the case $U > g$; the corresponding phase diagram in plane (n, h) is shown on Fig.3. For the phase 1, $\eta = -\frac{1}{2}$, which realizes at $h < \frac{Jn}{2}$ for $0 \leq n \leq 1$ and at $h < g - \frac{1-n}{2}J$ for $1 \leq n \leq 2$ we have:

$$\mu = \begin{cases} -\frac{g}{2}; & 0 < n < 1 \\ U - \frac{g}{2}; & 1 < n < 2 \\ \mu > U - \frac{g}{2}, & n = 2 \\ -\frac{g}{2} < \mu < U - \frac{g}{2}, & n = 1 \\ \mu < -\frac{g}{2}, & n = 0 \end{cases} \quad (36)$$

For the phase 4, $\eta = \frac{1}{2}$, where $h > g - \frac{1-n}{2}J$ for $0 < n < 1$; and $h > 2g - J + \frac{nn}{2}$ for $1 < n < 2$

$$\mu = \begin{cases} \frac{g}{2}; & 0 < n < 1 \\ U + \frac{g}{2}; & 1 < n < 2 \\ \mu > U + \frac{g}{2}, & n = 2 \\ \frac{g}{2} < \mu < U + \frac{g}{2}, & n = 1 \\ \mu < \frac{g}{2}, & n = 0 \end{cases} \quad (37)$$

In the case of intermediate phase 2, $\eta = \frac{1}{2}$, at $\frac{J}{2} < h < g - \frac{J}{2}$ the parameter φ at $T \rightarrow 0$ is approximated by the exponent

$$\varphi \approx \exp \left\{ \beta \left[h + J \left(\frac{1}{2} - n \right) - U \right] \right\}$$

and correspondingly $a \sim e^{-\beta \frac{g}{2}}$. As a result:

$$\mu = \frac{J}{2} - \frac{g}{2} - Jn + h, \quad 0 < n < 1, \quad (38)$$

and

$$\begin{aligned} \mu &= \frac{J}{2} - \frac{g}{2} + h, & n &= 0 \\ -\frac{g}{2} - \frac{J}{2} + h < \mu < U - \frac{g}{2}, & n &= 1 \end{aligned} \quad (39)$$

One can see that within this phase there is a possibility of descending dependence of μ on n .

$$\left(\frac{\partial\mu}{\partial n}\right)_{h,T} < 0 \quad (40)$$

That means the instability of homogenous state of the system. More convenient and stable thermodynamically is the state with phase separation, which is a mixture of states with different electron concentrations and different values of order parameter. In the case illustrated on Fig. 4a the phase 2 splits at $T=0$ into phase 4 ($n=0, \eta=\frac{1}{2}$) and phase 1 ($n=1, \eta=-\frac{1}{2}$) with weight coefficients $1-n$ and n respectively.

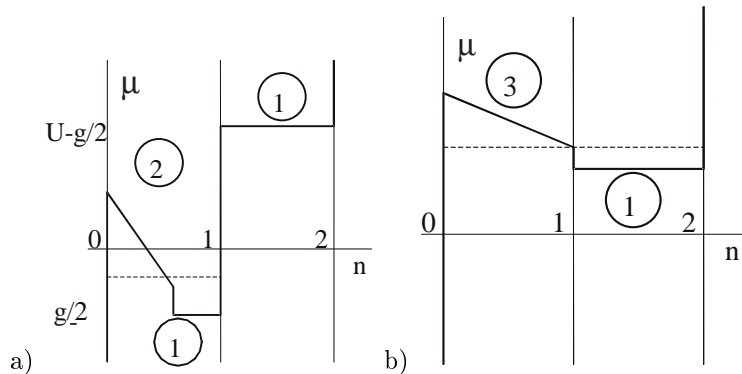


Figure 4. The dependence of chemical potential on the electron concentration n ($T=0$). a) $U > g$; $g > J/2$; $0 < h < J/2$; b) $J/2 < U < g - J/4$; $g > J/2$; $U < h < U + J/4$

On Fig. 4b another example is shown. In this case the descending character of $\mu(n)$ dependence takes place in the phase 3,

$$\mu = \frac{J}{4} + \frac{U}{2} - \frac{g}{2} - \frac{nJ}{4} + \frac{h}{2}, \quad (41)$$

The separation into phase 4 and phase 1, with concentrations $n=0$ and $n=2$ respectively, occurs.

Negative sign of derivative $\left(\frac{\partial\mu}{\partial n}\right)$ is typical for phase 2' as well. Here

$$\mu = U + \frac{3J}{2} - \frac{3g}{2} - nJ + h \quad (42)$$

Phase separated states are bordered by binodal lines. At $T=0$ they are:

$$\begin{aligned} n &= 0, & (0 < h < g) \\ n &= 1, & (0 < h < 2g) \\ n &= 2, & (g < h < 2g) \end{aligned} \quad (43)$$

at $U > g$, and

$$\begin{aligned} n &= 0, & (0 < h < 2g - U) \\ n &= 1, & (0 < h < U, 2g - U < h < 2g) \\ n &= 2, & (U < h < 2g) \end{aligned} \quad (44)$$

at $U < g$ (Fig.3). These boundaries surround the regions of existence of intermediate phases 2, 2', and 3. Mentioned phases might be stable only if there were some factors that will maintain the space homogeneity of electron concentration.

5. Phase transition at $\mu=\text{const}$.

The dependence of order parameter on field h and temperature θ , at the constant value of chemical potential, is determined according to equation (10). To investigate its possible solutions we will start with the case of zero temperature. The comparison of eigenvalues λ_r , $\lambda_{\bar{r}}$ allows us to find out the ground state of the system at fixed value of μ , and study its possible changes depending on the parameters g , U , J and field h values.

The obtained results are presented in the form of (H, μ) - diagrams. The areas where the ground of the system is realized in the form of one or other state (3) are shown on these diagrams. The form of mentioned diagrams depends on the relation between parameters U and g values (Fig. 5a $U > g$; Fig. 5b $U < g$). Transitions between regions $|r\rangle \leftrightarrow |p\rangle$, $|\tilde{r}\rangle \leftrightarrow |\tilde{p}\rangle$ lead to the change of average number of electrons only. At transitions $|r\rangle \leftrightarrow |\tilde{r}\rangle$ the flipping of pseudospin takes place, and at $|r\rangle \leftrightarrow |\tilde{p}\rangle$ ($r \neq p$) both processes occur.

The process of flipping of pseudospin at the crossing of H^* -line that defines the boundary of $|r\rangle \leftrightarrow |\tilde{r}\rangle$, is a phase transition. For the fixed value of μ the state $|r\rangle$ with $\eta = \frac{1}{2}$ exists at $h > 2H^* - \frac{J}{2}$, and state $|\tilde{r}\rangle$ with $\eta = -\frac{1}{2}$ - at $h > 2H^* + \frac{J}{2}$. Jump-like change of η between these two values, which corresponds to the first order phase transition, takes place at $h = 2H^*$. That's why, making substitution $H \rightarrow \frac{h}{2}$ one can consider the Fig. 5a and 5b as (h, μ) - phase diagrams at $T=0$, where H^* is a line of phase transitions.

We will consider now the case of non-zero temperature. Among all possible solutions $\eta = f(\theta, h, \mu)$ of equation (10), let us separate the

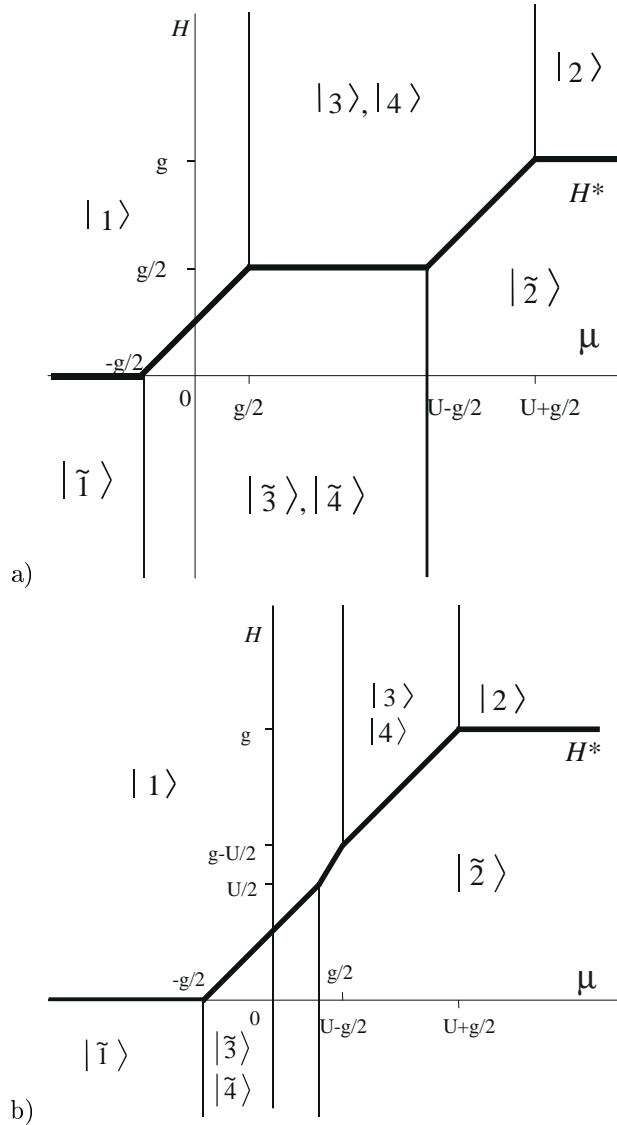


Figure 5. The ground state diagram (regime $\mu = const$). a) $U > g$; b) $U < g$

zero ones. In (θ, h) -plane they define the curves which are described by an equation

$$f(\theta, h; \mu) = 0, \quad (45)$$

where μ plays the role of some parameter. Function f has the following form

$$f = sh \left(\frac{\beta h}{2} \right) + e^{-\beta(U-2\mu)} sh\beta \left(\frac{h}{2} - g \right) + 2e^{\beta\mu} sh\beta \left(\frac{h}{2} - \frac{g}{2} \right) \quad (46)$$

From equation (45) one can get

$$h = \theta \ln \frac{\xi_1}{\xi_2}, \quad (47)$$

where

$$\begin{aligned} \xi_1 &= 1 + e^{-\beta(U-g-2\mu)} + 2e^{\beta(\frac{g}{2}+\mu)} \\ \xi_2 &= \xi_1|_{g \rightarrow -g} \end{aligned} \quad (48)$$

After a substitution of an expression for field h from (5.3) into equation (10) we will get an equation

$$\eta = \frac{1}{2} th \frac{\beta J \eta}{2}, \quad (49)$$

that defines the order parameter along the line $h = \theta \ln \frac{\xi_1}{\xi_2}$. Formula (49) has the standard form of molecular field equation. In addition to zero solution non-zero ones exist at $\theta < \theta_c = \frac{J}{4}$. One can make a conclusion that at the temperatures $\theta < \theta_c$ the relation (47) has a meaning of equation that describes the curve of phase equilibrium (first order phase transition curve), and temperature θ_c corresponds to the critical point. Critical value of h_c is given by expression

$$h_c = \frac{J}{4} \ln \frac{1 + e^{-\frac{4}{J}(U-g-2\mu)} + 2e^{\frac{4}{J}(\frac{g}{2}+\mu)}}{1 + e^{-\frac{4}{J}(U+g-2\mu)} + 2e^{-\frac{4}{J}(\frac{g}{2}-\mu)}} \quad (50)$$

The feature of the phase transition is that the curve of phase equilibrium generally is not parallel to the temperature axis. Particularly, at $g \gg J, U \gg J$

$$\begin{aligned} h_c &= 2\theta e^{\beta(\frac{g}{2}+\mu)} & \mu < -\frac{g}{2} \\ h_c &= \theta \ln 3 & \mu = -\frac{g}{2} \\ h_c &= 2g - \theta \ln 3 & \mu = U + \frac{g}{2} \\ h_c &= 2g - 2\theta e^{\beta(U+\frac{g}{2}-\mu)} & \mu > U + \frac{g}{2} \end{aligned} \quad (51)$$

The value $\mu = -\frac{U}{2}$ is an exception, at which $h_c = g$. At $\mu < \frac{U}{2}$ and $\mu > \frac{U}{2}$ the bents of coexistence curves are opposite.

The existence of a bent of the coexistence curve testifies the possibility of the first order phase transition at the change of temperature with a jump of order parameter η if the value of field h is within interval placed between $2H^*$ and h_c values.

With the help of expression (13), it is possible to find out the average electron concentration, which corresponds to the critical point at given value of chemical potential. Making substitution $\eta = 0$ and using the expression (50) for the critical field one can obtain

$$n_c = \nu(g) + \nu(-g), \quad (52)$$

where

$$\nu(g) = \frac{e^{-\frac{4}{T}(U+g-2\mu)} + e^{-\frac{4}{T}(\frac{g}{2}-\mu)}}{1 + e^{-\frac{4}{T}(U+g-2\mu)} + 2e^{-\frac{4}{T}(\frac{g}{2}-\mu)}} \quad (53)$$

Substitution $\frac{U}{2} - \mu \rightarrow \mu - \frac{U}{2}$ corresponds to the electron-hole transformation $n_c \rightarrow 2 - n_c$, which is in agreement with mentioned above symmetry of the model. At $\mu = \frac{U}{2}$ the critical concentration n_c is equal to unity.

At the temperatures below the critical value crossing the phase coexistence curve leads to the jump of electron concentration between values that correspond to phases, which are involved in phase separation (this corresponds to the break point on the dependence $\Omega(\mu)$). At the same time these values are points of binodal lines, which are determined according to the Maxwell rule from the plot of function $\mu(n)$. Illustrating samples of this are presented in Fig.6 and Fig.7. The plots presented are obtained using numerical calculations based on formulas (7), (10) and (13).

6. Conclusions.

The investigation performed shows that pseudospin-electron model with long-range interaction possesses some features, which differ it from the ordinary Ising model. They are:

- The possibility of the first order phase transition at the change of temperature and fixed value of field (regime $\mu = const$)
- Instability with respect to phase separation in the wide range of parameter h (regime $n = const$) with an appearance of regions with different electron concentration and different orientation of pseudospins.

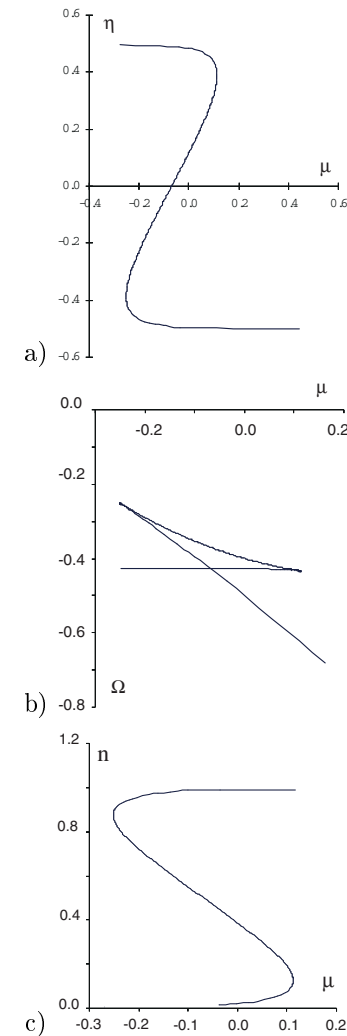


Figure 6. a) The μ dependence of $\langle S^z \rangle = \eta$ mean value. The parameter values: $h/J = 0.55$; $U/J = 1.5$; $g/J = 1$, $T/J = 0.1$. μ is given in dimensionless units: $\mu \rightarrow \mu/J$.

b) The μ dependence of thermodynamical potential Ω . The parameter values: $g/J = 1.0$, $U/J = 1.5$, $h/J = 0.55$, $T/J = 0.1$.

c) The μ dependence of concentration n . The parameter values: $h/J = 0.55$, $U/J = 1.5$, $g/J = 1.0$, $T/J = 0.1$.

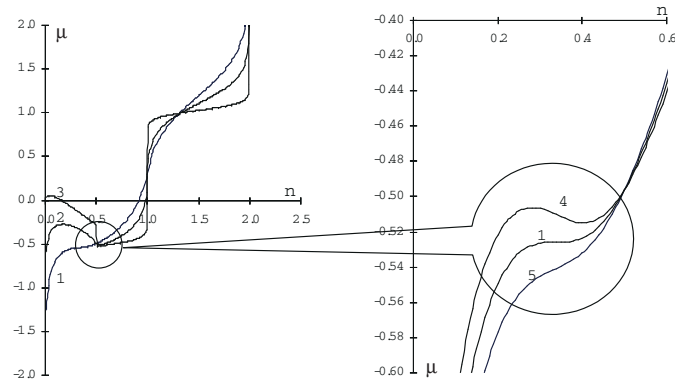


Figure 7. The n dependence of chemical potential μ . The parameter values: $g/J = 1.0$; $U/J = 1$; $h/J = 0.25$; [1 - $T/J = 0.25$, 2 - $T/J = 0.14$, 3 - $T/J = 0.03$, 4 - $T/J = 0.24$, 5 - $T/J = 0.26$]. μ is given in dimensionless units: $\mu \rightarrow \mu/J$.

The inclusion of electron transfer into consideration does not lead to any qualitative changes, because the contribution of the electron transfer into thermodynamics of the model is connected mainly with the formation of an additional interaction (besides the direct J_{ij} one) between pseudospins. The obtained results give the more substantiated interpretation of the behaviour of pair correlation function and dielectric susceptibility of the model in the case $t \neq 0$, $J = 0$ investigated in GRPA [6,8]. It is possible to conclude that the divergence of susceptibility $\chi_{ss}|_{\mu=const}$ and other related quantities at certain values of temperature and $h \sim g$ (at $U = \infty$) corresponds to the point of the high-temperature phase instability. The temperature of this instability is situated below the temperature of the first order phase transition that leads to the jump of $\langle S^z \rangle$. It is necessary to notice that thermodynamics of pseudospin-electron model in the frames of GRPA is studied not enough yet. This should be the subject of a separate investigation.

When the model is used for the description of the thermodynamics of oxygen subsystem in $YBa_2Cu_3O_{7-\delta}$ - crystals, the results of this work might be used as a basis for description of bistability phenomena in apex oxygen sublattices as well as for study of experimentally observed spatial nonuniformities and phase-separated states in monocrystalline specimens [9,10].

7. Acknowledgements

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ВЗАЄМОДІЄЮ МІЖ ПСЕВДСПІНАМИ

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