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Dynamics and thermodynamics of the model with local anharmonism in the case of absence of the electron Hubbard correlation.

II. The numerical research.

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Динаміка та термодинаміка моделі з локальним ангармонізмом у випадку відсутності електронної хаббардівської кореляції. II. Чисельне дослідження.

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Анотація. Проведено аналіз термодинамічних властивостей псевдоспін-електронної моделі у випадку відсутності електронної кореляції. Показано, що взаємодія електронів з псевдоспінами в режимі $\mu = \text{const}$ приводить до можливості фазового переходу першого роду при зміні температури із стрибком середнього значення псевдоспіна $\langle S^z \rangle$ і перебудовою електронного спектру. В режимі $n = \text{const}$ при певних значеннях параметрів має місце нестабільність щодо фазового розшарування в електронній підсистемі.

Dynamics and thermodynamics of the model with local anharmonism in the case of absence of the electron Hubbard correlation. II. The numerical research.

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Abstract. The analysis of the thermodynamic properties of the pseudospin-electron model in the case of absence of the electron correlation is performed. It is shown that interaction between the electron and pseudospin subsystems leads in the $\mu = \text{const}$ regime to the possibility of the first order phase transition at the temperature change with the jump of the pseudospin mean value $\langle S^z \rangle$ and reconstruction of the electron spectrum. In the regime $n = \text{const}$ an instability with respect to the phase separation in electron subsystem can take place for certain values of the model parameters.

1. Introduction.

The model under consideration takes into account the interaction of electrons with the local anharmonic mode of lattice vibrations. Such property is characteristic for the vibrations of the so-called apex oxygen ions O_{IV} along c -axis direction of the layered compounds of $YBa_2Cu_3O_7$ - type structure [1–3]. In the case of local double-well potential, the vibrational degrees of freedom can be presented by pseudospin variables. The Hamiltonian of the model, with the use of pseudospin variables for the description of anharmonic vibrations, has the following form [4].

$$H = \sum_i H_i + \sum_{ij\sigma} t_{ij} b_{i\sigma}^+ b_{j\sigma}, \quad (1)$$

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

where the single-site energy H_i includes Hubbard correlation U , interaction with anharmonic (pseudospin) mode (g - term), the energy of the tunnelling splitting (Ω - term) and energy of the anharmonic potential asymmetry (h - term); E_o defines the origin of energies of the single-electron states (for the case of grand canonical ensemble $E_o = -\mu$). The values $S^z = \pm 1/2$ correspond to the two possible positions of oxygen O_{IV} in the double-well potential. The second term in (1) describes electron transfer.

In the first part of this work [5] we have written the Hamiltonian of the model in the second quantized form (for the case $\Omega = 0$ and absence of the Hubbard correlation $U = 0$)

$$H = \sum_i \{ \varepsilon (n_{i\uparrow} + n_{i\downarrow}) + \tilde{\varepsilon} (\tilde{n}_{i\uparrow} + \tilde{n}_{i\downarrow}) - h S_i^z \} + \sum_{ij\sigma} t_{ij} (a_{i\sigma}^+ a_{j\sigma} + a_{i\sigma}^+ \tilde{a}_{j\sigma} + \tilde{a}_{i\sigma}^+ a_{j\sigma} + \tilde{a}_{i\sigma}^+ \tilde{a}_{j\sigma}) = H_o + H_{int}, \quad (3)$$

using the operators of the electron creation (annihilation) at the site with certain pseudospin orientation

$$\begin{aligned} a_{\sigma i} &= b_{\sigma i} (1/2 + S_i^z), & a_{\sigma i}^+ &= b_{\sigma i}^+ (1/2 + S_i^z), \\ \tilde{a}_{\sigma i} &= b_{\sigma i} (1/2 - S_i^z), & \tilde{a}_{\sigma i}^+ &= b_{\sigma i}^+ (1/2 - S_i^z). \end{aligned} \quad (4)$$

Here

$$\varepsilon = E_o + g/2, \quad \tilde{\varepsilon} = E_o - g/2, \quad (5)$$

are energies of the single-site states; H_o is the single-site (diagonal) term, H_{int} is the hopping terms.

The analytical calculation was performed by diagrammatic method in the mean field approximation [5]. Single-particle Green functions are taken in the Hubbard-I approximation. This corresponds to the omitting of the diagrams including semi-invariants of the higher than first order in the loop and also the connection of two loops by more than one semi-invariant.

Then the analytical equation for the mean value of pseudospin $\langle S^z \rangle$ was expressed in form

$$\langle S_i^z \rangle = \langle S_i^z \rangle_{MF} = \frac{1}{2} \tanh \left\{ \frac{\beta}{2} (h + \alpha_2 - \alpha_1) + \ln \frac{1 + e^{-\beta \varepsilon}}{1 + e^{-\beta \tilde{\varepsilon}}} \right\}. \quad (6)$$

Difference $\alpha_2 - \alpha_1$ in (6) corresponds to the internal effective self-consistent field acting on pseudospin

$$\alpha_2 - \alpha_1 = \frac{2}{N} \sum_{\vec{k}} t_{\vec{k}} \frac{\varepsilon - \tilde{\varepsilon}}{\varepsilon_I(t_{\vec{k}}) - \varepsilon_{II}(t_{\vec{k}})} \{ n(\varepsilon_{II}(t_{\vec{k}})) - n(\varepsilon_I(t_{\vec{k}})) \}, \quad (7)$$

$n(\varepsilon) = \frac{1}{1 + e^{\beta \varepsilon}}$ is Fermi distribution, $\varepsilon_{I,II}$ are energies of the single-electron excitations

$$\varepsilon_{I,II}(t_{\vec{k}}) = 1/2(2E_o + t_{\vec{k}}) \pm 1/2 \sqrt{g^2 + 4t_{\vec{k}} \langle S^z \rangle g + t_{\vec{k}}^2}. \quad (8)$$

Behaviour of the electron bands as function of the coupling constant is presented in Fig. 1. One can see that the gap in spectrum always exists. The widths of subbands depends on the mean value of pseudospin and in the case of strong coupling ($g \gg W$) subbands halfwidth is equal to $W(\frac{1}{2} \pm \langle S^z \rangle)$.

The diagram series for mean value $\langle n_i \rangle$ (using the perturbation theory, Wick's theorem and expansion in semi-invariants) can be presented in the form

$$\langle n_i \rangle = \blacksquare = \ominus - \text{diagram 1} + \frac{1}{2!} \text{diagram 2} - \frac{1}{3!} \text{diagram 3} + \dots + \sum_{\alpha} \text{diagram 4}, \quad (9)$$

with the analytical expression

$$\langle n \rangle = \frac{2}{N} \sum_{\vec{k}} \{ n(\varepsilon_I(t_{\vec{k}})) + n(\varepsilon_{II}(t_{\vec{k}})) \} - 2 \langle P^+ \rangle n(\tilde{\varepsilon}) - 2 \langle P^- \rangle n(\varepsilon). \quad (10)$$

The diagram series for the thermodynamical potential and the corresponding analytical expression are following

$$\beta\Delta\Omega = -\ln Z + \ln Z_o, \quad Z = Sp(e^{-\beta H}), \quad Z_o = Sp(e^{-\beta H_o}),$$

$$\beta\Delta\Omega = \left(\frac{1}{2} \text{diagram} + \frac{1}{3} \text{diagram} + \frac{1}{4} \text{diagram} + \dots \right) + \dots - \dots$$

$$\Delta\Omega = -\frac{2}{N\beta} \sum_{\vec{k}} \ln \frac{\cosh \frac{\beta}{2} \varepsilon_I(t_{\vec{k}}) \cosh \frac{\beta}{2} \varepsilon_{II}(t_{\vec{k}})}{(\cosh \frac{\beta}{2} \varepsilon) (\cosh \frac{\beta}{2} \tilde{\varepsilon})} \quad (12)$$

$$-\frac{1}{\beta} \ln \cosh \left\{ \frac{\beta}{2} (h + \alpha_2 - \alpha_1) + \ln \frac{1 + e^{-\beta\varepsilon}}{1 + e^{-\beta\tilde{\varepsilon}}} \right\} +$$

$$+\frac{1}{\beta} \ln \cosh \left\{ \frac{\beta}{2} h + \ln \frac{1 + e^{-\beta\varepsilon}}{1 + e^{-\beta\tilde{\varepsilon}}} \right\} + \langle S^z \rangle (\alpha_2 - \alpha_1).$$

We would like to remind, also, the diagram equation and analytical solution for the pseudospin correlator

$$\text{diagram} = \text{diagram} - \sum_{\alpha, \beta} \text{diagram} \quad (13)$$

$$\langle S^z S^z \rangle_{\vec{q}} = \frac{1/4 - \langle S^z \rangle^2}{1 + \sum_{\alpha, \beta} (-1)^{\alpha+\beta} \boxed{\Pi}_{\vec{q}}^{\alpha, \beta} \left(\frac{1}{4} - \langle S^z \rangle^2 \right)}, \quad (14)$$

where

$$\sum_{\alpha, \beta} (-1)^{\alpha+\beta} \boxed{\Pi}_{\vec{q}}^{\alpha, \beta} = \frac{2\beta}{N} \sum_{\vec{k}} \frac{t_{\vec{k}} t_{\vec{k}+\vec{q}} (\varepsilon - \tilde{\varepsilon})^2}{[\varepsilon_I(t_{\vec{k}}) - \varepsilon_{II}(t_{\vec{k}})] [\varepsilon_I(t_{\vec{k}+\vec{q}}) - \varepsilon_{II}(t_{\vec{k}+\vec{q}})]} \times$$

$$\times \left\{ \frac{n[\varepsilon_I(t_{\vec{k}})] - n[\varepsilon_I(t_{\vec{k}+\vec{q}})]}{\varepsilon_I(t_{\vec{k}}) - \varepsilon_I(t_{\vec{k}+\vec{q}})} + \frac{n[\varepsilon_{II}(t_{\vec{k}})] - n[\varepsilon_{II}(t_{\vec{k}+\vec{q}})]}{\varepsilon_{II}(t_{\vec{k}}) - \varepsilon_{II}(t_{\vec{k}+\vec{q}})} - \right. \quad (15)$$

$$\left. - \frac{n[\varepsilon_I(t_{\vec{k}})] - n[\varepsilon_{II}(t_{\vec{k}+\vec{q}})]}{\varepsilon_I(t_{\vec{k}}) - \varepsilon_{II}(t_{\vec{k}+\vec{q}})} - \frac{n[\varepsilon_{II}(t_{\vec{k}})] - n[\varepsilon_I(t_{\vec{k}+\vec{q}})]}{\varepsilon_{II}(t_{\vec{k}}) - \varepsilon_I(t_{\vec{k}+\vec{q}})} \right\}.$$

Our correlator is different from zero only in the static case. This is due to the fact that operator S^z commutes with Hamiltonian being the integral of motion.

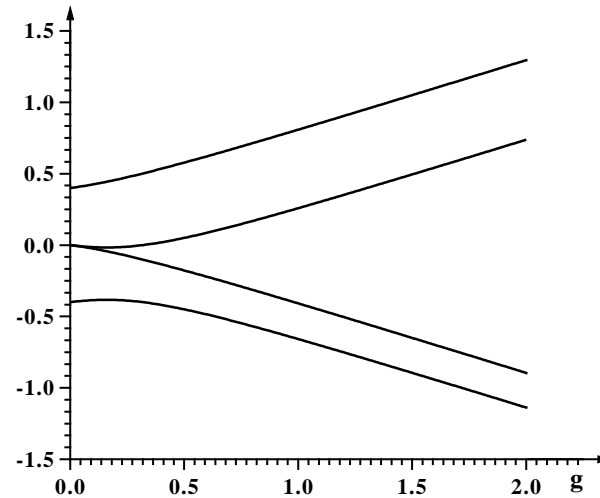


Figure 1. Electron bands boundaries ($W = 0.4$, $\langle S^z \rangle = 0.2$).

2. The numerical research in $\mu=\text{const}$ regime.

In investigation of the equilibrium conditions we shall separate two regimes: $\mu=\text{const}$ and $n=\text{const}$. The equilibrium is defined for the first regime by the minimum of thermodynamical potential: $\left(\frac{\partial \Omega}{\partial \langle S^z \rangle} \right)_{T, \mu, h} = 0$.

The $\mu=\text{const}$ regime corresponds to the case when the charge redistribution between conducting sheets CuO_2 and other structural elements (charge reservoir, e.g. nonstoichiometric in oxygen CuO chains in YBaCuO type structures) is allowed.

The dependences of order parameter $\langle S^z \rangle$ on field h and temperature T , at the constant value of chemical potential, are determined by equation (6). All integrals in (6) can be calculated analytically at zero temperature (below, all calculations will be performed for rectangular density of states, but we would like to remark that similar behaviour we can obtain in the case of semi-elliptic density of states).

We shall present all our results for the case of zero temperature as well as for the case of non-zero temperature.

The phase diagrams $\mu - h$ which indicate stability regions for states with $\langle S^z \rangle = \pm \frac{1}{2}$ are shown in Fig. 2 for $g \gg W$.

One can see two regions of the μ and h values where the states with $\langle S^z \rangle = \frac{1}{2}$ and $\langle S^z \rangle = -\frac{1}{2}$ are both stable. In the vicinity of these regions the phase transitions of the first order with the change of the longitudinal field h and/or chemical potential μ take place and they are shown by thick lines on phase diagrams Fig. 2.

The field dependencies of $\langle S^z \rangle$ and Ω near the phase transition point are presented in Figs. 3, 4. Their behaviour in the cases of $T = 0$ and $T \neq 0$ with the change of chemical potential is similar: S - like for mean value of pseudospin and the fish tail form for thermodynamical potential.

In the $\mu=\text{const}$ regime chemical potential can be situated in the electron bands or out of them with the change of field h (Fig. 5 dashed line) and in the vicinity of the phase transition point this results in the rapid change of the electron concentration (Fig. 6 dotted lines) due to the charge transfer from/to the reservoir (CuO planes). The widths of the electron subbands depend on the mean value of pseudospin which results in the presented above behaviours.

The phase transition point is presented by the inflection point on the dependence $\Omega(h)$ (Fig. 4 dotted lines). At the same time this value is determined according to the Maxwell rule from the plot of function $S^z(h)$.

With the temperature increase the region of the phase coexistence narrows and the corresponding phase diagram $T_c - h$ is shown in Fig. 7. The tilt of the coexistence curve testifies the possibility of the first order phase transition at the change of temperature with the jump of pseudospin mean value. (The phase diagram $T_c - \mu$ has a similar form). The existence of the shifted and tilted curve as result of the local pseudospin-electron interaction was obtained for the first time in [6] for pseudospin-

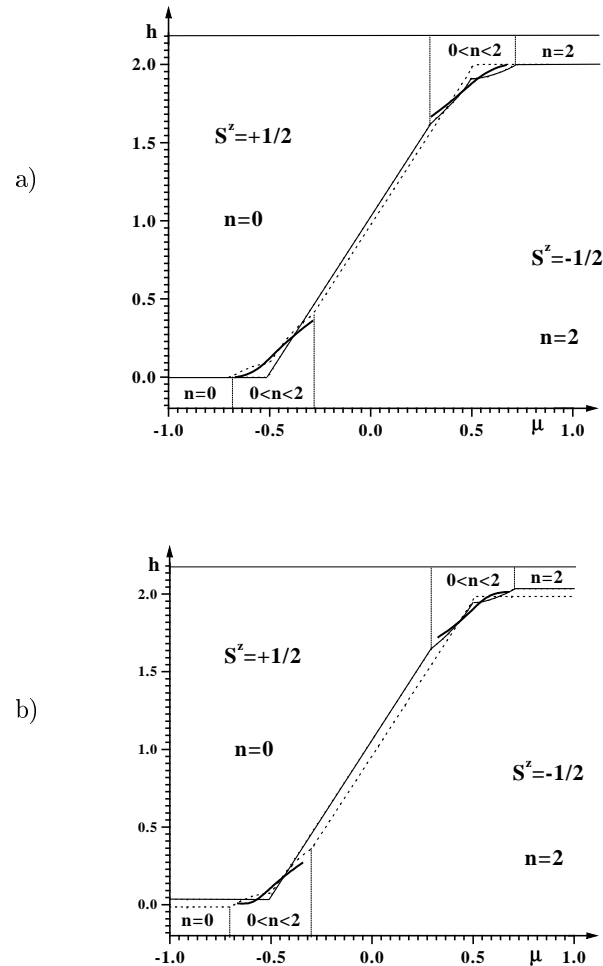


Figure 2. Phase diagram $\mu - h$. Dotted and thin solid lines surround regions with $S^z = \pm \frac{1}{2}$, respectively. Thick solid line indicate the first order phase transition points. a) the case of zero temperature; b) $T = 0.002$ ($W = 0.2$; $g = 1$).

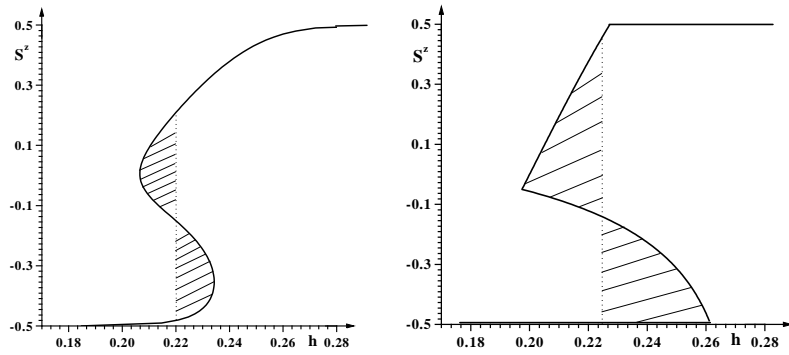


Figure 3. Field dependency of $\langle S^z \rangle$ ($W = 0.2$, $\mu = -0.4$, $g = 1.0$) for $\mu = \text{const}$ regime; $T = 0.01$ and $T = 0$.

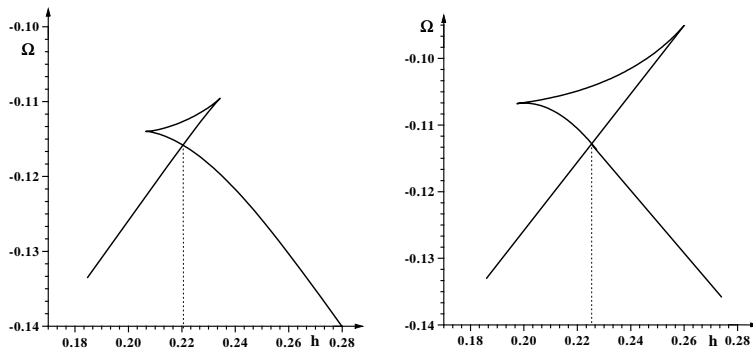


Figure 4. Field dependency of thermodynamical potential ($W = 0.2$, $\mu = -0.4$, $g = 1.0$); $T = 0.01$ and $T = 0$.

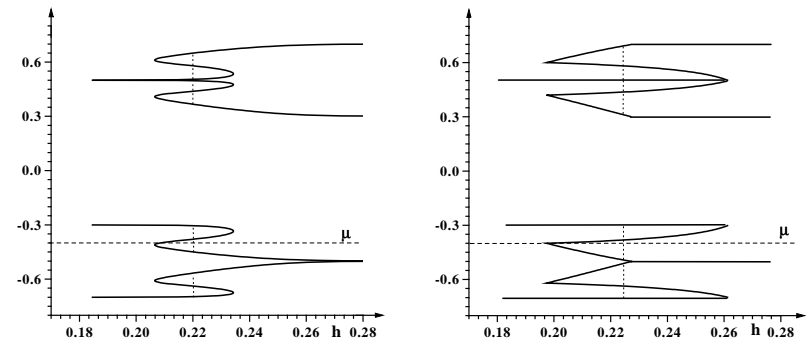


Figure 5. Field dependency of electron bands boundaries ($W = 0.2$, $\mu = -0.4$, $g = 1.0$); $T = 0.01$ and $T = 0$.

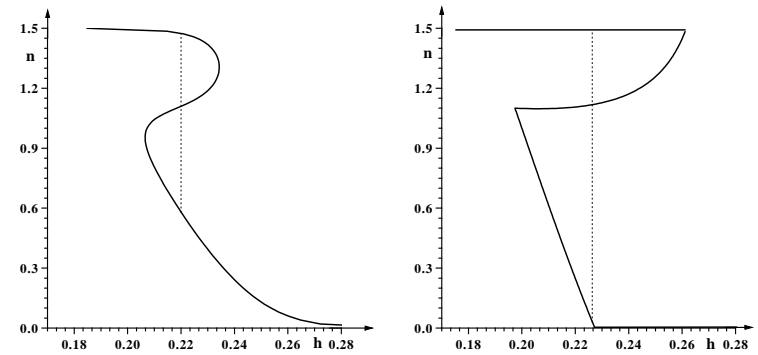


Figure 6. Field dependency of electron concentration ($W = 0.2$, $\mu = -0.4$, $g = 1.0$); $T = 0.01$ and $T = 0$.

electron model with direct interaction between pseudospins.

The analysis of the thermodynamical potential behaviour with the temperature increase (Fig. 8) shows that the lowest value of $\Omega(T)$ corresponds to the jump of the mean value of pseudospin (Fig. 9 dotted lines) from the branch which corresponds to the low temperature phase to the branch of the high temperature phase. The analysis of the $\langle S^z S^z \rangle$ behaviour with the temperature decrease shows that the high temperature phase is stable up to zero temperature. This means that vertical line on the T_c-h phase diagram only once cross the boundary of the phase stability.

In figures the case when the chemical potential is places in the lower subband is presented. There is no any specific behaviour when chemical potential is placed out of bands. And if chemical potential is placed in upper subband our results transform according to the internal symmetry of the Hamiltonian:

$$\mu \rightarrow -\mu, \quad h \rightarrow 2g - h, \quad n \rightarrow 2 - n, \quad S^z \rightarrow -S^z. \quad (16)$$

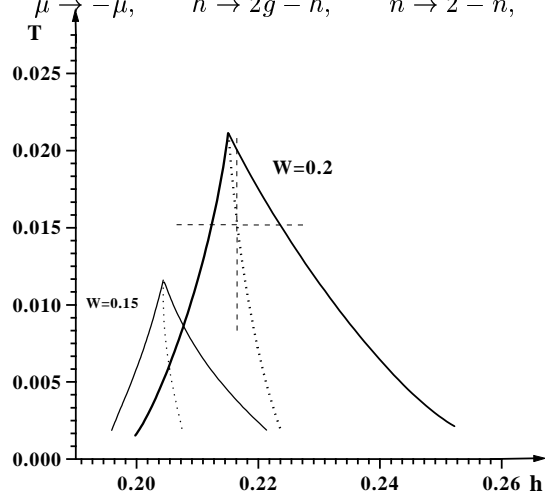


Figure 7. Phase diagram $T_c - h$ ($g = 1$, $\mu = -0.4$).

3. The numerical research in $n=\text{const}$ regime.

In the regime of the fixed value of electron concentration the first order phase transition with the jump of pseudospin mean value accompanied

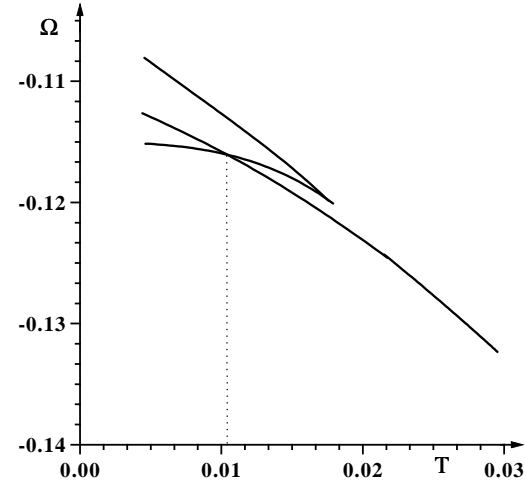


Figure 8. Temperature dependence of thermodynamical potential ($W = 0.2$, $h = 0.22$, $\mu = -0.4$, $g = 1$).

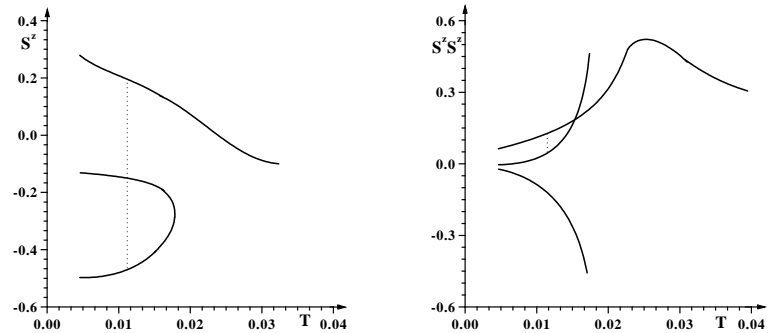


Figure 9. Dependence of the mean value of pseudospin and pseudospin-pseudospin correlation function on the temperature ($W = 0.2$, $h = 0.22$, $\mu = -0.4$, $g = 1$).

by the change of electron concentration transforms into the phase separation.

The dependence of the mean value of particle number (or electron concentration) on chemical potential is one of the factors that determines the thermodynamically stable states of system. One can see the regions with $d\mu/dn \leq 0$ where states with homogenous distribution of particle are unstable, which correspond the phase separation into the regions with different electron concentrations and pseudospin mean values (Fig. 10 and Fig. 11).

In the $n=\text{const}$ regime the equilibrium condition is determined by the minimum of free energy $F = \Omega + \mu N$. In the phase separated region free energy as a function of n deflects up (Fig. 11) and concentrations of the separated phases are determined by the tangent line touch points (these points, also, are points of binodal lines , which are determined according to the Maxwell rule from the function $\mu(n)$ see. Fig. 10).

Resulting phase diagram $T-n$ is shown in Fig. 12.

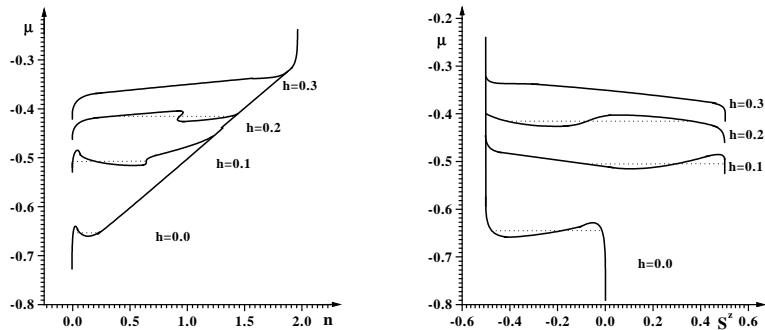


Figure 10. Dependence of the chemical potential μ on the electron concentration n and pseudospin mean-value $\langle S^z \rangle$ for different h values ($g = 1$, $W = 0.2$, $T = 0.01$).

4. Conclusions.

The investigation of the pseudospin–electron model in the case of absence of the electron correlation was performed in the mean field approximation using Hubbard–I approximation for the calculation of the single-particle Green function. In the first part of this paper we performed

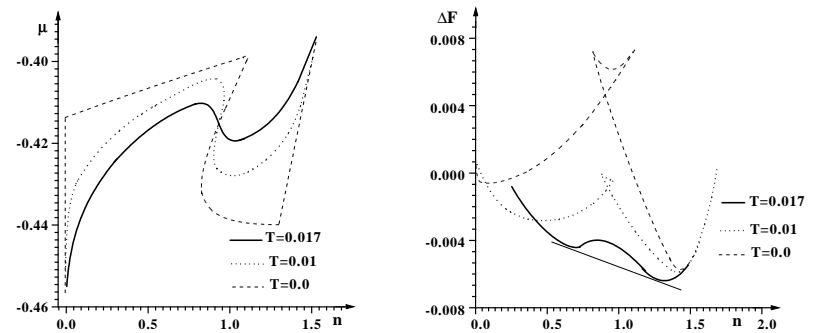


Figure 11. Dependence of the chemical potential μ on the electron concentration n and deviation of free energy from linear dependence for different T values ($g = 1$, $W = 0.2$, $h = 0.2$).

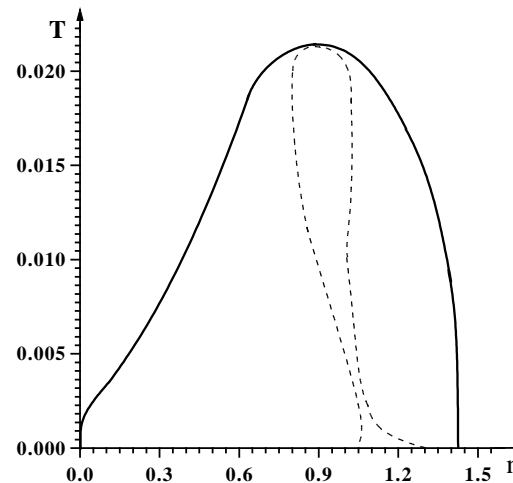


Figure 12. Phase diagram $T - n$ ($g = 1$, $W = 0.2$, $h = 0.2$) for phase separated state: solid line – binodal points, dashed line – spinodal points.

the analytical consideration for our model and all quantities have been obtained in the framework of one approximation.

As a result of numerical investigations we obtain:

1) the gap in the electron spectrum always exist (with the change of mean value of pseudospin the reconstruction of electron spectrum is realized);

2) the possibility of the first order phase transition with the change of the longitudinal field h (in consequence of this the S -like behaviour for mean value of pseudospin with the jump in the phase transition point (that corresponds to the inflected point on the dependence $\Omega(h)$) is obtained and in this point the concentration redistribute rapidly between the conducting sheets CuO_2 and charge reservoir (CuO planes) in YBaCuO type structures);

3) the phase coexistence curve is tilted from vertical line, therefore the possibility of the first order phase transition with the temperature change exists;

4) the high temperature phase is stable in the whole region of temperature (Fig. 9);

5) in the regime $n=\text{const}$ we have the regions with $d\mu/dn < 0$, which corresponds to the phase separation with the appearance of regions with different electron concentrations and different orientation of pseudospins.

References

1. Cohen R.E., Pickett W.E., Krakauer H. Theoretical determination of strong electron-phonon coupling in $\text{YBa}_2\text{Cu}_3\text{O}_7$ // *Phys. Rev. Lett.* – 1990. – **64**, N 21. – P.2575–2578.
2. Maruyama H., Ishii T., Bamba N., Maeda H., Koizumi A., Yoshikawa Y., Yamazaki H. Temperature dependence of the EXAFS spectrum in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ compounds // *Physica C*. – 1989. – **160**, N 5/6. – P. 524.
3. Conradson S.D., Raistrick I.D. The axial oxygen atom and superconductivity in $\text{YBa}_2\text{Cu}_3\text{O}_7$ // *Science*. – 1989. – **243**, N 4896. – P. 1340.
4. Stasyuk I.V., Shvaika A.M. Dielectric properties and electron spectrum of the Muller model in the HTSC theory. // *Acta Physica Polonica A*, **84**, 293 (1993).
5. I.V.Stasyuk, A.M.Shvaika, K.V.Tabunshchyk. Dynamics and thermodynamics of the model with local anharmonism in the case of absence of the electron Hubbard correlation.
I. The analytical consideration. // Preprint ICMP-98-21E – P. 1–18.

6. Stasyuk I.V., Havrylyuk Yu. Phase transitions in pseudospin-electron model with direct interaction between pseudospins. // Preprint ICMP-98-18E – P. 1–20.
7. Stasyuk I.V., Shvaika A.M. Pseudospin-Electron Model in Large Dimensions. // Preprint ICMP-98-20E – P. 1–16.
8. Stasyuk I.V., Shvaika A.M. Dielectric instability and local anharmonic model in the theory of high- T_c superconductivity. // *Acta Physica Polonica A*, **85**, 363 (1994).
9. Stasyuk I.V., Shvaika A.M. Dielectric instability and vibronic-type spectrum of local anharmonic model of high- T_c superconductors. // *Ferroelectrics*, **192**, – P. 1–10 (1997).
10. Muller K.A. // *Phase transition*. – 1988. – (Special issue).
11. Bishop A.R., Martin R.L., Muller K.A., Tesanovic Z. Superconductivity in oxides: Toward a unified picture // *Z. Phys. B – Condensed Matter*. – 1989. – **76**, N 1. – P. 17–24.
12. Hirsch J.E., Tang S. Effective interactions in an oxygen-hole metal // *Phys. Rev. B*. – 1989. – **40**, N 4. – P. 2179–2186.
13. Frick M., von der Linden W., Morgenstern I., Raedt H. Local anharmonic vibrations, strong correlations and superconductivity: A quantum simulation study // *Z. Phys. B – Condensed Matter*. – 1990. – **81**, N 2. – P. 327–335.
14. Izyumov Yu.A., Letfulov B.M. // Spin fluctuations and superconducting states in the Hubbard model with a strong Coulomb repulsion. *J. Phys.: Condens. Matter*, **3**, 5373 (1991).

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ДИНАМІКА ТА ТЕРМОДИНАМІКА МОДЕЛІ З ЛОКАЛЬНИМ
АНГАРМОНІЗМОМ У ВИПАДКУ ВІДСУТНОСТІ ЕЛЕКТРОННОЇ
ХАББАРДІВСЬКОЇ КОРЕЛЯЦІЇ. II. ЧИСЕЛЬНЕ ДОСЛІДЖЕННЯ.

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