Національна академія наук України

ІНСТИТУТ ФІЗИКИ КОНДЕНСОВАНИХ СИСТЕМ

ICMP–98–21E

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.

ЛЬВІВ

УДК: 538.945

PACS: 71.10.Fd, 71.38.+i, 77.80.Bh, 63.20.Ry

Динаміка та термодинаміка моделі з локальним ангармонізмом у випадку відсутності електронної хаббардівської кореляції. I. Аналітичний розгляд.

І.В.Стасюк, А.М.Швайка, К.В.Табунщик

Анотація. В роботі досліджується динаміка та термодинаміка моделі з локальним ангармонізмом у випадку відсутності електронної (хаббардівської) кореляції. Розраховані часові кореляційні функції, середні значення операторів псевдоспіну і кількості частинок та термодинамічний потенціал. Разрахунок проведений діаграмним методом у наближенні середнього поля. Одночастинкові функції Гріна взяті у наближенні Хаббард–I.

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

I.V.Stasyuk, A.M.Shvaika, K.V.Tabunshchyk

Abstract. Dynamics and thermodynamics of the model with local anharmonism in the case of absence of the electron (Hubbard) correlation is investigated in the present work. The correlation functions, mean values of pseudospin and particle number as well as the thermodynamical potential are calculated. The calculation is performed by diagrammatic method in the mean field approximation. Single–particle Green functions are taken in the Hubbard–I approximation.

1. Introduction.

The model considering the interaction of electrons with the local anharmonic mode of lattice vibrations is used in the last years in the theory of high–temperature superconducting crystals. Particularly, 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 (see, [1-3]). An important role of the apex oxygen and its anharmonic vibrations in the phase transition into superconducting state has been already mentioned [4,5] and the possible connection between the superconductivity and lattice instability of ferroelectric type in high–T_c superconducting compounds is under discussion [6,7]. In the case of local double–well potential, the vibrational degrees of freedom can be presented by pseudospin variables. The Hamiltonian of the derived in this way pseudospin–electron model has the following form [8]

$$H = \sum_i H_i + \sum_{ij\sigma} t_{ij} b^+_{i\sigma} b_{j\sigma} \ , \tag{1.1}$$

and includes besides the terms describing electron transfer ($\sim t_{ij}$), the electron correlation (U–term), interaction with anharmonic mode (g–term), the energy of the tunnelling splitting (Ω–term) and energy of the anharmonic potential asymmetry (h–term) in the single–site part

$$H_i = U n_{i\uparrow} n_{i\downarrow} + E_o(n_{i\uparrow} + n_{i\downarrow}) + g(n_{i\uparrow} + n_{i\downarrow}) S^z_i - \Omega S^x_i - h S^z_i \ . \tag{1.2}$$

Here, E_o gives the origin for energies of the electron states at lattice site ($E_o = -\mu$).

In this paper, which consists of two parts, our aim is to obtain the expressions for correlation functions which determine the dielectric susceptibility, mean values of pseudospin and particle number operators as well as the thermodynamical potential in the case $\Omega = 0$ and absence of the Hubbard correlation $U = 0$.

In the second part of the paper we shell perform numerical calculations for the analytical expressions obtained in the first part. We shall investigate values of pseudospin and particle number operators with the change of the asymmetry parameter h ($T = const$) or with the change of temperature T ($h = const$) for the cases of the fixed chemical potential value (regime $\mu = const$) and constant mean value particle number. We shell present also some result for the case $T = 0$.

2. Hamiltonian and initial relations.

We shall write the Hamiltonian of the model and the operators which correspond to physical quantities in the second quantized form using the operators of the electron creation (annihilation) at the site with the certain pseudospin orientation

$$\begin{array}{ll} a_{\sigma i} = b_{\sigma i}(1/2 + S^z_i) \ , & a^+_{\sigma i} = b^+_{\sigma i}(1/2 + S^z_i) \ , \\ \tilde{a}_{\sigma i} = b_{\sigma i}(1/2 - S^z_i) \ , & \tilde{a}^+_{\sigma i} = b^+_{\sigma i}(1/2 - S^z_i) \ . \end{array} \tag{2.1}$$

Then we obtain the following expression for the initial Hamiltonian

$$\begin{aligned} H = & \sum_i \{\varepsilon(n_{i\uparrow} + n_{i\downarrow}) + \tilde{\varepsilon}(\tilde{n}_{i\uparrow} + \tilde{n}_{i\downarrow}) - h S^z_i\} + \\ & + \sum_{ij\sigma} t_{ij}(a^+_{i\sigma} a_{j\sigma} + a^+_{i\sigma} \tilde{a}_{j\sigma} + \tilde{a}^+_{i\sigma} a_{j\sigma} + \tilde{a}^+_{i\sigma} \tilde{a}_{j\sigma}) \ = \\ & = H_o + H_{int}, \end{aligned} \tag{2.2}$$

where

$$\varepsilon = E_o + g/2 \, , \, \tilde{\varepsilon} = E_o - g/2 \, , \tag{2.3}$$

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

The introduced operators satisfy following commutation rules

$$\begin{array}{ll} \{\tilde{a}^+_{i\sigma}, \tilde{a}_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}(1/2 - S^z_i) \ , & \{\tilde{a}^+_{i\sigma}, a_{j\sigma'}\} = 0 \ , \\ \{a^+_{i\sigma}, a_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}(1/2 + S^z_i) \ , & \{a^+_{i\sigma}, \tilde{a}_{j\sigma'}\} = 0 \ . \end{array} \tag{2.4}$$

In order to calculate pseudospin mean values we shall use the standard representation of the statistical operator in form

$$e^{-\beta H} = e^{-\beta H_o} \hat{\sigma}(\beta) \, , \tag{2.5}$$

$$\hat{\sigma}(\beta) = T_\tau \exp\left\{ - \int_0^\beta H_{int}(\tau) d\tau \right\} \ . \tag{2.6}$$

Which gives the following expressions for $\langle S^z_l \rangle$

$$\langle S^z_l \rangle = \frac{1}{\langle \hat{\sigma}(\beta) \rangle_o} \langle S^z_l \hat{\sigma}(\beta) \rangle_o = \langle S^z_l \hat{\sigma}(\beta) \rangle^c_o \, . \tag{2.7}$$

Here, the operators are given in the interaction representation

$$A(\tau) = e^{\tau H_o} A e^{-\tau H_o} \, ; \tag{2.8}$$

the averaging $\langle \ldots \rangle_o$ is performed over the statistical distribution with Hamiltonian H_o, and symbol $\langle \ldots \rangle^c_o$ denotes the keeping of the connected diagrams.

3. Perturbation theory for pseudospin mean values and diagram technique.

The expansion of the exponent in (2.6) in powers of H_{int} (2.2) leads, after the substitution in equation (2.7), to the expression that has the form of the sum of infinite series with the terms presented by the averages of the T–products of the electron creation (annihilation) operators at the site with the certain pseudospin orientation in the interaction representation. The evaluation of such averages can be performed using Wick's theorem.

In our case this theorem has some differences from the standart formulation. Namelly, result of each pairing of operators (2.1) contains an operator factors, i.e.

$$\overleftarrow{a_i(\tau')a_o^+(\tau)} = \hat{g}(\tau'-\tau)\delta_{io}P_i^+, \quad \overleftarrow{\tilde{a}_i(\tau')\tilde{a}_o^+(\tau)} = \tilde{g}(\tau'-\tau)\delta_{io}P_i^-, \tag{3.1}$$

$$\overrightarrow{a_o^+(\tau)a_i(\tau')} = -\hat{g}(\tau'-\tau)\delta_{io}P_i^+, \quad \overrightarrow{\tilde{a}_o^+(\tau)\tilde{a}_i(\tau')} = -\tilde{g}(\tau'-\tau)\delta_{io}P_i^-.$$

Finally, this gives the possibility to express result in term of the products of nonperturbated Green functions

$$\hat{g}_{io}(\tau-\tau') = \frac{\langle T_\tau a_i(\tau)a_o^+(\tau')\rangle_o}{\langle\{a_i a_o^+\}\rangle_o} = e^{\varepsilon(\tau'-\tau)}\delta_{oi}\begin{cases}\frac{1}{1+e^{-\beta\varepsilon}} & :\ \tau>\tau',\\ \frac{-1}{1+e^{\beta\varepsilon}} & :\ \tau'>\tau,\end{cases} \tag{3.2}$$

$$\tilde{g}_{io}(\tau-\tau') = \frac{\langle T_\tau \tilde{a}_i(\tau)\tilde{a}_o^+(\tau')\rangle_o}{\langle\{\tilde{a}_i\tilde{a}_o^+\}\rangle_o} = e^{\tilde{\varepsilon}(\tau'-\tau)}\delta_{oi}\begin{cases}\frac{1}{1+e^{-\beta\tilde{\varepsilon}}} & :\ \tau>\tau',\\ \frac{-1}{1+e^{\beta\tilde{\varepsilon}}} & :\ \tau'>\tau,\end{cases}$$

$$\tilde{g}_{io}(\tau-\tau') = \tilde{g}(\tau-\tau')\delta_{io}\,, \quad \hat{g}_{io}(\tau-\tau') = \hat{g}(\tau-\tau')\delta_{io}\,,$$

and averages of the certain number of the projection operators

$$P_i^+ = \frac{1}{2} + S_i^z\,, \qquad P_i^- = \frac{1}{2} - S_i^z. \tag{3.3}$$

Let us demonstrate this procedure for the case of evaluation of $\langle S_l^z\rangle$, for one of the terms which appear in the fourth order of the perturbation theory

$$\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \int_0^\beta d\tau_4 \sum_{ij i_1 j_1} \sum_{i_2 j_2 i_3 j_3} t_{ij}t_{i_1 j_1}t_{i_2 j_2}t_{i_3 j_3} \times \tag{3.4}$$
$$\times\langle T_\tau S_l^z a_i^+(\tau_1)a_j(\tau_1)\tilde{a}_{i_1}^+(\tau_2)a_{j_1}(\tau_2)a_{i_2}^+(\tau_3)\tilde{a}_{j_2}(\tau_3)a_{i_3}^+(\tau_4)a_{j_3}(\tau_4)\rangle_o\,.$$

The stepwise pairing of the certain operator with the other ones gives the possibility to reduce expression (3.4) to the sum of the averages of the smaller number of operators

$$\langle T_\tau S_l^z a_i^+(\tau_1)a_j(\tau_1)\tilde{a}_{i_1}^+(\tau_2)a_{j_1}(\tau_2)a_{i_2}^+(\tau_3)\tilde{a}_{j_2}(\tau_3)a_{i_3}^+(\tau_4)a_{j_3}(\tau_4)\rangle_o =$$

$$= \langle T_\tau S_l^z\ \overbrace{a_i^+(\tau_1)a_j(\tau_1)\tilde{a}_{i_1}^+(\tau_2)a_{j_1}(\tau_2)a_{i_2}^+(\tau_3)\tilde{a}_{j_2}(\tau_3)a_{i_3}^+(\tau_4)}a_{j_3}(\tau_4)\rangle_o +$$

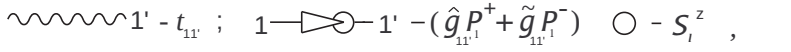
$$+\langle T_\tau S_l^z\ \overbrace{a_i^+(\tau_1)a_j(\tau_1)\tilde{a}_{i_1}^+(\tau_2)}a_{j_1}(\tau_2)\ a_{i_2}^+(\tau_3)\tilde{a}_{j_2}(\tau_3)a_{i_3}^+(\tau_4)a_{j_3}(\tau_4)\rangle_o =$$

$$= -\hat{g}_{ij_3}(\tau_1-\tau_4)\langle T_\tau S_l^z P_{j_3}^+ a_j(\tau_1)\tilde{a}_{i_1}^+(\tau_2)a_{j_1}(\tau_2)a_{i_2}^+(\tau_3)\tilde{a}_{j_2}(\tau_3)a_{i_3}^+(\tau_4)\rangle_o - \tag{3.5}$$
$$-\hat{g}_{ij_1}(\tau_1-\tau_2)\langle T_\tau S_l^z P_{j_1}^+ a_j(\tau_1)\tilde{a}_{i_1}^+(\tau_2)a_{i_2}^+(\tau_3)\tilde{a}_{j_2}(\tau_3)a_{i_3}^+(\tau_4)a_{j_2}(\tau_3)\rangle_o\,.$$

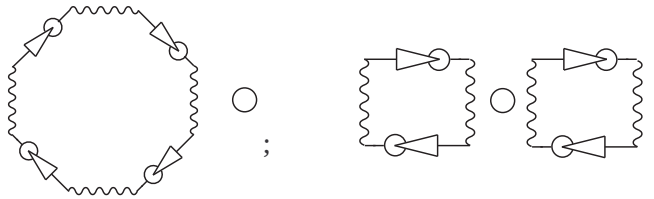
The successive applications of the pairing procedure for (3.5) leads, finally, to

$$-\hat{g}_{ij_1}(\tau_1-\tau_2)\tilde{g}_{i_1 j_2}(\tau_2-\tau_3)\hat{g}_{i_3 j}(\tau_4-\tau_1)\hat{g}_{i_2 j_1}(\tau_3-\tau_2)\langle T_\tau S_l^z P_j^+ P_{j_1}^+ P_{j_2}^- P_{j_3}^+\rangle_o -$$
$$-\hat{g}_{ij_3}(\tau_1-\tau_4)\tilde{g}_{i_1 j_2}(\tau_2-\tau_3)\hat{g}_{i_2 j}(\tau_3-\tau_1)\hat{g}_{i_3 j_1}(\tau_4-\tau_2)\langle T_\tau S_l^z P_j^+ P_{j_1}^+ P_{j_2}^- P_{j_3}^+\rangle_o +$$
$$+\hat{g}_{ij_3}(\tau_1-\tau_4)\tilde{g}_{i_1 j_2}(\tau_2-\tau_3)\hat{g}_{i_2 j_1}(\tau_3-\tau_2)\hat{g}_{i_3 j}(\tau_4-\tau_1)\langle T_\tau S_l^z P_j^+ P_{j_1}^+ P_{j_2}^- P_{j_3}^+\rangle_o\,. \tag{3.6}$$

We introduce the diagrammatic notations

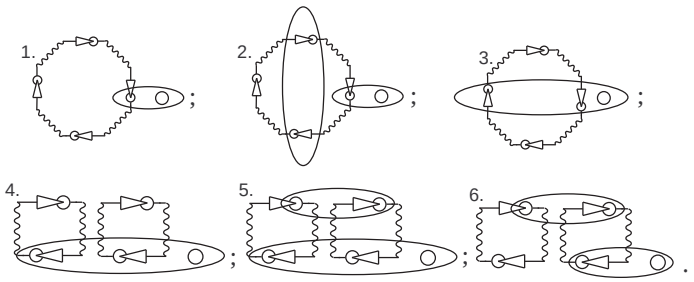


and diagrams



correspond to the expression (3.6).

The expansion of (3.6) in semi–invariants leads to the multiplication of diagrams (semi–invariants are represented by the ovals surrounding corresponding vertices with diagonal operators and contain the δ–symbol on site indexes). For example,



We shall neglect diagrams of types 2, 3, 5 i.e. the types including semi–invariants of the higher than first order in the loop (this means that chain fragments form the single–electron Green functions in the Hubbard–I approximation) and also the connection of two loops by more than one semi–invariant (this approximation means that selfconsistent field is taken into account in the zero approximation).

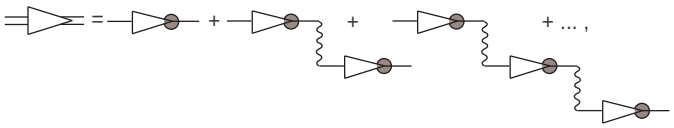
Let us proceed to the momentum–frequency representation in the expressions for the Green functions determined on finite interval $0<\tau<\beta$ when they can be expanded in Fourier series with discrete frequencies

$$\hat{g}(\tau) = \frac{1}{\beta}\sum_n e^{i\omega_n\tau} g(\omega_n);$$

$$\tilde{g}(\tau) = \frac{1}{\beta}\sum_n e^{i\omega_n\tau} \tilde{g}(\omega_n); \qquad (3.7)$$

$$\hat{g}(\omega_n) = -\frac{1}{i\omega_n - \varepsilon}; \qquad \tilde{g}(\omega_n) = -\frac{1}{i\omega_n - \tilde{\varepsilon}}; \qquad \omega_n = \frac{2n+1}{\beta}\pi\,.$$

The characteristic feature of the already presented diagrams and diagrams that correspond to other orders of the perturbation theory is the presence of chain fragments. The simplest series of chain diagrams is

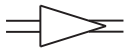


(3.8)

where

$$= g(\omega_n) = \frac{\langle P^+\rangle}{i\omega_n - \varepsilon} + \frac{\langle P^-\rangle}{i\omega_n - \tilde{\varepsilon}}\,, \qquad (3.9)$$

and corresponds to Hubbard–I approximation for single–electron Green function. The expression

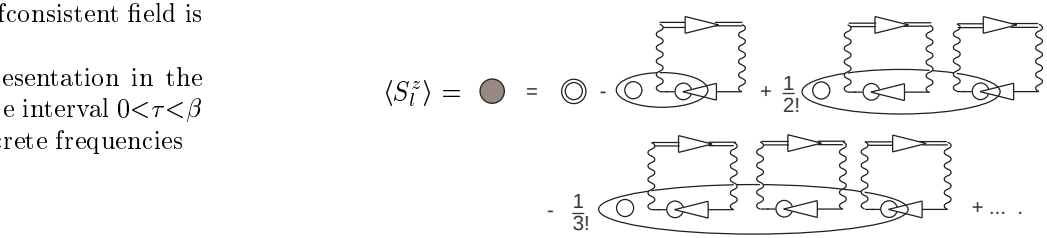


$$= G_{\vec{k}}(\omega_n) = \frac{1}{g^{-1}(\omega_n) - t_{\vec{k}}}\,, \qquad (3.10)$$

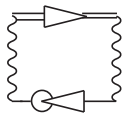
in the momentum–frequency representation corresponds to the sum of graphs (3.8). The poles of function $G_{\vec{k}}(\omega_n)$ determine the spectrum of the single–electron excitations

$$\varepsilon_{II,I}(t_{\vec{k}}) = 1/2(2E_o + t_{\vec{k}}) \mp 1/2\sqrt{g^2 + 4t_{\vec{k}}\langle S^z\rangle g + t_{\vec{k}}^2}\,, \qquad (3.11)$$

Let us now return to the problem of summation of the diagram series for average $\langle S_l^z\rangle$ taking into account the above mentioned arguments. The diagram series has the form

$\langle S_l^z\rangle =$  (3.12)

The analytical expressions for loop has the next form



$$= \frac{2}{N}\sum_{n,\vec{k}} \frac{t_{\vec{k}}^2}{g^{-1}(\omega_n) - t_{\vec{k}}} \left(\frac{P_i^+}{i\omega_n - \varepsilon} + \frac{P_i^-}{i\omega_n - \tilde{\varepsilon}}\right) =$$

$$= \beta(\alpha_1 P_i^+ + \alpha_2 P_i^-)\,, \qquad (3.13)$$

where we used the following notations

$$\alpha_1 = \frac{2}{N\beta}\sum_{n,\vec{k}} \frac{t_{\vec{k}}^2}{(g^{-1}(\omega_n) - t_{\vec{k}})} \frac{1}{(i\omega_n - \varepsilon)}\,,$$

$$\alpha_2 = \frac{2}{N\beta}\sum_{n,\vec{k}} \frac{t_{\vec{k}}^2}{(g^{-1}(\omega_n) - t_{\vec{k}})}\frac{1}{(i\omega_n - \tilde{\varepsilon})}\,.$$

Using decomposition into simple fractions and summation over frequency we obtained

$$\alpha_1 = \frac{2}{N}\sum_{\vec{k}} t_{\vec{k}}(A_1 n(\varepsilon_I(t_{\vec{k}})) + B_1 n(\varepsilon_{II}(t_{\vec{k}})))\,,$$

$$\alpha_2 = \frac{2}{N}\sum_{\vec{k}} t_{\vec{k}}(A_2 n(\varepsilon_I(t_{\vec{k}})) + B_2 n(\varepsilon_{II}(t_{\vec{k}})))\,,$$

where

$$A_1 = \frac{\varepsilon_I(t_{\vec{k}}) - \tilde{\varepsilon}}{\varepsilon_I(t_{\vec{k}}) - \varepsilon_{II}(t_{\vec{k}})}\,, \qquad B_1 = \frac{\varepsilon_{II}(t_{\vec{k}}) - \tilde{\varepsilon}}{\varepsilon_{II}(t_{\vec{k}}) - \varepsilon_I(t_{\vec{k}})}\,,$$

$$A_2 = \frac{\varepsilon_I(t_{\vec{k}}) - \varepsilon}{\varepsilon_I(t_{\vec{k}}) - \varepsilon_{II}(t_{\vec{k}})}\,, \qquad B_2 = \frac{\varepsilon_{II}(t_{\vec{k}}) - \varepsilon}{\varepsilon_{II}(t_{\vec{k}}) - \varepsilon_I(t_{\vec{k}})}\,.$$

The equation for $\langle S_l^z\rangle$ can be presented in the form

$$\langle S_l^z\rangle = \langle S_l^z\rangle_o - \langle S_l^z\beta(\alpha_1 P_l^+ + \alpha_2 P_l^-)\rangle_{oc} + \\ + \frac{1}{2!}\langle S_l^z\beta^2(\alpha_1 P_l^+ + \alpha_2 P_l^-)^2\rangle_{oc} - \ldots = \langle S_l^z e^{-\beta(\alpha_1 P_l^+ + \alpha_2 P_l^-)}\rangle_{oc}\,.$$

Let us introduce

$$H_{MF} = \sum_i H_i^{MF}\,,$$

where

$$H_i^{MF} = H_{i\,o} + \alpha_1 P_i^+ + \alpha_2 P_i^-\,.$$

Then the analytical equation for $\langle S_l^z\rangle$ can be expresed in the form

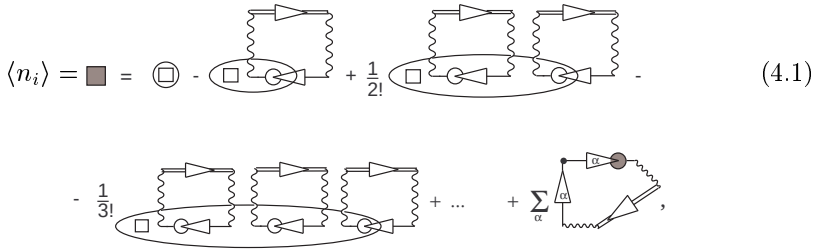
$$\langle S_l^z\rangle = \langle S_l^z\rangle_{MF} = \frac{Sp(S_l^z e^{-\beta H_{MF}})}{Sp(e^{-\beta H_{MF}})} = \qquad (3.14)$$
$$= \frac{1}{2}\tanh\left\{\frac{\beta}{2}(h + \alpha_2 - \alpha_1) + \ln\frac{1 + e^{-\beta\varepsilon}}{1 + e^{-\beta\tilde{\varepsilon}}}\right\}\,.$$

Difference $\alpha_2 - \alpha_1$ corresponds to the internal effective self–consistent field acting on pseudospin

$$\alpha_2 - \alpha_1 = \frac{2}{N}\sum_{\vec{k}} t_{\vec{k}}\frac{\varepsilon - \tilde{\varepsilon}}{\varepsilon_I(t_{\vec{k}}) - \varepsilon_{II}(t_{\vec{k}})}\{n(\varepsilon_I(t_{\vec{k}})) - n(\varepsilon_{II}(t_{\vec{k}}))\}\,. \qquad (3.15)$$

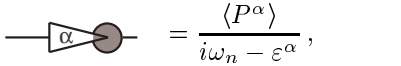
4. Mean value of particle number.

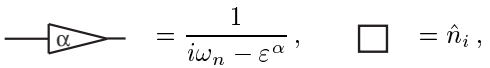
The diagram series for average $\langle n_i\rangle$ (using the perturbation theory, Wick's theorem and expansion in semi–invariants) can be presented in the form



(4.1)

where





$$P^\alpha = (P^+; P^-)\,,$$
$$\varepsilon_\alpha = (\varepsilon; \tilde{\varepsilon})\,,$$

and the last term appears due to the pairing of the electron creation (annihilation) operators with the operator of particle number.

Analytical expression for (4.1) can be obtained starting from formulas (3.8), (3.9)

$$\langle n_i\rangle = \langle n_i\rangle_{MF} + \frac{2}{N\beta}\sum_{n,\vec{k},\alpha}\frac{t_{\vec{k}}^2}{(g^{-1}(\omega_n) - t_{\vec{k}})}\frac{\langle P^\alpha\rangle}{(i\omega_n - \varepsilon^\alpha)^2}\,, \qquad (4.2)$$

where

$$\langle n_i\rangle_{MF} = \frac{Sp(n_i e^{-\beta H_{MF}})}{Sp(e^{-\beta H_{MF}})}\,.$$

After simple transformation we obtain next relation

$$\langle n\rangle_{MF} - n(\varepsilon) - n(\tilde{\varepsilon}) = 2\langle S^z\rangle(n(\varepsilon) - n(\tilde{\varepsilon}))\,, \qquad (4.3)$$

or

$$\langle n\rangle_{MF} = 2\langle P^+\rangle n(\varepsilon) + 2\langle P^-\rangle n(\tilde{\varepsilon})\,,$$

where $n(\varepsilon) = \dfrac{1}{1+e^{\beta\varepsilon}}$ is Fermi distribution.

Using decomposition into simple fractions, summation over frequency and relation (4.3) we can present average $\langle n\rangle$ in the form

$$\langle n\rangle = \frac{2}{N}\sum_{\vec{k}}\{n(\varepsilon_I(t_{\vec{k}})) + n(\varepsilon_{II}(t_{\vec{k}}))\} - 2\langle P^+\rangle n(\tilde{\varepsilon}) - 2\langle P^-\rangle n(\varepsilon)\,. \quad (4.4)$$

5. Thermodynamical potential.

In order to calculate the thermodynamical potential let us introduce the parameter $\lambda \in [0,1]$ in the initial Hamiltonian

$$H_\lambda = H_o + \lambda H_{int}\,, \quad (5.1)$$

such that $H \to H_o$ for $\lambda = 0$ and $H \to H_o + H_{int}$ for $\lambda = 1$.

Hence

$$Z_\lambda = Sp(e^{-\beta H_\lambda}) = Sp(e^{-\beta H_o}\hat{\sigma}_\lambda(\beta)) = Z_o\langle\hat{\sigma}_\lambda(\beta)\rangle_o\,,$$

where

$$\hat{\sigma}_\lambda(\beta) = T_\tau \exp\left\{-\lambda\int_0^\beta H_{int}(\tau)d\tau\right\}\,,$$

and

$$\Omega_\lambda = -\frac{1}{\beta}\ln Z_o - \frac{1}{\beta}\ln\langle\hat{\sigma}_\lambda(\beta)\rangle_o\,, \quad (5.2)$$

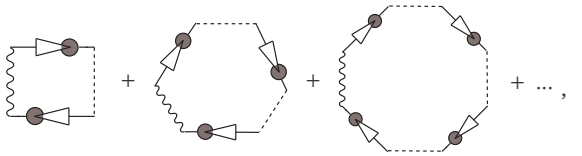
$$\Delta\Omega_\lambda = \Omega_\lambda - \Omega_o = -\frac{1}{\beta}\ln\langle\hat{\sigma}_\lambda(\beta)\rangle_o\,.$$

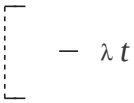
Here Ω_o is the thermodynamical potential calculated with the single–site (diagonal) part of the initial Hamiltonian.

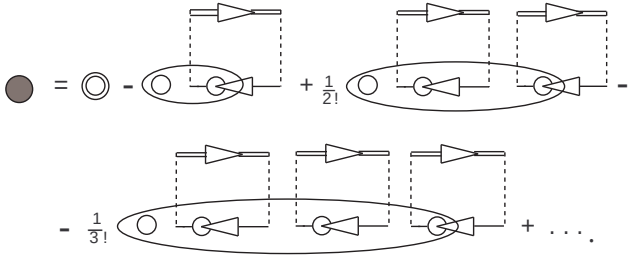
Therefore

$$\Delta\Omega = \int_0^1 d\lambda\left(\frac{d\Omega_\lambda}{d\lambda}\right)\,. \quad (5.3)$$

For the value $d\Omega_\lambda/d\lambda$, we can write immediately the diagram series in the next form

$\beta\dfrac{d\Omega_\lambda}{d\lambda} =$  (5.4)

where  and also



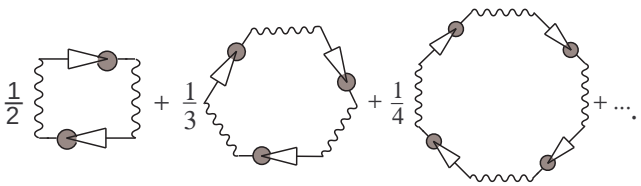
The expression (5.3) can be presented in the form (using the diagram series (5.4))

$$\Delta\Omega = \frac{2}{N\beta}\sum_{n,\vec{k}}\int_0^1 \lambda t_{\vec{k}}^2 g_\lambda^2(\omega_n)\frac{1}{1-\lambda t_{\vec{k}} g_\lambda(\omega_n)}d\lambda =$$

$$= -\frac{2}{N\beta}\sum_{n,\vec{k}}\ln(1 - t_{\vec{k}}g(\omega_n)) - \frac{2}{N\beta}\sum_{n,\vec{k}}\int_0^1 \frac{\lambda t_{\vec{k}}\frac{dg_\lambda(\omega_n)}{d\lambda}}{1-\lambda t_{\vec{k}} g_\lambda(\omega_n)}d\lambda\,. \quad (5.5)$$

The first term in expression (5.5) may be written in the diagram form

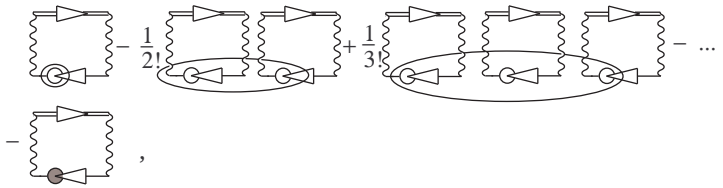
as



(5.6)

The series (5.6) describes an electron gas which energy spectrum is defined by the total pseudospins field. This series is in conformity with the so–called one loop–approximation.

The second term in expression (5.5) can be integrated to the following diagram series



(5.7)

and appears due to the presence of pseudospin subsystem.

Finally, the diagram series for $\beta\Delta\Omega$ may be written as the sum of expressions (5.6) and (5.7), the corresponding analytical expression is the following

$$\Delta\Omega = -\frac{2}{N\beta}\sum_{\vec{k}} \ln \frac{(\cosh\frac{\beta}{2}\varepsilon_I(t_{\vec{k}}))(\cosh\frac{\beta}{2}\varepsilon_{II}(t_{\vec{k}}))}{(\cosh\frac{\beta}{2}\varepsilon)(\cosh\frac{\beta}{2}\tilde{\varepsilon})} - \tag{5.8}$$

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

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

Here, the decomposition in simple fractions and summation over frequency were done.

Then, since the thermodynamical potential is the function of argument $\langle S^z\rangle$, let us check the consistency of approximations made for $\langle S^z\rangle$,

$\langle n\rangle$ and thermodynamical potential Ω. For this purpose one should obtain average $\langle S^z\rangle$ and average $\langle n\rangle$ from the expression for grand thermodynamical potential

$$\frac{d\Omega}{d(-\mu)} = \frac{2}{N}\sum_{\vec{k}}\{n(\varepsilon_I(t_{\vec{k}}))+n(\varepsilon_{II}(t_{\vec{k}}))\}-2\langle P^+\rangle n(\tilde{\varepsilon})-2\langle P^-\rangle n(\varepsilon)\,,$$

$$\frac{d\Omega}{d(-h)} = \frac{1}{2}\tanh\left\{\frac{\beta}{2}(h+\alpha_2-\alpha_1)+\ln\frac{1+e^{-\beta\varepsilon}}{1+e^{-\beta\tilde{\varepsilon}}}\right\}.$$

We thus obtain

$$\frac{d\Omega}{d(-\mu)} = \langle n\rangle\,, \qquad \frac{d\Omega}{d(-h)} = \langle S^z\rangle\,.$$

Therefore, the calculation of the mean values of the pseudospin and particle number operators as well as the thermodynamical potential is performed in the same approximation which corresponds to the mean field one.

6. Pseudospin, electron, and mixed correlators.

In this section our aim is to calculate correlators

$$K^{ss}_{lm}(\tau-\tau') = \langle T\tilde{S}^z_l(\tau)\tilde{S}^z_m(\tau')\rangle_c\,,$$

$$K^{sn}_{lm}(\tau-\tau') = \langle T\tilde{S}^z_l(\tau)\tilde{n}_m(\tau')\rangle_c\,,$$

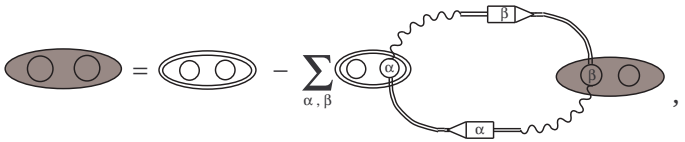
$$K^{nn}_{lm}(\tau-\tau') = \langle T\tilde{n}_l(\tau)\tilde{n}_m(\tau')\rangle_c$$

constructed of the operators given in the Heisenberg representation with imaginary time argument.

Let us present the diagram series for correlation function (in the momentum–frequency representation) within the generalized random phase approximation. In our case (absence of the Hubbard correlation) this approximation is reduced, because the so–called ladder diagrams (see.[10]) with antiparallel lines disappear. This reduce allow to take into account mean values of pseudospin found self–consistently within the mean field approximation.

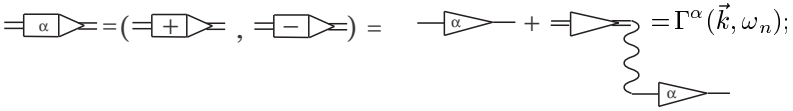
We would like to remind that we have neglected diagrams which include semi–invariants of the higher than first order in the loop and

also connection of two loops by more than one semi–invariant.



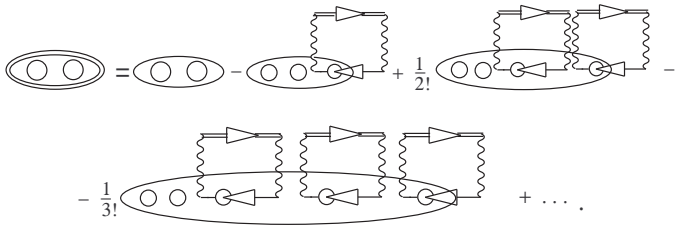
(6.1)

where, we define



$$P^{\alpha} = (P^{+}, P^{-});\ \alpha = (0,1);\ \varepsilon^{\alpha} = (\varepsilon, \tilde{\varepsilon}); \qquad \textcircled{\alpha} = P^{\alpha}; \qquad \bigcirc = S^{z}\ .$$

Here, the first term in equation (6.1) takes into account the direct influence on pseudospins of the internal effective self–consistent field and is given by

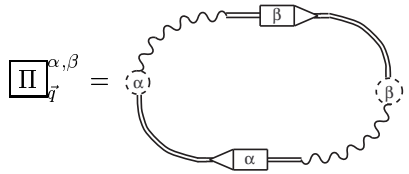


(6.2)

Series (6.2) means second–order semi–invariant which renormalized due to the 'single–tale' parts, and thus is calculate by H_{MF}.

The second term in equation (6.1) describes the interaction between pseudospins which is mediated by electrons (energy of electron spectrum is defined by the total pseudospin field).

We introduce the shortened notations



(6.3)

Solution of equation (6.1) can be written in the analytical form

$$\langle S^z S^z \rangle_{\vec{q}} = \frac{1/4 - \langle S^z \rangle^2}{1 + \sum\limits_{\alpha,\beta} (-1)^{\alpha+\beta} \boxed{\Pi}^{\alpha,\beta}_{\vec{q}} \left(\frac{1}{4} - \langle S^z \rangle^2\right)}\,, \tag{6.4}$$

where

$$\boxed{\Pi}^{\alpha,\beta}_{\vec{q}} = \frac{2}{N} \sum_{\vec{k}} t_{\vec{k}} t_{\vec{k}+\vec{q}} \Gamma^{\alpha}(\vec{k}, \omega_n) \Gamma^{\beta}(\vec{k}+\vec{q}, \omega_n)\,, \tag{6.5}$$

$$\Gamma^{\alpha}(\vec{k}, \omega_n) = \frac{1}{(i\omega_n - \varepsilon^{\alpha})} \frac{1}{(1 - t_{\vec{k}} g(\omega_n))}\,. \tag{6.6}$$

Decomposition of the function $\Gamma^{\alpha}(\vec{k}, \omega_n)$ into simple fractions and subsequent evaluation of the sum over frequency leads to the next expression

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

$$\times \left\{ \frac{n[\varepsilon_I(t_{\vec{k}})] - n[\varepsilon_I(t_{\vec{k}+\vec{q}})]}{\varepsilon_I(t_{\vec{k}}) - \varepsilon_I(t_{\vec{k}+\vec{q}})} + \frac{n[\varepsilon_{II}(t_{\vec{k}})] - n[\varepsilon_{II}(t_{\vec{k}+\vec{q}})]}{\varepsilon_{II}(t_{\vec{k}}) - \varepsilon_{II}(t_{\vec{k}+\vec{q}})} - \right. \tag{6.7}$$

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

After the substitution (6.7) in equation (6.4) we obtain, finally, expression for $\langle S^z S^z \rangle$.

This formula for the uniform case ($\vec{q} = 0$) can be rewritten as

$$\langle S^z S^z \rangle_{\vec{q}=0} = (1/4 - \langle S^z \rangle^2) \times \tag{6.8}$$

$$\times\left\{1-\left(\frac{4\beta}{N}\sum_{\vec{k}}t_{\vec{k}}^2\frac{(\varepsilon-\tilde{\varepsilon})^2}{[\varepsilon_I(t_{\vec{k}})-\varepsilon_{II}(t_{\vec{k}})]^3}\{n[\varepsilon_I(t_{\vec{k}})]-n[\varepsilon_{II}(t_{\vec{k}})]\}+\right.\right.$$

$$\left.\left.+\frac{\beta^2}{2N}\sum_{\vec{k}}\frac{t_{\vec{k}}^2(\varepsilon-\tilde{\varepsilon})^2}{[\varepsilon_I(t_{\vec{k}})-\varepsilon_{II}(t_{\vec{k}})]^2}\left\{\frac{1}{\cosh^2\frac{\beta\varepsilon_I(t_{\vec{k}})}{2}}+\frac{1}{\cosh^2\frac{\beta\varepsilon_{II}(t_{\vec{k}})}{2}}\right\}\right)(\frac{1}{4}-\langle S^z\rangle^2)\right\}^{-1}.$$

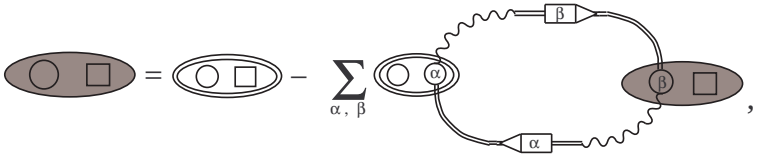
Expression (6.8) can be obtained from the derivative $d\langle S^z\rangle/d(\beta h)$. This means that mean values of pseudospin and pseudospin correlators are derived in the same approximation.

For mixed correlator the diagram series has the form

$\langle S^z n\rangle =$ 

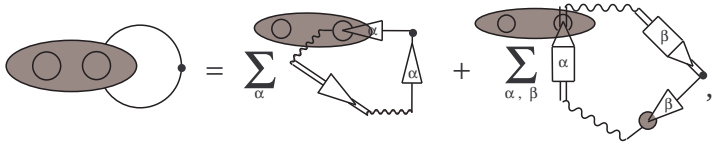
, (6.9)

where

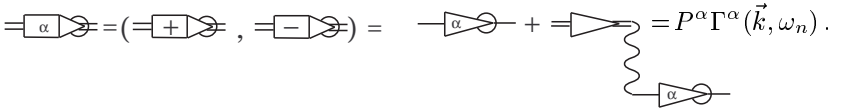
$I =$ 

, (6.10)

and

$II =$ 

, (6.11)



$= P^{\alpha}\Gamma^{\alpha}(\vec{k},\omega_n)\,.$

Solution of equation (6.10) can be written in the analytical form

$$I = 2(n(\varepsilon)-n(\tilde{\varepsilon}))\langle S^zS^z\rangle_{\vec{q}}\,. \tag{6.12}$$

Here we start from formula (6.4) and from the next relation

$$\frac{\langle S^z n\rangle_{MF}-\langle S^z\rangle\langle n\rangle}{\frac{1}{4}-\langle S^z\rangle^2} = 2(n(\varepsilon)-n(\tilde{\varepsilon}))\,. \tag{6.13}$$

The second term in the diagram series (6.9) we can present as

$$II = \frac{2}{N}\langle S^zS^z\rangle_{\vec{q}}\sum_{\vec{k}}\frac{t_{\vec{k}}(\varepsilon-\tilde{\varepsilon})}{\varepsilon_I(t_{\vec{k}})-\varepsilon_{II}(t_{\vec{k}})}\times$$

$$\times\left[\frac{n[\varepsilon_I(t_{\vec{k}})]-n[\varepsilon_I(t_{\vec{k}+\vec{q}})]}{\varepsilon_I(t_{\vec{k}})-\varepsilon_I(t_{\vec{k}+\vec{q}})}+\frac{n[\varepsilon_I(t_{\vec{k}})]-n[\varepsilon_{II}(t_{\vec{k}+\vec{q}})]}{\varepsilon_I(t_{\vec{k}})-\varepsilon_{II}(t_{\vec{k}+\vec{q}})}-\right. \tag{6.14}$$

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

Let us introduce the shortened notations for the expression (6.14)

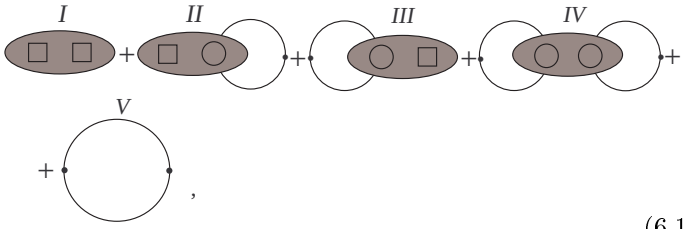
$$II = \langle S^zS^z\rangle_{\vec{q}}\times[\oplus]_{\vec{q}}\,. \tag{6.15}$$

In this way we obtain

$$\langle S^z n\rangle_{\vec{q}} = 2(n(\varepsilon)-n(\tilde{\varepsilon}))\langle S^zS^z\rangle_{\vec{q}}+\langle S^zS^z\rangle_{\vec{q}}\times[\oplus]_{\vec{q}}\,. \tag{6.16}$$

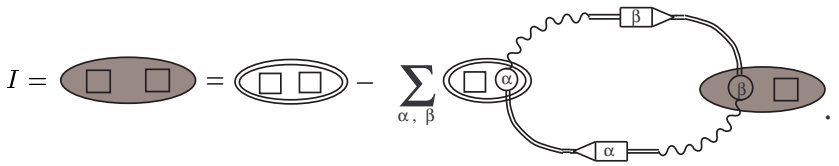
From our diagram series we can see: the correlators containing pseudospin variable S^z are different from zero only in the static case. This is due to the fact that the operator S^z commutes with Hamiltonian being the integral of motion.

For electron correlator our diagram series has the form

$\langle nn\rangle_{\vec{q},\omega} =$ 

, (6.17)

and only last term is not equal to zero for non–zero frequencies. Let us consider series (6.17) term by term



(6.18)

After simple transformation we can obtain the next relation

$$\langle nn\rangle_{MF} - \langle n\rangle^2 - \frac{1}{2}\left(\frac{\langle P^+\rangle}{\cosh^2\frac{\beta\varepsilon}{2}} + \frac{\langle P^-\rangle}{\cosh^2\frac{\beta\tilde{\varepsilon}}{2}}\right) = \tag{6.19}$$

$$= \frac{(\langle nS^z\rangle_{MF} - \langle n\rangle\langle S^z\rangle)^2}{\langle P^+\rangle\langle P^-\rangle}\,.$$

This relation makes possible to write immediately the simple analytic expression for series (6.18)

$$I = \left\{[2(n(\varepsilon) - n(\tilde{\varepsilon}))]^2\langle S^zS^z\rangle_{\vec{q}} + \frac{1}{2}\left(\frac{\langle P^+\rangle}{\cosh^2\frac{\beta\varepsilon}{2}} + \frac{\langle P^-\rangle}{\cosh^2\frac{\beta\tilde{\varepsilon}}{2}}\right)\right\}\delta(\omega)\,. \tag{6.20}$$

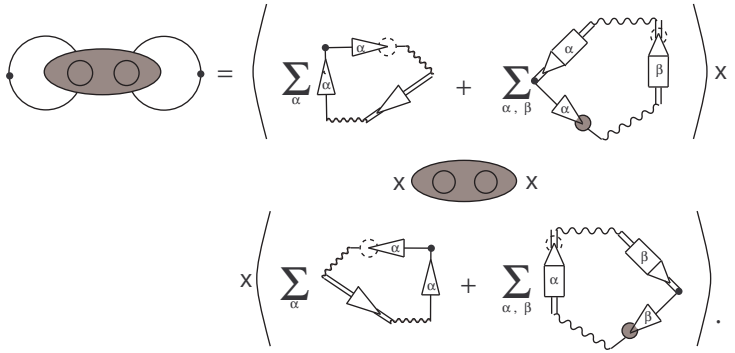
Analytical expressions for *II*–term can be obtained starting from formulae (6.11) – (6.15)

$$II = \left\{2[n(\varepsilon) - n(\tilde{\varepsilon})]\langle S^zS^z\rangle_{\vec{q}} \times [\oplus]_{\vec{q}}\right\}\delta(\omega)\,. \tag{6.21}$$

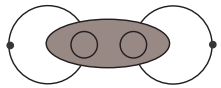
Using the expression (6.16) we can unite (6.21) and (6.20)

$$I + II = \left\{2(n(\varepsilon) - n(\tilde{\varepsilon}))\langle S^zn\rangle_{\vec{q}} + \frac{1}{2}\left(\frac{\langle P^+\rangle}{\cosh^2\frac{\beta\varepsilon}{2}} + \frac{\langle P^-\rangle}{\cosh^2\frac{\beta\tilde{\varepsilon}}{2}}\right)\right\}\delta(\omega)\,. \tag{6.22}$$

The diagram series for the fourth term in (6.17) has form



And can be written as

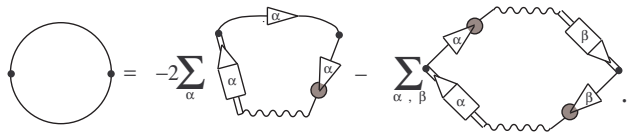


$$= [\oplus]_{\vec{q}} \times \langle S^zS^z\rangle_{\vec{q}} \times [\oplus]_{\vec{q}} \cdot \delta(\omega)\,. \tag{6.23}$$

Ones more using the formula (6.16) we unite *III*–term and *IV*–term

$$III + IV = \langle nS^z\rangle_{\vec{q}} \times [\oplus]_{\vec{q}} \cdot \delta(\omega)\,. \tag{6.24}$$

Last term can be presented in the form



(6.25)

Let us the take down final formula for electron correlator for the uniform ($\vec{q} = 0$) and static ($\omega = 0$) case

$$\langle nn\rangle = 2(n(\varepsilon) - n(\tilde{\varepsilon}))\langle S^zn\rangle_{\vec{q}=0} + \frac{1}{2}\left(\frac{\langle P^+\rangle}{\cosh^2\frac{\beta\varepsilon}{2}} + \frac{\langle P^-\rangle}{\cosh^2\frac{\beta\tilde{\varepsilon}}{2}}\right) + \tag{6.26}$$

$$+\frac{\beta}{2N}\sum_{\vec{k}}\frac{t_{\vec{k}}(\varepsilon-\tilde{\varepsilon})}{\varepsilon_I(t_{\vec{k}})-\varepsilon_{II}(t_{\vec{k}})}\left\{\frac{1}{\cosh^2\frac{\beta\varepsilon_{II}(t_{\vec{k}})}{2}}-\frac{1}{\cosh^2\frac{\beta\varepsilon_I(t_{\vec{k}})}{2}}\right\}\langle S^z n\rangle_{\vec{q}=0}+$$

$$+\frac{1}{2N}\sum_{\vec{k}}\left\{\frac{1}{\cosh^2\frac{\beta\varepsilon_{II}(t_{\vec{k}})}{2}}+\frac{1}{\cosh^2\frac{\beta\varepsilon_I(t_{\vec{k}})}{2}}\right\}-\frac{1}{2}\left\{\frac{1}{\cosh^2\frac{\beta\varepsilon}{2}}+\frac{1}{\cosh^2\frac{\beta\tilde{\varepsilon}}{2}}\right\}.$$

Same result we can obtain from the derivative $d\langle n\rangle/(d\beta\mu)$. Thus all our quantities: mean values of the pseudospin and particle number operators, thermodynamical potential as well as correlation functions are derived in the framework of one approximation which corresponds to the mean field approximation.

In the second part of the paper we shell perform numerical calculations for the analytical expressions obtained in the first part. We shall investigate values of pseudospin and particle number operators with the change of the asymmetry parameter h ($T = const$) or with the change of temperature T ($h = const$) for the cases of the fixed chemical potential value (regime $\mu = const$) and constant mean value particle number.

References

1. Cohen R.E., Pickett W.E., Krakauer H. Theoretical determination of strong electron–phonon coupling in $YBa_2Cu_3O_7$ // *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 $YBa_2Cu_3O_{7-\delta}$ compounds //*Physica C.* – 1989. – **160**, N 5/6. – P. 524.
3. Conradson S.D., Raistrick I.D. The axial oxygen atom and superconductivity in $YBa_2Cu_3O_7$ //*Science.* – 1989. – **243**, N 4896. – P. 1340.
4. Muller K.A. // *Phase transition.* – 1988. – (Special issue).
5. 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.
6. Hirsch J.E., Tang S. Effective interactions in an oxygen–hole metal //*Phys. Rev. B.* – 1989. – **40**, N 4. – P. 2179–2186.
7. 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.

8. 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).
9. 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).
10. 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).
11. Stasyuk I.V., Trachenko K.O. Investigation of locally anharmonic models of structural phase transitions. Seminumerical approach.// *Cond. Matt. Phys.*, (1997), N 9, 89.
12. 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).
13. Gervais F. Oxygen polarizability in ferroelectrics. A clue to understanding superconductivity in oxides? // *Ferroelectrics.* – 1992. – **130**. – P. 45–76.
14. Kurtz S.K., Hardy J.R., Floken J.W. Structural phase transition, ferroelectricity and high–temperature superconductivity. // *Ferroelectrics.* – 1988. – 87. – P. 29–40.

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/)

Ігор Васильович Стасюк
Андрій Михайлович Швайка
Кирило Вікторович Табунщик

Динаміка та термодинаміка моделі з локальним ангармонізмом у випадку відсутності електронної хаббардівської кореляції. I. Аналітичний розгляд.

Роботу отримано 10 вересня 1998 р.

Затверджено до друку Вченою радою ІФКС НАН України

Рекомендовано до друку семінаром відділу квантової статистики

Виготовлено при ІФКС НАН України