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ENERGY SPECTRUM OF PSEUDOSPIN-ELECTRON MODEL
IN THE DYNAMICAL MEAN-FIELD THEORY

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Енергетичний спектр псевдоспін-електронної моделі в
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Енергетичний спектр псевдоспін-електронної моделі в методі динамічного середнього поля

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Анотація. Досліджується псевдоспін-електронна модель у випадку відсутності кулонівської взаємодії на вузлі. За допомогою діаграмної техніки та з використанням теореми Віка отримано аналітичні вирази для розрахунку спектральних функцій моделі в рамках методу динамічного середнього поля (ДСП). Також досліджено вплив поля асиметрії h та тунельного розщеплення рівнів на появу та кількість зон в електронному спектрі.

Energy spectrum of pseudospin-electron model in the dynamical mean-field theory

I.V.Stasyuk, V.O.Krasnov

Abstract. Pseudospin-electron model in the case of Coulomb interaction absence is investiagted. Analytic equations for specral densities within the framework of the dynamical mean field theory (DMFT) using diagrammatic series and Wick's theorem are established. The effect of the asymmetry field h and tunneling-like splitting level in the local anharmonic well on the existence and number of electron subbands is investigated.

1. Introduction

Pseudospin-electron model (PEM) is one of models which are used in physics of the strongly-correlated electron systems in recent years. Application of the model to high-temperature superconductors allows, for example, to describe thermodynamics of anharmonic oxygen ion subsystem and explain the occurrence of inhomogeneous states and the bistability phenomena (see in [1]). In this model we take into consideration the dynamics of locally anharmonic structure elements (using pseudospin variables to describe them), interaction between pseudospins and electrons; and the asymmetry of local anharmonic potential wells. The electron subsystem is described by the Hubbard Hamiltonian.

In DMFT method the Hamiltonian with strong correlations is taken in the infinite space dimension ($d \to \infty$) limit; this leads to reformulation of the problem and transition to solution of the single-site problem described by effective Hamiltonian [2–4]. Only for simplest cases such as mobile particles in the Falicov-Kimball model one can solve analytically this problem. An exact solution exists also for pseudospin-electron model in the case of absence of transverse filed [5]. There are also some approximate analytical approaches, such as: Hubbard-I, Hubbard-III, alloy analogy (AA), modified alloy analogy (MAA) etc., see [6, 7].

The alloy analogy approximation for the single-site problem is used for pseudo-spin-electron model in this article. Our task is to study electron spectrum and find the conditions of appearing of a gap. Our problem is solved in the limit of infinite value of single-site electron interaction. The performed previously consideration of this problem in the Hubbard-I approximation [8] revealed complicated structure of the spectrum and presence of some number of subbands.

Also, in [9] the electron energy spectrum of the pseudospin-electron model allowing for interaction of the near energy subbands was considered. The effective single-site problem was solved within the auxiliary fermion field approach with the help of procedure of different-time decoupling of the higher order Green's functions [6]; the alloy analogy approximation was used. And a special case of two near subbands was considered.

2. Hamiltonian of the model and its transformation

The Hamiltonian of the pseudospin-electron model is:

$$H = \sum_i H_i + \sum_{<i,j>,\sigma} t_{ij} a^+_{i\sigma} a_{j\sigma} \tag{2.1}$$

where in the single-site part of the Hamiltonian Ω is the tunneling-like level splitting, g is the pseudospin-electron interaction constant and h is asymmetry of the local anharmonic potential:

$$H_i = -\mu(n_{i,\uparrow} + n_{i,\downarrow}) + g(n_{i,\uparrow} + n_{i,\downarrow})S_i^z - \Omega S_i^x - hS_i^z \qquad (2.2)$$

The second term in (2.1) describes the electron site-to-site hopping.

The term $Un_\uparrow n_\downarrow$ is not included as we invesigate our problem in the limit of infinite potential of single-site electron interaction $U \to \infty$, where all states with double cite occupation are absent. The single-site Hamiltonian is considered as the zero-order ones with respect to the electron transfer. It is useful to introduce the following standard single-site basis $|R\rangle = |n_{i,\uparrow}, n_{i,\downarrow}, S_i^z\rangle$, with six eigenvectors [10]:

$$|1\rangle = |0, 0, \frac{1}{2}\rangle, \quad |3\rangle = |0, 1, \frac{1}{2}\rangle, \quad |4\rangle = |1, 0, \frac{1}{2}\rangle, \qquad (2.3)$$

$$|\widetilde{1}\rangle = |0, 0, -\frac{1}{2}\rangle, \quad |\widetilde{3}\rangle = |0, 1, -\frac{1}{2}\rangle, \quad |\widetilde{4}\rangle = |1, 0, -\frac{1}{2}\rangle$$

Using Hubbard X-operators, which act in the space of such eigenvectors, we can write down the electron annihilation (creation) operators and pseudospin operators as follows [8]

$$c_{i,\uparrow} = X_i^{14} + X_i^{\widetilde{14}} \qquad (2.4)$$
$$c_{i,\downarrow} = X_i^{13} + X_i^{\widetilde{13}}$$

Then, the single-site part of the Hamiltonian can be expressed by means of X-operators in the way:

$$H_i = (-\mu + \frac{g}{2} - \frac{h}{2})(X_i^{33} + X_i^{44}) + (-\mu - \frac{g}{2} + \frac{h}{2})(X_i^{\widetilde{33}} + X_i^{\widetilde{44}}) +$$
$$+ \frac{h}{2}(X_i^{\widetilde{11}} - X_i^{11}) + \frac{\Omega}{2}(X_i^{1\widetilde{1}} + X_i^{\widetilde{1}1} + X_i^{3\widetilde{3}} + X_i^{\widetilde{3}3} + X_i^{4\widetilde{4}} + X_i^{\widetilde{4}4}) \quad (2.5)$$

This Hamiltonian is diagonal in the case $\Omega = 0$, but if tunneling splitting is non-zero we have to use a transformation

$$\begin{pmatrix} R \\ \widetilde{R} \end{pmatrix} = \begin{pmatrix} \cos\phi_r & \sin\phi_r \\ -\sin\phi_r & \cos\phi_r \end{pmatrix} \begin{pmatrix} r \\ \widetilde{r} \end{pmatrix} \qquad (2.6)$$

to diagonalize it. Here

$$\cos(2\phi_r) = \frac{n_r g - h}{\sqrt{(n_r g - h)^2 + \Omega^2}} \quad , n_1 = 0, n_3 = n_4 = 1 \quad (2.7)$$

In that way we have

$$H = \sum_{i,r} \varepsilon_r X_i^{rr} + \sum_{<i,j>,\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} \qquad (2.8)$$

$$\varepsilon_{1,\widetilde{1}} = \pm\frac{1}{2}\sqrt{h^2 + \Omega^2},$$

$$\varepsilon_{3,\widetilde{3}} = \varepsilon_{4,\widetilde{4}} = -\mu \pm \frac{1}{2}\sqrt{(g-h)^2 + \Omega^2}$$

Where

$$c_{i,\uparrow} = \cos\phi_{41}(X_i^{14} + X_i^{\widetilde{14}}) + \sin\phi_{41}(X_i^{1\widetilde{4}} - X_i^{\widetilde{1}4})$$
$$c_{i,\downarrow} = \cos\phi_{31}(X_i^{13} + X_i^{\widetilde{13}}) + \sin\phi_{31}(X_i^{1\widetilde{3}} - X_i^{\widetilde{1}3}) \qquad (2.9)$$
$$\cos\phi_{41} = \cos(\phi_4 - \phi_1) \quad \cos\phi_{31} = \cos(\phi_3 - \phi_1)$$
$$\sin\phi_{41} = \sin(\phi_4 - \phi_1) \quad \sin\phi_{31} = \sin(\phi_3 - \phi_1).$$

3. Dynamical mean field theory approach

The transition to the $d = \infty$ limit in the DMFT approach is accompanied by the scaling of the electron transfer parameter:

$$t = \frac{t^*}{\sqrt{d}} \qquad (3.1)$$

In particular, the self-energy part of the electron Green's function becomes a purely local [3, 4]:

$$\Sigma_{ij,\sigma}(\omega) = \Sigma_\sigma \delta_{ij}, \qquad d = \infty \qquad (3.2)$$

The Fourier-transform $\Sigma_{ij,\sigma}(\omega)$ is hence momentum-independent:

$$\Sigma_\sigma(\vec{k}, \omega) = \Sigma_\sigma(\omega) \qquad (3.3)$$

The electron Green's function in (k, ω) representation

$$G_k^\sigma(\omega) = \sum_{i-j} e^{i\vec{k}(\vec{R}_i - \vec{R}_j)} G_{ij,\sigma}(\omega) \qquad (3.4)$$

can be expressed as:

$$G_k^\sigma(\omega) = \frac{1}{[\Xi_\sigma(\omega)]^{-1} - t_k} \qquad (3.5)$$

where $\Xi_\sigma(\omega)$ is the part, which is irreducible (in the diagrammatic representation) according to Larkin. To calculate the $\Xi_\sigma(\omega)$ function the effective single-site problem is used. The transition to this problem corresponds to the replacement

$$e^{-\beta H} \to e^{-\beta H_{eff}} = e^{-\beta H_0} \times T exp\{-\int_0^\beta d\tau \int_0^\beta d\tau' \times$$

$$\sum_\sigma J_\sigma(\tau - \tau')a_\sigma^+(\tau)a_\sigma(\tau')\} \equiv e^{-\beta H_0}\widetilde{\sigma}(\beta) \qquad (3.6)$$

where

$$H_0 = H_i \qquad (3.7)$$

and $J_\sigma(\tau - \tau')$ - is an effective time-depended field (coherent potential) which is determined self-consistently from the condition that the same self-energy part $\Xi_\sigma(\omega)$ determines the lattice function $G_k^\sigma(\omega)$ as well as the Green's function $G_\sigma^{(a)}(\omega)$ of the effective single-site problem:

$$G_\sigma^{(a)}(\omega) = \frac{1}{[\Xi_\sigma(\omega)]^{-1} - J_\sigma(\omega)} \qquad (3.8)$$

In this case:

$$G_\sigma^{(a)} = G_{ii,\sigma}(\omega) = \frac{1}{N}\sum_k G_k^\sigma(\omega) \qquad (3.9)$$

The set of simultaneous equations (3.5, 3.8, 3.9) becomes closed when it is supplemented with the functional dependence

$$G_\sigma^{(a)}(\omega) = f([J_\sigma(\omega)]) \qquad (3.10)$$

which is obtained as the result of solving the effective single-site problem with the statistical operator $\exp(-\beta H_{eff})$.

4. Reformulation of Wick's theorem for single-site problem.

To find out the relation (3.10) let us calculate the electron Green's function using an expansion in powers of coherent potential $J_\sigma(\omega)$. In zero approximation:

$$\langle Tc_\uparrow(\tau)c_\uparrow^+(\tau')\rangle_0 = -\langle TX^{\widetilde{14}}(\tau)X^{\widetilde{41}}(\tau')\rangle_0 - \langle TX^{14}(\tau)X^{41}(\tau')\rangle_0$$

$$-\langle TX^{1\widetilde{4}}(\tau)X^{\widetilde{41}}(\tau')\rangle_0 - \langle TX^{\widetilde{14}}(\tau)X^{4\widetilde{1}}(\tau')\rangle_0 \qquad (4.1)$$

Here

$$-\langle TX^{14}(\tau)X^{41}(\tau')\rangle_0 = -g_0^{14}(\tau - \tau')\langle X^{11} + X^{44}\rangle_0 \qquad (4.2)$$

Where in the frequency representation $g_0^{14}(\omega_n) = -(i\omega_n - \lambda_{41})^{-1}$, etc. ($\lambda_{pq} = \varepsilon_p - \varepsilon_q$). In this case

$$-\langle Tc_\uparrow(\tau)c_\uparrow^+(\tau)\rangle_0 = g_0^{14}(\tau - \tau')\langle X^{11} + X^{44}\rangle_0 +$$

$$+g_0^{\widetilde{14}}(\tau - \tau')\langle X^{\widetilde{11}} + X^{\widetilde{44}}\rangle_0 + g_0^{1\widetilde{4}}(\tau - \tau')\langle X^{\widetilde{11}} + X^{44}\rangle_0 +$$

$$+g_0^{1\widetilde{4}}(\tau - \tau')\langle X^{11} + X^{\widetilde{44}}\rangle_0 \qquad (4.3)$$

Now, using Wick's theorem for Hubbard operators we can see that:

$$\overset{\frown}{X^{41}(\tau')X^{14}(\tau)} = -g_0^{14}(\tau - \tau')(X^{11} + X^{44})_{\tau'}$$

$$\overset{\frown}{X^{\widetilde{41}}(\tau')X^{14}(\tau)} = 0$$

$$\overset{\frown}{X^{\widetilde{41}}(\tau')X^{14}(\tau)} = -g_0^{14}(\tau - \tau')X^{\widetilde{44}}(\tau')$$

$$\overset{\frown}{X^{4\widetilde{1}}(\tau')X^{14}(\tau)} = -g_0^{14}(\tau - \tau')X^{1\widetilde{1}}(\tau')$$

As the result of such a procedure the X-operators of Bose-type appear.

The next step is to introduce alloy-analogy approximation (see [6,7]). In this case this means neglecting all non-diagonal Hubbard operators in the Wick's pairing. Such an approximation leads to the next result

$$\overset{\frown}{c_\uparrow^+(\tau')X^{14}(\tau)} = -g_0^{14}(\tau - \tau')(X^{11} + X^{44})_{\tau'}\cos\phi_{41}$$

$$\overset{\frown}{c_\downarrow^+(\tau')X^{14}(\tau)} = 0$$

$$\overset{\frown}{c_\uparrow^+(\tau')X^{\widetilde{14}}(\tau)} = -g_0^{\widetilde{14}}(\tau - \tau')(X^{\widetilde{11}} + X^{\widetilde{44}})_{\tau'}\cos\phi_{41}$$

$$\overset{\frown}{c_\downarrow^+(\tau')X^{\widetilde{14}}(\tau)} = 0$$

$$\overset{\frown}{c_\uparrow^+(\tau')X^{1\widetilde{4}}(\tau)} = g_0^{1\widetilde{4}}(\tau - \tau')(X^{\widetilde{11}} + X^{44})_{\tau'}\sin\phi_{41}$$

$$\overset{\frown}{c_\downarrow^+(\tau')X^{1\widetilde{4}}(\tau)} = 0$$

$$\overset{\frown}{c_\uparrow^+(\tau')X^{1\widetilde{4}}(\tau)} = -g_0^{1\widetilde{4}}(\tau - \tau')(X^{11} + X^{\widetilde{44}})_{\tau'}\sin\phi_{41}$$

$$\overset{\frown}{c_\downarrow^+(\tau')X^{1\widetilde{4}}(\tau)} = 0$$

$$(4.4)$$

And now using (2.9) we have:

$$\overrightarrow{c_\uparrow^+(\tau')c_\uparrow(\tau)} = -g_0^{14}(\tau-\tau')(X^{11}+X^{44})_{\tau'}\cos^2\phi_{41} -$$
$$-g_0^{\widetilde{14}}(\tau-\tau')(X^{\widetilde{11}}+X^{\widetilde{44}})_{\tau'}\cos^2\phi_{41} -$$
$$-g_0^{\widetilde{14}}(\tau-\tau')(X^{\widetilde{11}}+X^{44})_{\tau'}\sin^2\phi_{41} -$$
$$-g_0^{1\widetilde{4}}(\tau-\tau')(X^{11}+X^{\widetilde{44}})_{\tau'}\sin^2\phi_{41} \qquad (4.5)$$

This result shows us that in the case of alloy-analogy approximation the Fermi-operators pairing decomposes into the sum of terms, that are projections on single-site states (because of X^{rr} operators action). And this is main difference from ideal fermions case, where we have a Green's functions as the result of pairing.

Now we can rewrite

$$\overrightarrow{c_\uparrow^+(\tau')c_\uparrow(\tau)} = -[g_0^{14}(\tau-\tau')\cos^2\phi_{41}+g_0^{1\widetilde{4}}(\tau-\tau')(\sin\phi_{41}]X^{11}(\tau')$$
$$-[g_0^{\widetilde{14}}(\tau-\tau')\cos^2\phi_{41}+g_0^{\widetilde{14}}(\tau-\tau')(\sin\phi_{41}]X^{\widetilde{11}}(\tau') \qquad (4.6)$$
$$-[g_0^{14}(\tau-\tau')\cos^2\phi_{41}+g_0^{\widetilde{14}}(\tau-\tau')(\sin\phi_{41}]X^{44}(\tau')$$
$$-[g_0^{\widetilde{14}}(\tau-\tau')\cos^2\phi_{41}+g_0^{\widetilde{44}}(\tau-\tau')(\sin\phi_{41}]X^{\widetilde{44}}(\tau') \equiv$$
$$-g_{0\uparrow}^{(1)}X^{11}(\tau') - g_{0\uparrow}^{(\widetilde{1})}X^{\widetilde{11}}(\tau') - g_{0\uparrow}^{(4)}X^{44}(\tau') - g_{0\uparrow}^{(\widetilde{4})}X^{\widetilde{44}}(\tau')$$
$$= -\sum_r g_{0\uparrow}^{(r)}X^{rr}(\tau')$$

5. Expansions in terms of coherent potential.

In general, for electron Green's function of effective one-site problem we have:

$$\Upsilon_\sigma(\tau-\tau') = -\frac{\langle Tc_\sigma(\tau)c_\sigma^+(\tau')e^{-\beta H_{eff}}\rangle}{\langle e^{-\beta H_{eff}}\rangle} = -\frac{\langle Tc_\sigma(\tau)c_\sigma^+(\tau')\widetilde{\sigma}(\beta)\rangle_0}{\langle\widetilde{\sigma}(\beta)\rangle_0} \quad (5.1)$$

Numerator and denominator in this expression will be calculated separately using an expansion in terms of coherent potential $J_\sigma(\tau-\tau')$. The first step is to calculate the second order in this expansion - with four operators of creation and annihilation of electrons:

$$\langle Tc_\uparrow(\tau)c_\uparrow^+(\tau')c_\uparrow^+(\tau_1)c_\uparrow(\tau_2)\rangle_0 = -\langle T\overrightarrow{c_\uparrow^+(\tau)c_\uparrow(\tau)}\overrightarrow{c_\uparrow^+(\tau_1)c_\uparrow(\tau_2)}\rangle_0 +$$
$$+\langle T\overrightarrow{c_\uparrow^+(\tau_1)c_\uparrow(\tau)}\overrightarrow{c_\uparrow^+(\tau')c_\uparrow(\tau_2)}\rangle_0 =$$

$$-\sum_r g_{0\uparrow}^{(r)}(\tau-\tau')g_{0\uparrow}^{(r)}(\tau_2-\tau_1)\langle X^{rr}\rangle_0 +$$
$$+\sum_r g_{0\uparrow}^{(r)}(\tau-\tau_1)g_{0\uparrow}^{(r)}(\tau_2-\tau')\langle X^{rr}\rangle_0 \qquad (5.2)$$

and

$$\langle Tc_\uparrow(\tau)c_\uparrow^+(\tau')c_\downarrow^+(\tau_1)c_\downarrow(\tau_2)\rangle_0 = -\langle T\overrightarrow{c_\uparrow^+(\tau')c_\uparrow(\tau)}\overrightarrow{c_\downarrow^+(\tau_1)c_\downarrow(\tau_2)}\rangle_0 =$$
$$= -\sum_r g_{0\uparrow}^{(r)}(\tau-\tau')g_{0\downarrow}^{(r)}(\tau_2-\tau_1)\langle X^{rr}\rangle_0 \qquad (5.3)$$

Here pairing of Fermi-operators is performed according to (4.6). The diagonal X-operators, which appear along this procedure, we multiply using the rule $X^{rr}X^{pp} = X^{rr}\delta_{rp}$. As the result - only averages $\langle X^{rr}\rangle_0$ are present.

We can also consider third order in our expansion - with six operators of creation and annihilation of electrons:

$$\langle Tc_\uparrow(\tau)c_\uparrow^+(\tau')c_\uparrow^+(\tau_1)c_\uparrow(\tau_2)c_\uparrow^+(\tau_3)c_\uparrow(\tau_4)\rangle_0 =$$
$$= -\langle T\overrightarrow{c_\uparrow^+(\tau')c_\uparrow(\tau)}c_\uparrow^+(\tau_1)c_\uparrow(\tau_2)c_\uparrow^+(\tau_3)c_\uparrow(\tau_4)\rangle_0 +$$
$$+\langle Tc_\uparrow^+(\tau')\overrightarrow{c_\uparrow^+(\tau_1)c_\uparrow(\tau)}c_\uparrow(\tau_2)c_\uparrow^+(\tau_3)c_\uparrow(\tau_4)\rangle_0 +$$
$$+\langle Tc_\uparrow^+(\tau')c_\uparrow^+(\tau_1)c_\uparrow(\tau_2)\rangle_0\overrightarrow{c_\uparrow^+(\tau_3)c_\uparrow(\tau)}c_\uparrow(\tau_4)\rangle_0 =$$

$$-\langle T\overrightarrow{c_\uparrow^+(\tau')c_\uparrow(\tau)}\overrightarrow{c_\uparrow^+(\tau_1)c_\uparrow(\tau_2)}\overrightarrow{c_\uparrow^+(\tau_3)c_\uparrow(\tau_4)}\rangle_0 +$$
$$+\langle T\overrightarrow{c_\uparrow^+(\tau')c_\uparrow(\tau)}\overrightarrow{c_\uparrow^+(\tau_1)c_\uparrow(\tau_4)}\overrightarrow{c_\uparrow^+(\tau_3)c_\uparrow(\tau_2)}\rangle_0 +$$
$$+\langle T\overrightarrow{c_\uparrow^+(\tau')c_\uparrow(\tau_2)}\overrightarrow{c_\uparrow^+(\tau_1)c_\uparrow(\tau)}\overrightarrow{c_\uparrow^+(\tau_3)c_\uparrow(\tau_4)}\rangle_0 -$$
$$-\langle T\overrightarrow{c_\uparrow^+(\tau')c_\uparrow(\tau_4)}\overrightarrow{c_\uparrow^+(\tau_1)c_\uparrow(\tau)}\overrightarrow{c_\uparrow^+(\tau_3)c_\uparrow(\tau_2)}\rangle_0 +$$
$$+\langle T\overrightarrow{c_\uparrow^+(\tau')c_\uparrow(\tau_4)}\overrightarrow{c_\uparrow^+(\tau_1)c_\uparrow(\tau_2)}\overrightarrow{c_\uparrow^+(\tau_3)c_\uparrow(\tau)}\rangle_0 -$$
$$-\langle T\overrightarrow{c_\uparrow^+(\tau')c_\uparrow(\tau_2)}\overrightarrow{c_\uparrow^+(\tau_3)c_\uparrow(\tau)}\overrightarrow{c_\uparrow^+(\tau_1)c_\uparrow(\tau_4)}\rangle_0 - \qquad (5.4)$$

And finally

$$\langle Tc_\uparrow(\tau)c_\uparrow^+(\tau')c_\uparrow^+(\tau_1)c_\uparrow(\tau_2)c_\uparrow^+(\tau_3)c_\uparrow(\tau_4)\rangle_0 =$$
$$= \sum_r g_{0\uparrow}^{(r)}(\tau-\tau')g_{0\uparrow}^{(r)}(\tau_2-\tau_1)g_{0\uparrow}^{(r)}(\tau_4-\tau_3)\langle X^{rr}\rangle_0 -$$

$$-\sum_r g_{0\uparrow}^{(r)}(\tau-\tau')g_{0\uparrow}^{(r)}(\tau_4-\tau_1)g_{0\uparrow}^{(r)}(\tau_2-\tau_3)\langle X^{rr}\rangle_0 -$$

$$-\sum_r g_{0\uparrow}^{(r)}(\tau_2-\tau')g_{0\uparrow}^{(r)}(\tau-\tau_1)g_{0\uparrow}^{(r)}(\tau_4-\tau_3)\langle X^{rr}\rangle_0 +$$

$$+\sum_r g_{0\uparrow}^{(r)}(\tau_4-\tau')g_{0\uparrow}^{(r)}(\tau-\tau_1)g_{0\uparrow}^{(r)}(\tau_2-\tau_3)\langle X^{rr}\rangle_0 -$$

$$-\sum_r g_{0\uparrow}^{(r)}(\tau_4-\tau')g_{0\uparrow}^{(r)}(\tau_2-\tau_1)g_{0\uparrow}^{(r)}(\tau-\tau_3)\langle X^{rr}\rangle_0 +$$

$$+\sum_r g_{0\uparrow}^{(r)}(\tau_2-\tau')g_{0\uparrow}^{(r)}(\tau-\tau_3)g_{0\uparrow}^{(r)}(\tau_4-\tau_1)\langle X^{rr}\rangle_0 \qquad (5.5)$$

The similar procedure is also actual in the case of higher order terms. Using the diagrammatic series we can separate connected and disconnected "vacuum" (without external verteces) parts of diagrams. First of them are create geometric progression in the frequency representation. Second ones, after infinite series summation, give exponential contributions from diagrams in subspaces $|r\rangle$. The latter look like closed rings of different length (created by unperturbed Green's function and coherent potential lines).

So, for numerator in Green's function $\langle Tc_\uparrow(\tau)c_\uparrow^+(\tau')\rangle_{num}$ we will have after calculation

$$\langle Tc_\uparrow(\tau)c_\uparrow^+(\tau')\rangle_{num} = \sum_r \Big[g_{0\uparrow}^{(r)}(\omega_n) - g_{0\uparrow}^{(r)}(\omega_n)J_\uparrow(\omega_n)g_{0\uparrow}^{(r)}(\omega_n) +$$

$$+g_{0\uparrow}^{(r)}(\omega_n)J_\uparrow(\omega_n)g_{0\uparrow}^{(r)}(\omega_n)J_\uparrow(\omega_n)g_{0\uparrow}^{(r)}(\omega_n) - \dots \Big] \langle X^{rr}\rangle_0 e^{Q_r} =$$

$$= \sum_r \frac{g_{0\uparrow}^{(r)}(\omega_n)}{1+g_{0\uparrow}^{(r)}(\omega_n)J_\uparrow(\omega_n)}\langle X^{rr}\rangle_0 e^{Q_r} \qquad (5.6)$$

Here, Q_r in analytical form is

$$Q_r = \sum_{\omega_n}\sum_\sigma g_{0\sigma}^{(r)}(\omega_n)J_\sigma(\omega_n) - \frac{1}{2}\Big[\sum_{\omega_n}\sum_\sigma g_{0\sigma}^{(r)}(\omega_n)J_\sigma(\omega_n) \Big]^2 +$$

$$\frac{1}{3}\Big[\sum_{\omega_n}\sum_\sigma g_{0\sigma}^{(r)}(\omega_n)J_\sigma(\omega_n) \Big]^3 - \dots \qquad (5.7)$$

and using $-\ln(1+x) = -x + \frac{x^2}{2} - \frac{x^3}{3} + \frac{x^4}{4} - \dots$ we have

$$Q_r = \sum_{\omega_n}\sum_\sigma \ln(1+g_{0\sigma}^{(r)}(\omega_n)J_\sigma(\omega_n)) \qquad (5.8)$$

This means:

$$Q_1 = \sum_{\omega_n}\ln(1+g_{0\uparrow}^{(1)}(\omega_n)J_\uparrow(\omega_n)) + \sum_{\omega_n}\ln(1+g_{0\downarrow}^{(1)}(\omega_n)J_\downarrow(\omega_n))$$

$$Q_{\widetilde{1}} = \sum_{\omega_n}\ln(1+g_{0\uparrow}^{(\widetilde{1})}(\omega_n)J_\uparrow(\omega_n)) + \sum_{\omega_n}\ln(1+g_{0\downarrow}^{(\widetilde{1})}(\omega_n)J_\downarrow(\omega_n))$$

$$Q_3 = \sum_{\omega_n}\ln(1+g_{0\downarrow}^{(3)}(\omega_n)J_\downarrow(\omega_n))$$

$$Q_{\widetilde{3}} = \sum_{\omega_n}\ln(1+g_{0\downarrow}^{(\widetilde{3})}(\omega_n)J_\downarrow(\omega_n))$$

$$Q_4 = \sum_{\omega_n}\ln(1+g_{0\uparrow}^{(4)}(\omega_n)J_\uparrow(\omega_n))$$

$$Q_{\widetilde{4}} = \sum_{\omega_n}\ln(1+g_{0\uparrow}^{(\widetilde{4})}(\omega_n)J_\uparrow(\omega_n)) \qquad (5.9)$$

The next step is to calculate the denominator $\langle\widetilde{\sigma}(\beta)\rangle_0$

$$\langle\widetilde{\sigma}(\beta)\rangle_0 = 1 - \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_\sigma J_\sigma(\tau_1-\tau_2)\langle Tc_\sigma^+(\tau_1)c_\sigma(\tau_2)\rangle_0 +$$

$$+\frac{1}{2!}\int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_4 \sum_\sigma\sum_{\sigma'} J_\sigma(\tau_1-\tau_2)J_{\sigma'}(\tau_3-\tau_4) \times \qquad (5.10)$$

$$\times \langle Tc_\sigma^+(\tau_1)c_\sigma(\tau_2)c_{\sigma'}^+(\tau_3)c_{\sigma'}(\tau_4)\rangle_0 - \dots$$

In diagrammatic representation this series is expressed through the set of "vacuum" diagrams. And the number of such diagrams in the n-th order of perturbation theory very fast increases with increasing of n. The final result could be expressed as contributions Q_r of mentioned above ring diagrams. In such a case, we have

$$\langle\sigma(\beta)\rangle_0 = 1 + \sum_r \Big[Q_r + \frac{1}{2!}Q_r^2 + \frac{1}{3!}Q_r^3 + \dots \Big]\langle X^{rr}\rangle_0 =$$

$$= \sum_r e^{Q_r}\langle X^{rr}\rangle_0 \qquad (5.11)$$

Finally, our analytical result is

$$\langle Tc_\uparrow^+ c_\uparrow\rangle = \frac{\sum_r \frac{g_{0\uparrow}^{(r)}(\omega_n)}{1+g_{0\uparrow}^{(r)}(\omega_n)J_\uparrow(\omega_n)}\langle X^{rr}\rangle_0 e^{Q_r}}{\sum_p e^{Q_p}\langle X^{pp}\rangle_0} \qquad (5.12)$$

and for spin $\sigma = \downarrow$

$$\langle Tc_{\downarrow}^+ c_{\downarrow} \rangle = \frac{\sum_r \frac{g_{0\downarrow}^{(r)}(\omega_n)}{1+g_{0\downarrow}^{(r)}(\omega_n)J_{\downarrow}(\omega_n)} \langle X^{rr} \rangle_0 e^{Q_r}}{\sum_p e^{Q_p} \langle X^{pp} \rangle_0} \tag{5.13}$$

6. Electron energy spectrum

Now, we have the closed system of equations to solve our problem: to calculate the Green's function $G_{\uparrow}^{(a)}(\omega)$ and the coherent potential $J_{\uparrow}(\omega)$

$$G_k^{\sigma}(\omega) = \frac{1}{[\Xi_{\sigma}(\omega)]^{-1} - t_k}$$

$$G_{\sigma}^{(a)}(\omega) = \frac{1}{[\Xi_{\sigma}(\omega)]^{-1} - J_{\sigma}(\omega)} = \frac{1}{N} \sum_k G_k^{\sigma}(\omega) \tag{6.1}$$

$$G_{\sigma}^{(a)}(\omega) = \frac{\sum_r \frac{g_{0\sigma}^{(r)}(\omega_n)}{1+g_{0\sigma}^{(r)}(\omega_n)J_{\sigma}(\omega_n)} \langle X^{rr} \rangle_0 e^{Q_r}}{\sum_p e^{Q_p} \langle X^{pp} \rangle_0}$$

To sum over the $\overrightarrow{k}$ we use the semi-elliptical density of states $\rho_0(t) = \frac{2}{\pi W^2}\sqrt{W^2 - t^2}$. In this case $J_{\sigma}(\omega) = \frac{W^2}{4}G_{\sigma}^{(a)}(\omega)$ [5], and our final equation for coherent potential $J_{\sigma}(\omega)$ is the following

$$J_{\sigma}(\omega_n) = \frac{W^2}{4} \frac{\sum_r \frac{g_{0\sigma}^{(r)}(\omega_n)}{1+g_{0\sigma}^{(r)}(\omega_n)J_{\sigma}(\omega_n)} \langle X^{rr} \rangle_0 e^{Q_r}}{\sum_p e^{Q_p} \langle X^{pp} \rangle_0}$$

In a usual way we perform analytical continuation on real axis ($i\omega_n \to \omega - i\delta$) and only solutions with $\Im J_{\sigma}(\omega) > 0$ must be considered.

Possibility of existence of four, three or two separate subbands or joining into the single one (when a gap in spectrum disappears) depends on the model parameter values. All these cases are shown in the Figure 1.

Band boundaries are determined form the condition $\Im J_{\sigma}(\omega) \to 0$. In figure 2 their dependence on coupling constant g are presented. And in figure 3 the dependence electron band boundaries on tunneling level splitting are presented.

At the regime of constant chemical potential we can calculate an electron concentration mean value as:

$$\langle n_{\uparrow} \rangle = \frac{1}{\beta} \sum_m G_{\uparrow}(\omega_m) e^{-i\omega_n * 0} \tag{6.2}$$
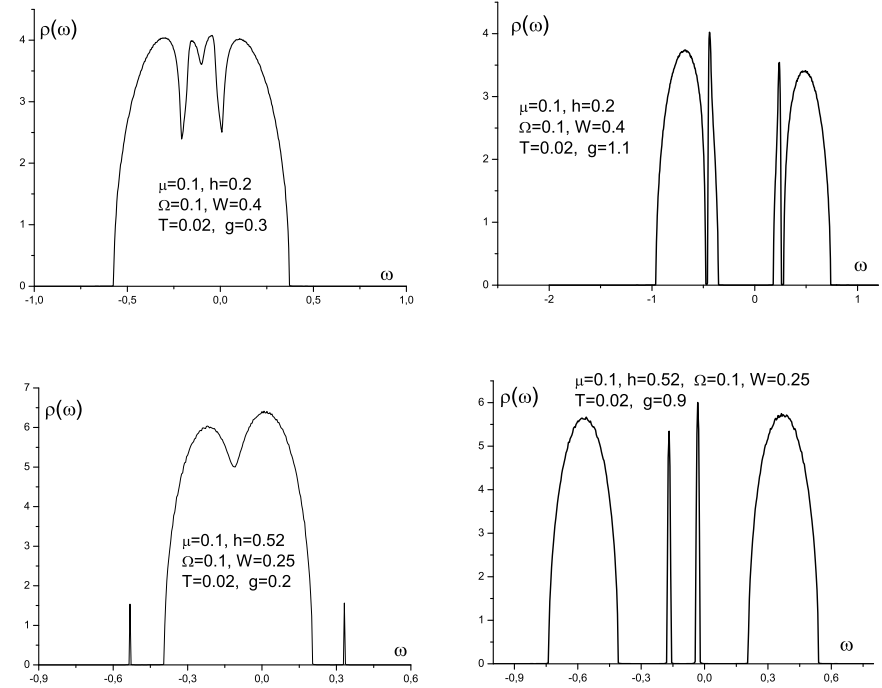

Fig.1 Density of states $\rho(\omega)$ at various values of the the tunneling-like level splitting, the pseudospin-electron interaction and asymmetry of the local anharmonic potential
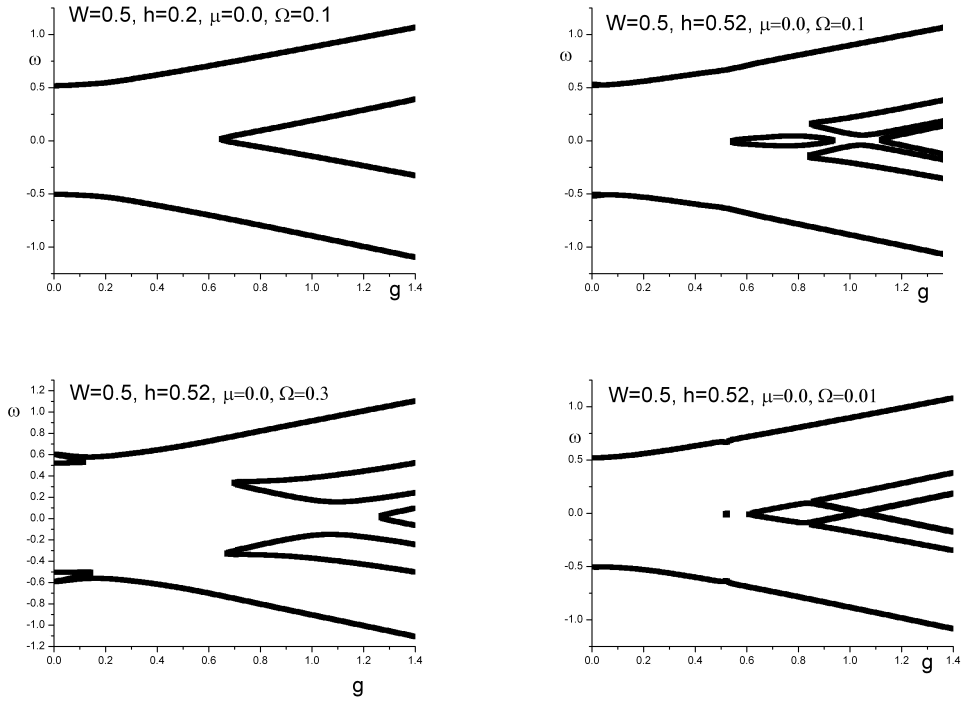
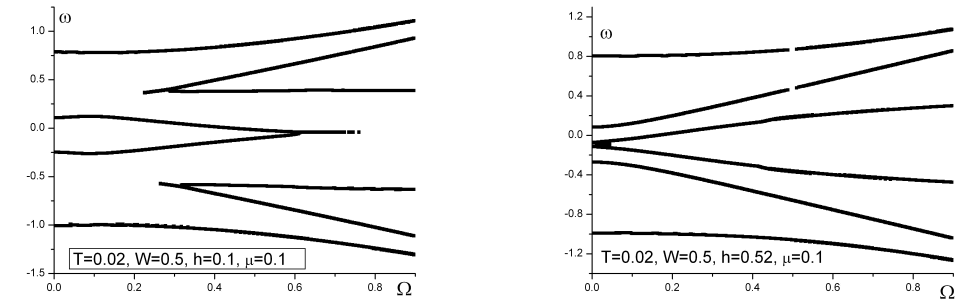Fig.2 Electron band boundaries

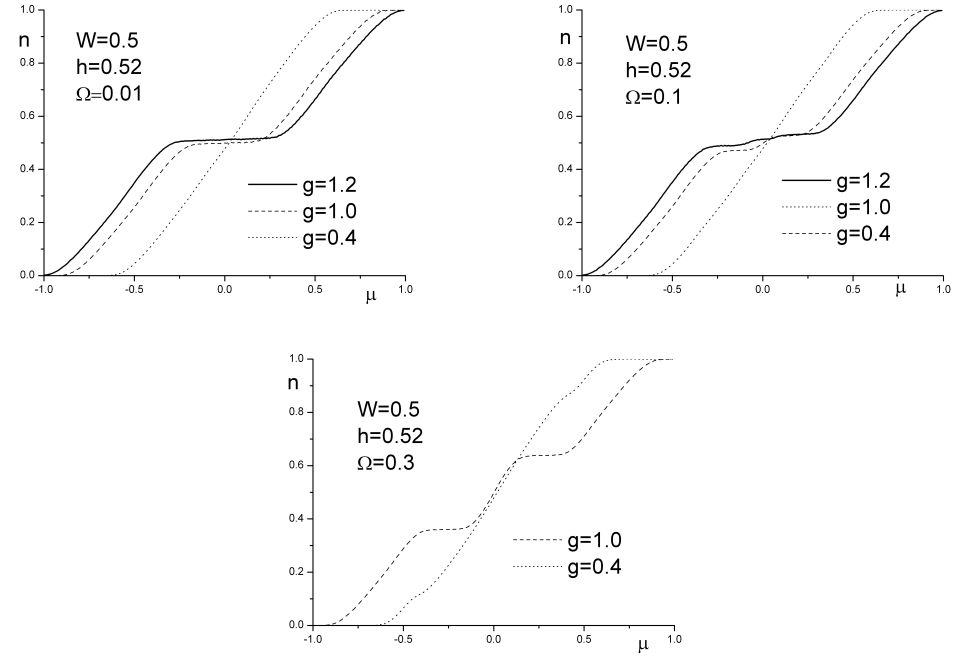Fig.3 Electron band boundaries

Fig.4 Electron concentration mean value

Several dependencies of electron mean value on chemical potential with different values of the model parameters are presented on figure 4.

7. Conclusions

The electron energy spectrum of the pseudospin-electron model is considered. For this purpose the dynamical mean field method is applied. The effective single-site problem is solved within original approach based on use of diagrammatic series and Wick's theorem are established; the alloy analogy approximation is used.

The obtained results show that in the real system, which exhibit the local anharmonicity of lattice vibrations, the metal-insulator transition, determined by the short-ranged electron correlation, is influenced by that anharmonic subsystem. Changing the parameters of local anharmonicity (e.g, the shape of potential well), one can affect the conditions of appearing a gap.

The more complete analysis of reconstruction of energy spectrum will be a subject of our subsequent consideration.

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