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Band electron spectrum and thermodynamical properties of the pseudospin-electron model with tunneling splitting of levels

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Електронній спектр та термодинамічні властивості псевдоспін-електронної моделі тунельним розщепленням рівнів

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Анотація. Розглянуто псевдоспін-електронну модель з тунельним розщепленням рівнів. Для її дослідження використано узагальнення методу динамічного середнього поля на системи з корельованим переносом. В наближенні типу сплаву проведено чисельні дослідження електронної густини станів. Також досліджено залежність концентрації електронів та середнього значення псевдоспінів від хімічного потенціалу, поля асиметрії та тунелювання. Показано що в наближенні типу сплаву модель демонструє фазовий перехід першого роду у феромагнітний стан при зміні хімічного потенціалу.

Band electron spectrum and thermodynamical properties of the pseudospin-electron model with tunneling splitting of levels

O.Ya. Farenyuk, A.M. Shvaika

Abstract. The pseudospin-electron model with tunneling splitting of levels is considered. Generalization of dynamical mean-field method for systems with correlated hopping was applied to the investigation of the model. Within the alloy-analogy approximation the numerical investigations were conducted and electron spectrum was calculated. The dependences of the electron concentrations and average pseudospin values on chemical potential, asymmetry field and tunneling were obtained. It was shown, that in alloy-analogy approximation the model possess the first order phase transition to ferromagnetic state with the change of chemical potential and second order phase transition with the change of temperature.

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1. Introduction

One of the main models for describing strongly correlated electron systems is the Hubbard model and it's extensions and modifications. The model is often generalized by introducing of additional degrees of freedom. In particular, it is supposed that interaction of electrons with a lattice vibrations is important for describing high-temperature superconductors [1] and proton-electron interaction in molecular and crystalline systems with hydrogen bonds [2]. Because anharmonicity in such a systems is principally local, it can be considered by using pseudospin formalism. Important particular case of anharmonic vibrations is local potential with two minima, which corresponds to absolute pseudospin value 1/2. The pseudospin-electron model (PEM) [3] is generalization of the Hubbard model which includes pseudospins with absolute value 1/2.

The Hamiltonian of the model has the following form:

$$H = \sum_i H_i + H_t + H_{ss}, \tag{1.1}$$

$$H_t = \sum_{i,j,\sigma} t_{ij} a^+_{i\sigma} a_{j\sigma}, \tag{1.2}$$

$$H_{ss} = -\frac{1}{2} \sum_{i,j} J_{ij} S^z_i S^z_j, \tag{1.3}$$

$$H_i = U n_{i\uparrow} n_{i\downarrow} + g n_i, S^z_i - h S^z_i - \Omega S^x_i - \mu n_i, \tag{1.4}$$

where H_i is the single-site Hamiltonian, H_t is electron transfer and H_{ss} is direct pseudospin-pseudospin interaction. $n_{i\sigma} = a^+_{i\sigma} a_{j\sigma}$ is the σ-spin electron number operator, $g n_i S^z_i$ represents interaction with the anharmonic mode (pseudospin). U is Coulomb repulsion of the electrons at one site. ΩS^x_i describes tunneling splitting of vibration mode and $h S^z_i$ is asymmetry of the anharmonic potential.

PEM was investigated in many special cases. Among them are:

- a model with the inclusion of the direct pseudospin-pseudospin interaction (but without electron transfer ($t_{ij} = 0$)) [4,5]
- PEM in the case of absence of the direct pseudospin-pseudospin interaction ($J_{ij} = 0$), when pseudospins interact through the electron subsystem [6].

Special attention was paid to electron spectra [7], the pseudospin and collective dynamics [8], effective electron-electron interaction [9], correlation functions ($\langle S^z S^z \rangle$, $\langle S^z n \rangle$, $\langle nn \rangle$), possibility of the phase separation

and charge-ordered phases [6]. Phase transitions between states with different electron concentrations and with different pseudospin orientations were also studied.

In the case of direct pseudospin-pseudospin interaction PEM is investigated mainly within the mean field approximation (MFA) [4] and the transfer matrixes formalism [5]. PEM without direct pseudospin-pseudospin is investigated using generalized random phase approximation (GRPA) [10] and dynamic mean-field theory (DMFT) [11]. Many special cases of such modification of PEM were studied:

- simplified PEM with $U = 0$ and $\Omega = 0$ or $\Omega \neq 0$ [8,12],
- a model with the infinitely large Coloumb interaction $U \to \infty$ [13, 14]
- PEM with $\Omega \neq 0$ but symmetric anharmonic potential $h = 0$ [7],
- two-sublattice PEM [15].

The simplified PEM ($U = 0$ and $\Omega = 0$) corresponds to the Falicov-Kimball (FK) model but differ in thermodynamic equilibrium conditions[1] [11].

This paper presents investigation of the PEM with tunneling splitting of levels without direct pseudospin-pseudospin interaction. Generalization of dynamical mean-field method for systems with correlated hopping was applied to the investigation of the model. Within the alloy-analogy approximation the numerical investigations were conducted and electron spectrum was calculated. The dependences of the electron concentrations and average pseudospin values on chemical potential, asymmetry field and tunneling probability were obtained.

Special attention was paid to the phase transition to the ferromagnetic state with the change of chemical potential and temperature. Different aspects of possibility of ferromagnetism in PEM model were analyzed.

2. Analysis of the Hamiltonian

In the case of narrow bands ($t \ll U$) and absence of the direct pseudospin-pseudospin interaction, the single-site Hamiltonian (1.4) plays a role of an initial approximation, so it is useful to introduce the

[1] $S^z = const$ for the FK model and $h = const$ for the PEM.

Hubbard operators $X_i^{RS} \equiv |i,R\rangle\langle i,S|$ which acts in the space spanned by the state vectors, defined as:

$$|i,p\rangle = |n_{i\uparrow}, n_{i\downarrow}, S_i^z\rangle. \tag{2.1}$$

Then single-site Hamiltonian H_i can be expressed as [16]:

$$H_i = \sum_{p=1}^{4} \lambda_p X_i^{pp} - \frac{\Omega}{2} \sum_{p=1}^{4} (X_i^{p\tilde{p}} + X_i^{\tilde{p}p}), \tag{2.2}$$

where:

$$\lambda_{1,\tilde{1}} = \mp\frac{h}{2},\ \lambda_{2,\tilde{2}} = -2\mu + U \pm (g - \frac{h}{2}),\ \lambda_{3,\tilde{3}} = \lambda_{4,\tilde{4}} = -\mu \pm (g-h). \tag{2.3}$$

This Hamiltonian is diagonal for $\Omega = 0$ (no tunneling splitting of the vibrational modes). For $\Omega \neq 0$ we can diagonalize it by using following unitary transformation [16]:

$$\begin{pmatrix} |R\rangle \\ |\tilde{R}\rangle \end{pmatrix} = \begin{pmatrix} \cos(\phi_r) & \sin(\phi_r) \\ -\sin(\phi_r)\cos(\phi_r) & \end{pmatrix} \begin{pmatrix} |r\rangle \\ |\tilde{r}\rangle \end{pmatrix}, \tag{2.4}$$

where:

$$\cos(2\phi_r) = \frac{n_r g - h}{\sqrt{(n_r g - h)^2 + \Omega^2}}; \quad \sin(2\phi_r) = \frac{\Omega}{\sqrt{(n_r g - h)^2 + \Omega^2}}. \tag{2.5}$$

Then we have:

$$H_i = \sum_p \lambda_p X_i^{pp} \tag{2.6}$$

and

$$\lambda_{r,\tilde{r}} = U\delta_{r,2} - \mu n_r \pm \frac{1}{2}\sqrt{(n_r g - h)^2 + \Omega^2}. \tag{2.7}$$

Here n_r denotes number of electrons for state r : $n_1 = 0$, $n_2 = 2$, $n_3 = 1$, $n_4 = 1$; $n_r = n_{\tilde{r}}$. After transformation (2.4) Hubbard operators are also transformed:

$$\begin{pmatrix} X^{RS} + X^{\tilde{R}\tilde{S}} \\ X^{R\tilde{S}} - X^{\tilde{R}S} \end{pmatrix} = \begin{pmatrix} \cos(\phi_r - \phi_s) & -\sin(\phi_r - \phi_s) \\ \sin(\phi_r - \phi_s) & \cos(\phi_r - \phi_s) \end{pmatrix} \begin{pmatrix} X^{rs} + X^{\tilde{r}\tilde{s}} \\ X^{r\tilde{s}} - X^{\tilde{r}s} \end{pmatrix}, \tag{2.8}$$

$$\begin{pmatrix} X^{RS} - X^{\tilde{R}\tilde{S}} \\ X^{R\tilde{S}} + X^{\tilde{R}S} \end{pmatrix} = \begin{pmatrix} \cos(\phi_r + \phi_s) & \sin(\phi_r + \phi_s) \\ -\sin(\phi_r + \phi_s)\cos(\phi_r + \phi_s) & \end{pmatrix} \begin{pmatrix} X^{rs} - X^{\tilde{r}\tilde{s}} \\ X^{r\tilde{s}} + X^{\tilde{r}s} \end{pmatrix}. \tag{2.9}$$

In the new basis total Hamiltonian can be written as:

$$H = \sum_i \sum_r \lambda_r X_i^{rr} + \sum_{ij} \sum_\sigma t_{ij\sigma} a_{i\sigma}^+ a_{j\sigma}. \tag{2.10}$$

Here creation (destruction) operators are defined as:

$$a_\sigma^+ = \sum_{mn} A_{mn}^\sigma X_i^{mn}, \qquad a_\sigma = \sum_{mn} A_{mn}^\sigma X_i^{nm}, \tag{2.11}$$

where:

$$\begin{array}{llll} A_{41}^\uparrow = & A_{\tilde{4}\tilde{1}}^\uparrow = \cos(\phi_{41}), & A_{23}^\uparrow = & A_{\tilde{2}\tilde{3}}^\uparrow = \cos(\phi_{23}), \\ A_{\tilde{4}1}^\uparrow = & -A_{4\tilde{1}}^\uparrow = \sin(\phi_{41}), & A_{\tilde{2}3}^\uparrow = & -A_{2\tilde{3}}^\uparrow = \sin(\phi_{23}), \\ A_{31}^\downarrow = & A_{\tilde{3}\tilde{1}}^\downarrow = \cos(\phi_{31}), & A_{24}^\downarrow = & A_{\tilde{2}\tilde{4}}^\downarrow = -\cos(\phi_{24}), \\ A_{\tilde{3}1}^\downarrow = & -A_{3\tilde{1}}^\downarrow = \sin(\phi_{31}), & A_{\tilde{2}4}^\downarrow = & -A_{2\tilde{4}}^\downarrow = -\sin(\phi_{24}), \end{array} \tag{2.12}$$

and all other are equal to zero. Here the designation $\phi_{pq} = \phi_p - \phi_q$ is used.

One can see, that for the diagonalized Hamiltonian, hopping integral value depends on states of neighboring lattice sites. Hopping of that kind is called correlated hopping and can be dealed with using matrix representations of all quantities [17]. In our case, hopping term can be rewritten in the following way:

$$H_t = \sum_{ij} \sum_\sigma t_{ij\sigma} a_{i\sigma}^+ a_{j\sigma}, \tag{2.13}$$

$$t_{ij\sigma} a_{i\sigma}^+ a_{j\sigma} = \left((Y_{i\tau(\sigma)}^1)^+, (Y_{i\tau(\sigma)}^2)^+, (Y_{i\tau(\sigma)}^3)^+, (Y_{i\tau(\sigma)}^4)^+ \right) \hat{t}_{ij\sigma} \begin{pmatrix} Y_{i\tau(\sigma)}^1 \\ Y_{i\tau(\sigma)}^2 \\ Y_{i\tau(\sigma)}^3 \\ Y_{i\tau(\sigma)}^4 \end{pmatrix}, \tag{2.14}$$

where:

$$\begin{array}{ll} Y_{i\tau(\uparrow)}^1 = X_{i\tau}^{14} + X_{i\tau}^{\tilde{1}\tilde{4}}, & Y_{i\tau(\uparrow)}^2 = X_{i\tau}^{1\tilde{4}} - X_{i\tau}^{\tilde{1}4}, \\ Y_{i\tau(\uparrow)}^3 = X_{i\tau}^{32} + X_{i\tau}^{\tilde{3}\tilde{2}}, & Y_{i\tau(\uparrow)}^4 = X_{i\tau}^{3\tilde{2}} - X_{i\tau}^{\tilde{3}2}, \\ Y_{i\tau(\downarrow)}^1 = X_{i\tau}^{13} + X_{i\tau}^{\tilde{1}\tilde{3}}, & Y_{i\tau(\downarrow)}^2 = X_{i\tau}^{1\tilde{3}} - X_{i\tau}^{\tilde{1}3}, \\ Y_{i\tau(\downarrow)}^3 = X_{i\tau}^{42} + X_{i\tau}^{\tilde{4}\tilde{2}}, & Y_{i\tau(\downarrow)}^4 = X_{i\tau}^{4\tilde{2}} - X_{i\tau}^{\tilde{4}2}, \end{array}$$

and the designation $X_{i\tau}^{pq} \equiv X_i^{pq}(\tau)$ was used.

The correlated hopping matrix for the model is:

$$\hat{t}_{ij\sigma} = t_{ij} \left(\gamma_\sigma^T \otimes \gamma_\sigma \right), \tag{2.15}$$

$$\gamma_\uparrow = (\cos\phi_{41}, \sin\phi_{41}, \cos\phi_{23}, \sin\phi_{23}),$$
$$\gamma_\downarrow = (\cos\phi_{31}, \sin\phi_{31}, -\cos\phi_{24}, -\sin\phi_{24}).$$

So, one can see that correlated hopping, introduced by tunneling splitting is simple enough, because rank of direct product of vectors is always equal to one:

$$\operatorname{rank}\left(\gamma_\sigma^T \otimes \gamma_\sigma\right) = 1. \tag{2.16}$$

3. Temperature Green Functions. Perturbation theory in terms of electronic hopping

Investigation of the model is performed using temperature Green functions.

Single-site Hamiltonian (1.4) was selected as a zero-order Hamiltonian. Thus statistical operator can be written as:

$$\hat\rho = e^{-\beta\hat H_0}\hat\sigma(\beta), \tag{3.1}$$

where

$$\hat\sigma(\beta) = T\exp\left\{-\int_0^\beta d\tau\int_0^\beta d\tau'\sum_{ij\sigma} t_{ij\sigma}(\tau-\tau')a_{i\sigma}^+(\tau)a_{j\sigma}(\tau')\right\}, \qquad H_0 = \sum_i H_i. \tag{3.2}$$

For the grand canonical potential functional we have:

$$\Omega = -\frac{1}{\beta}\ln \operatorname{Sp}\hat\rho = \Omega_0 - \frac{1}{\beta}\ln\langle\hat\sigma(\beta)\rangle_0, \tag{3.3}$$

$$\Omega_0 = -\frac{1}{\beta}\ln \operatorname{Sp} e^{-\beta H_0}. \tag{3.4}$$

So we can define single-electron Green's function as:

$$G_{ij\sigma}(\tau-\tau') = -\langle T a_{i\sigma}(\tau)a_{j\sigma}^+(\tau')\rangle = \frac{\delta\Omega}{\delta t_{ji\sigma}(\tau'-\tau)}, \tag{3.5}$$

and mean values are

$$\langle n\rangle = \frac{1}{N}\sum_{i\sigma}\langle n_{i\sigma}\rangle = -\frac{1}{N}\frac{d\Omega}{d\mu}, \tag{3.6}$$

$$\langle S^z\rangle = \frac{1}{N}\sum_{i}\langle S_i^z\rangle = -\frac{1}{N}\frac{d\Omega}{dh}, \tag{3.7}$$

$$\langle S^x\rangle = \frac{1}{N}\sum_{i}\langle S_i^x\rangle = -\frac{1}{N}\frac{d\Omega}{d\Omega_H}. \tag{3.8}$$

Here mean values are define by

$$\langle\ldots\rangle = \frac{1}{Z}\operatorname{Sp}(\ldots\hat\rho), \tag{3.9}$$

$$Z = \operatorname{Sp}\hat\rho, \tag{3.10}$$

or

$$\langle\ldots\rangle = \frac{1}{\langle\hat\sigma(\beta)\rangle_0}\langle\ldots\hat\sigma(\beta)\rangle_0 = \langle\ldots\hat\sigma(\beta)\rangle_{0c}, \tag{3.11}$$

where

$$\langle\ldots\rangle_0 = \frac{1}{Z_0}\operatorname{Sp}(\ldots e^{-\beta H_0}), \tag{3.12}$$

$$Z_0 = \operatorname{Sp} e^{-\beta H_0}. \tag{3.13}$$

Let us introduce corresponding matrix Green functions[2] and other quantities [17]. According to (2.13), (2.14) and (2.15) matrix form of Green's function $\hat G_{ij,\sigma}(\tau-\tau')$ is defined as:

$$\hat G_{ij,\sigma}^{\mu\nu}(\tau-\tau') = \beta\frac{\delta\Omega}{\delta\hat t_{ij,\sigma}^{\nu\mu}(\tau-\tau')}, \tag{3.14}$$

where μ, ν are matrix indices. Then total Green's function (3.5) is equal to:

$$G_\sigma = \operatorname{Sp}\left(\frac{d\hat t_\sigma}{dt_\sigma}\hat G_\sigma\right) = \operatorname{Sp}\left(\left(\gamma_\sigma^T\otimes\gamma_\sigma\right)\hat G_\sigma\right) = \gamma_\sigma\hat G_\sigma\gamma_\sigma^T. \tag{3.15}$$

According to (2.14) and using (3.14) we can write elements of the 4×4 matrix Green's function:

$$G_{ij,\sigma}^{\mu\nu}(\tau-\tau') = -\langle T_\tau Y_{i\tau(\sigma)}^\mu\left(Y_{j\tau'(\sigma)}^\nu\right)^+\rangle. \tag{3.16}$$

It is obvious, that for each matrix element of Green's function we will have sum of T–products of Hubbard operators like $\langle T_\tau X_i^{pq}(\tau)X_{i'}^{p'q'}(\tau')X_{i_1}^{p_1q_1}(\tau_1)X_{i_1'}^{p_1'q_1'}(\tau_1')\ldots\rangle_0$. We can calculate them by the consecutive pairing according to the corresponding Wick's theorem [18]. Zero-order Green functions, which corresponds to (3.16) are explicitly defined in appendix A.

[2] Related to correlated hopping.

4. Dynamical mean field theory of correlated hopping

Because only limited number of lattice models can be solved exactly, one must use some approximations to describe model behavior. Dynamical Mean-Field Theory (DMFT), which is exact in the limit of infinite spatial dimensions $d \to \infty$, is one of the most popular approaches [19]. The DMFT is based on local (single-site) nature of the self-energy in the limit $d \to \infty$. But, for systems with correlated hopping self-energy becomes unlocal [20], so it is necessary to modify standard DMFT approach. Let us recall that self-energy appears in the Dyson equation for the one-electron Green's function, and represents many-electron interactions, which are taken into account as perturbations. There is another natural approach — perturbation theory over electron hopping $t_{ij\sigma}$. In this case fundamental equation for the one-electron Green's function is the Larkin equation [17]:

$$\hat{G}_{\mathbf{k}\sigma}(\omega) = \hat{\Xi}_{\mathbf{k}\sigma}(\omega) + \hat{\Xi}_{\mathbf{k}\sigma}(\omega)\hat{t}_{\mathbf{k}\sigma}\hat{G}_{\mathbf{k}\sigma}(\omega), \tag{4.1}$$

where $\Xi_{ij}(\omega)$ is an irreducible part of the Green's function that can not be divided into parts by cutting one hopping line. Formal solution of Larkin equation gives us the Larkin representation of the Green function:

$$\hat{G}_{\mathbf{k}}(\omega) = \left[1 - \hat{\Xi}_{\mathbf{k}}(\omega)\hat{t}_{\mathbf{k}}\right]^{-1}\hat{\Xi}_{\mathbf{k}}(\omega) = \left[\hat{\Xi}_{\mathbf{k}}^{-1}(\omega) - \hat{t}_{\mathbf{k}}\right]^{-1}. \tag{4.2}$$

It was shown in [21], that $\Xi_{ij}(\omega)$ is local in the $d \to \infty$ limit[3]:

$$\Xi_{\sigma}(\omega_n, \mathbf{k}) = \Xi_{\sigma}(\omega_n), \tag{4.3}$$

and this statement is more general than the one about the local nature of the self-energy [17].

Such matrix representation allows to reformulate the Dynamical Mean-Field Theory of the systems with correlated hopping in the terms of local quantities. Equivalency of the irreducible part $\hat{\Xi}_{\sigma}(\omega)$ for the lattice problem and the single-impurity problem leads to the following equation for coherent potential $J_{\sigma}(\omega)$ [17]:

$$\frac{1}{N}\sum_{\mathbf{k}}\left[\hat{\Xi}_{\sigma}^{-1}(\omega) - \hat{t}_{\mathbf{k}\sigma}\right]^{-1} = \left[\hat{\Xi}_{\sigma}^{-1}(\omega) - \hat{J}_{\sigma}(\omega)\right]^{-1} = \hat{G}_{imp,\sigma}(\omega), \tag{4.4}$$

[3]when hopping integral is scaled by $t_{ij} \to \frac{t_{ij}}{\sqrt{d}}$ in order to obtain finite density of states.

which is the matrix generalization of the Brandt-Mielsch [22] equation for the auxiliary Kadanoff-Baym field. Right side of (4.4) is the Larkin representation of the single-site Green's function $\hat{G}_{imp,\sigma}(\omega)$ for the single-impurity problem with statistical operator:

$$\hat{\rho} = e^{-\beta\hat{H}_0}T\exp\left\{-\int_0^{\beta}d\tau\int_0^{\beta}d\tau'\sum_{ij\sigma}J_{\sigma}(\tau-\tau')a_{\sigma}^{+}(\tau)a_{\sigma}(\tau')\right\}. \tag{4.5}$$

The grand canonical potential of the lattice in terms of the quantities for the impurity model [17] is:

$$\frac{\Omega_{lat}}{N} = \Omega_{imp} - \frac{1}{\beta}\sum_{\nu}\left\{\frac{1}{N}\sum_{\mathbf{k},\sigma}\ln\det\left[1 - \hat{\Xi}_{\sigma}(i\omega_\nu)\hat{t}_{\mathbf{k}\sigma}\right]\right.$$
$$\left. - \ln\det\left[1 - \hat{\Xi}_{\sigma}(i\omega_\nu)\hat{J}_{\sigma}(i\omega_\nu)\right]\right\}, \tag{4.6}$$

where Ω_{imp} is the grand canonical potential for the impurity model. Ω_{imp} can be calculated by applying Wick's theorem, but now we have averages of the products of diagonal Hubbard operators at the same site, so we can multiply them and reduce their product to a single Hubbard operator. Finally we get [18]:

$$\Omega_{imp} = -\frac{1}{\beta}\ln\sum_{p}e^{-\beta\Omega_{(p)}}, \tag{4.7}$$

where $\Omega_{(p)}$ is grand canonical potential for subspace $|p\rangle$. Now we can find single-electron Green's function for impurity model by:

$$\hat{G}_{imp,\sigma}(i\omega_n) = \frac{\delta\Omega_{imp}}{\delta\hat{J}_{\sigma}(i\omega_n)} = \sum_{p}w_p\hat{G}_{\sigma(p)}(i\omega_n), \tag{4.8}$$

$$\hat{G}_{\sigma(p)}^{\mu\nu}(i\omega_n) = \frac{\delta\Omega_{(p)}}{\delta\hat{J}_{\sigma}^{\nu\mu}(i\omega_n)} \tag{4.9}$$

where $\hat{G}_{\sigma(p)}^{\mu\nu}(i\omega_n)$ are single-electron Green's functions for subspaces characterized by the statistical weights

$$w_p = \frac{e^{-\beta\Omega_{(p)}}}{\sum_q e^{-\beta\Omega_{(q)}}}. \tag{4.10}$$

As a result single-site (impurity) problem naturally splits into eight subspaces $|p\rangle = |1\rangle, \ldots |\tilde{4}\rangle$ (see also [18]). We also can introduce an irreducible parts of Green's functions in subspaces $\hat{\Xi}_{\sigma(p)}(i\omega_n)$ by

$$\hat{G}_{\sigma(p)}(i\omega_n) = \left[\hat{\Xi}_{\sigma(p)}^{-1}(i\omega_n) - \hat{J}_{\sigma}(i\omega_n)\right]^{-1}. \tag{4.11}$$

Because matrix of electron hopping is direct product (2.15), one can proof that equality (4.4) conserves after transforming it into scalar form by relations:

$$\hat{t_\sigma} = \gamma_\sigma^T t \gamma_\sigma \Longrightarrow \hat{J}_\sigma = J \cdot (\gamma_\sigma^T \otimes \gamma_\sigma) \Leftrightarrow J_\sigma = \gamma_\sigma^T \hat{J}_\sigma \gamma_\sigma. \tag{4.12}$$

The same transformations are also applied to all other matrix quantities, like Green functions and irreducible parts. As a result we can easily switch to scalar form and back for all equations. For example, equation (4.4) can be transformed in the following way:

$$\frac{1}{N}\sum_{\mathbf{k}} \gamma \left[\hat{\Xi}_\sigma^{-1}(\omega) - \hat{t}_{\mathbf{k}\sigma}\right]^{-1} \gamma^T = \sum_p w_p \gamma \left[\hat{\Xi}_{\sigma(p)}^{-1}(\omega) - \hat{J}_\sigma(\omega)\right]^{-1} \gamma^T.$$

Then, for left and right part after using obvious relation:

$$\hat{A}(\gamma^T \otimes \gamma)\hat{B} = \hat{A}\gamma^T \cdot \gamma \hat{B}$$

we have:

$$\begin{aligned}\gamma \left[\hat{\Xi}_\sigma^{-1} - \hat{t}_{\mathbf{k}\sigma}\right]^{-1} \gamma^T &= \gamma \left(\hat{\Xi}_\sigma + \hat{\Xi}_\sigma \left[t_{\mathbf{k}\sigma}(\gamma^T \otimes \gamma)\right] \hat{\Xi}_\sigma + \ldots\right) \gamma^T \\ &= \left(\gamma \Xi_\sigma \gamma^T\right) + \left(\gamma \Xi_\sigma \gamma^T\right) t_{\mathbf{k}\sigma} \left(\gamma \Xi_\sigma \gamma^T\right) + \ldots = \left[\gamma \hat{\Xi}_\sigma^{-1} \gamma^T - t_{\mathbf{k}\sigma}\right]^{-1}\end{aligned}$$

and

$$\gamma \left[\hat{\Xi}_{\sigma(p)}^{-1} - \hat{J}_\sigma\right]^{-1} \gamma^T = \left[\gamma \hat{\Xi}_{\sigma(p)}^{-1} \gamma^T - J_\sigma\right]^{-1}.$$

So scalar form of equation (4.4) can be written as:

$$\begin{aligned}\frac{1}{N}\sum_{\mathbf{k}} \left[\gamma \hat{\Xi}_\sigma^{-1} \gamma^T - t_{\mathbf{k}\sigma}\right]^{-1} &= \left[\gamma \hat{\Xi}_\sigma^{-1} \gamma^T - J_\sigma\right]^{-1} \\ &= \sum_p w_p \left[\gamma \hat{\Xi}_{\sigma(p)}^{-1} \gamma^T - J_\sigma\right]^{-1}.\end{aligned} \tag{4.13}$$

This interchangeability of representations allows us to use whatever form is more convenient in each situation.

5. Alloy-analogy approximation. Numerical calculations

For the pseudospin-electron model with tunneling splitting perturbation theory expansion is very large and inconvenient — for example, third order contribution has near 30000 terms. For obtaining results on behave of the model, we used very simple approximation:

$$\hat{\Xi}_{\sigma(p)}(\omega_n) = \hat{g}_{\sigma(p)}(\omega_n), \tag{5.1}$$

a so-called alloy-analogy approximation. Here $\hat{g}_{\sigma(p)}(\omega_n)$ are zero-order matrix Green functions for subspaces obtained from (3.16).

Then, for the grand canonical potentials for subspaces one can obtain [18]:

$$\Omega_{(p)} = \lambda_p - \frac{1}{\beta}\sum_{n\sigma} \ln\det\left(1 - \hat{\Xi}_{\sigma(p)}(\omega_n)\hat{J}_\sigma(\omega_n)\right). \tag{5.2}$$

For numerical calculations scalar form of equations is more convenient. Starting from (5.2) and using (4.12) one can obtain grand canonical potential for subspaces, expressed in scalar quantities:

$$\Omega_{(p)} = \lambda_p - \frac{1}{\beta}\sum_{n\sigma} \ln\left(1 - \Xi_{\sigma(p)}(\omega_n)J_\sigma(\omega_n)\right), \tag{5.3}$$

where:

$$\Xi_{\sigma(p)} = \gamma_\sigma \hat{\Xi}_{\sigma(p)} \gamma_\sigma^T. \tag{5.4}$$

The first step of the numerical analysis is solving of the equation (4.4) for coherent potential, when irreducible part is defined by (5.1). This equation may have more then one solution, but it is rather complex and contains integrations. It is more convenient to introduce equation for statistical weights w_p, treating them as self-consistency parameters and then use it's solutions for calculating Green functions and coherent potential (see also [23]).

Equation for w_p has following form:

$$w_p = \frac{\exp(-\beta\Omega_{(p)}(\{w_l\}))}{\sum_q \exp(-\beta\Omega_{(q)}(\{w_{l'}\}))}. \tag{5.5}$$

$\Omega_{(p)}(\{w_l\})$ is calculated according to (5.3) using coherent potential $J_\sigma(\omega)$ which is obtained by iterative algorithm, described in details in appendix D. Green functions can be obtained from the same iterative process.

Initial examination of the solutions space of (5.5) was made using Multi-Niche Crowding (MNC) variant of the genetic algorithms (GA) [24]. It allowed us to find all possible potential solutions. Then the candidates were checked and refined using modified Newton method[4].

It was shown that for rather large U the model shows transition to the ferromagnetic state.

[4] The GA are mostly too slow to rich high precision.

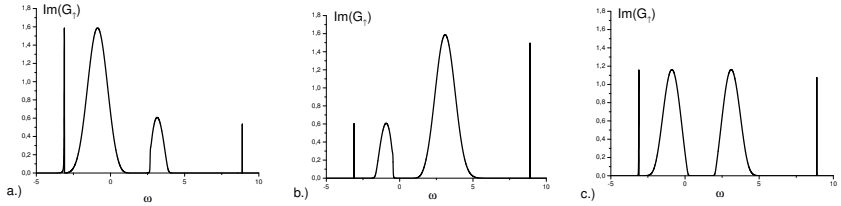

Figure 1. Electron spectrum. Numerical parameters: $h = -2.0$, $g = 1.85$, $\Omega = 1.01$, $U = 4.0$, $\mu = -0.33$, $T = 0.01$, $W = 1.0$, (a),(b) and (c) corresponds to different solutions:

a	b	c
$w_{\tilde{3}} = 0.160$	$w_{\tilde{3}} = 0.840$	$w_{\tilde{3}} = 0.5$
$w_{\tilde{4}} = 0.840$	$w_{\tilde{4}} = 0.160$	$w_{\tilde{4}} = 0.5$
other $w_p = 0$		
$n = 0.833$	$n = 0.833$	$n = 0.881$
$n_\uparrow - n_\downarrow = 0.518$	$n_\uparrow - n_\downarrow = 0.518$	$n_\uparrow - n_\downarrow = 0$
$S^z = -0.48$	$S^z = -0.48$	$S^z = -0.48$
$\Omega_{lat} = -1.95$	$\Omega_{lat} = -1.95$	$\Omega_{lat} = -1.93$

Typical situation is the existence of three solution sets for self-consistency parameters w_p (Figure 1). One of them corresponds to the paramagnetic phase and two other to the ferromagnetic ordering.

Average value of electron concentrations can be obtained in two different ways. One of them is differentiation of the Grand canonical potential by the chemical potential μ. The other way is based on using density of states:

$$n_\sigma = \frac{1}{\beta} \sum_n G_\sigma(i\omega_n). \tag{5.6}$$

For the AA approach thermodynamically obtained concentrations can get unphysical values for some values of the chemical potential, so the second one was used.

Figure 2 presents typical behavior of the electron concentration, depending on chemical potential. One can see that ferromagnetism exists for electron concentrations near the half-filling, both for $n < 1$ and $n > 1$. Gaps on $\mu - n$ diagram corresponds to the unperturbed levels, where present iterative algorithm of calculations fails for AA approximation.

The critical Coulombian repulsion U, shown on Figure 3 is much lower than for ordinary Hubbard model according to [25,26]. Indeed, numerous studies [27–29] revealed that different forms of correlated hopping

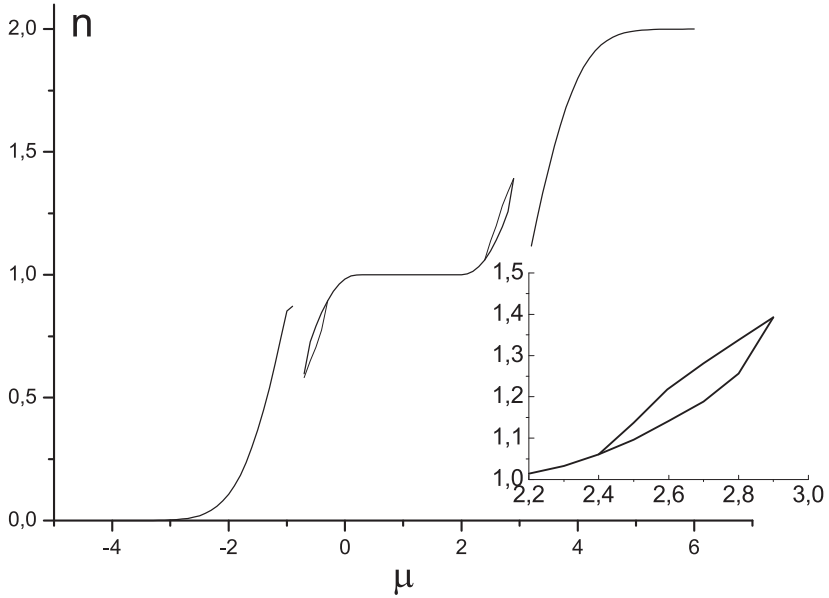

Figure 2. $\mu - n$ diagram. $h = -2.0$, $g = 1.85$, $\Omega = 1.01$, $U = 4.0$, $T = 0.01$, $W = 1.0$

favors ferromagnetism including lowering of the critical U and stabilizing of ferromagnetic ordering.

In addition the model possess phase transition with the change of the temperature. Figure 4 shows change of the magnetization $n_\uparrow - n_\downarrow$ with the temperature.

6. Conclusions

The pseudospin-electron model with tunneling splitting of the vibration mode was investigated. It was shown that correlated hopping formalism is useful for investigating systems with transverse field. The numerical results were obtained within alloy-analogy approximation.

Possibility of the ferromagnetism within alloy-analogy approximation was shown. Ferromagnetism in Hubbard-like models is still controversial [30–32]. In fact, Hubbard model first was proposed as model for describing ferromagnetism in metals. It manifests ferromagnetism for large values of U within mean-field theory [25]. Some other approximations

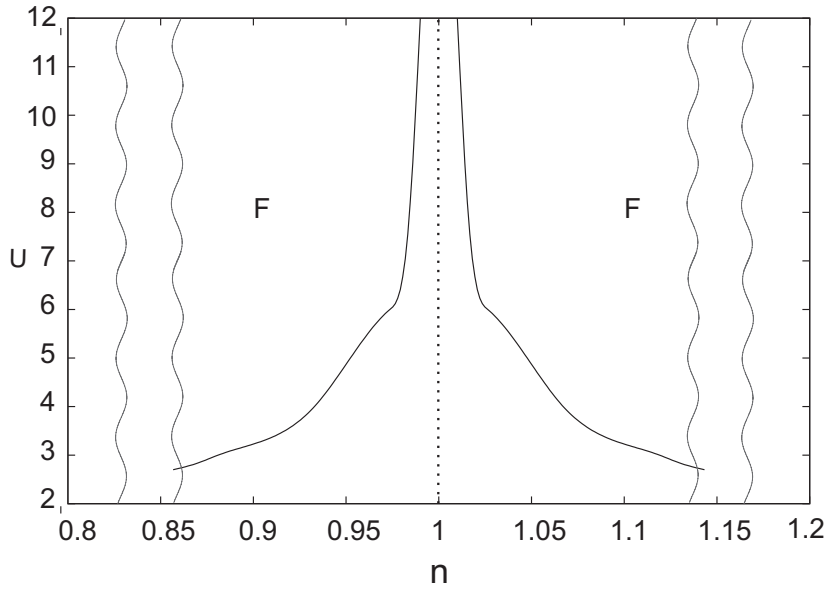

Figure 3. Magnetic phase diagram. F denotes regions where ferromagnetism exists. Wavy lines serve as the boundaries of regions, where AA approximation fails. $h = -2.0$, $g = 1.85$, $\Omega = 1.01$, $T = 0.01$, $W = 1.0$

leads to ferromagnetism too. Gutzwiller method leads to the ferromagnetism even in case of the Gaussian density of states [26] for substantially large U. It is generally accepted that ferromagnetic phase cannot develop in the AA approximation because it lacks mechanism for spin-dependent shift of the center of gravity of the Hubbard bands [23,33]. However in recent years other mechanisms of ferromagnetic ordering, where there is no shift in the relative position of the Hubbard bands, were considered [34]. One of them is connected with the redistribution of the electron densities between spin-up and spin-down electrons. Our scheme of solving the equations for the Green functions leads to the ferromagnetism of that kind.

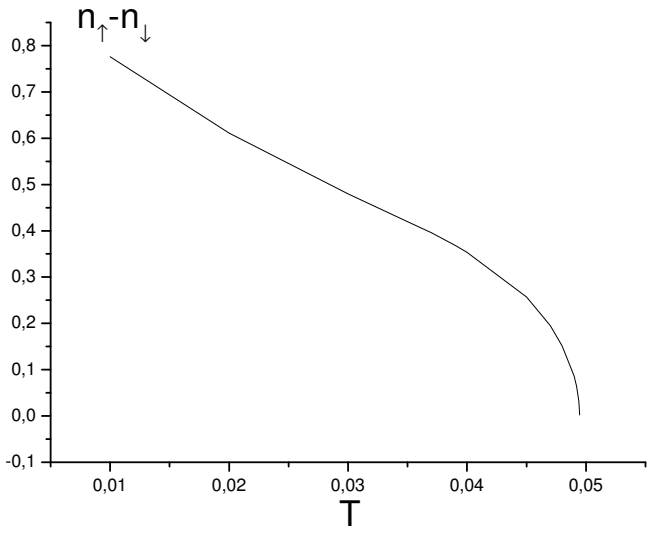

Figure 4. Dependence of magnetization on temperature. $h = -2.0$, $g = 1.85$, $\Omega = 1.01$, $\mu = 1.62$, $U = 8.0$, $T = 0.01$, $W = 1.0$

A. Zero-order matrix Green functions

$$\hat{g}_{\uparrow(1)}(\omega_n) = \begin{pmatrix} \frac{1}{i\omega_n - \lambda_{41}} & 0 & 0\,0 \\ 0 & \frac{1}{i\omega_n - \lambda_{\tilde{4}\tilde{1}}} & 0\,0 \\ 0 & 0 & 0\,0 \\ 0 & 0 & 0\,0 \end{pmatrix}, \quad \hat{g}_{\downarrow(1)}(\omega_n) = \begin{pmatrix} \frac{1}{i\omega_n - \lambda_{31}} & 0 & 0\,0 \\ 0 & \frac{1}{i\omega_n - \lambda_{\tilde{3}\tilde{1}}} & 0\,0 \\ 0 & 0 & 0\,0 \\ 0 & 0 & 0\,0 \end{pmatrix}$$

$$\hat{g}_{\uparrow(\tilde{1})}(\omega_n) = \begin{pmatrix} \frac{1}{i\omega_n - \lambda_{4\tilde{1}}} & 0 & 0\,0 \\ 0 & \frac{1}{i\omega_n - \lambda_{4\tilde{1}}} & 0\,0 \\ 0 & 0 & 0\,0 \\ 0 & 0 & 0\,0 \end{pmatrix}, \quad \hat{g}_{\downarrow(\tilde{1})}(\omega_n) = \begin{pmatrix} \frac{1}{i\omega_n - \lambda_{\tilde{3}\tilde{1}}} & 0 & 0\,0 \\ 0 & \frac{1}{i\omega_n - \lambda_{3\tilde{1}}} & 0\,0 \\ 0 & 0 & 0\,0 \\ 0 & 0 & 0\,0 \end{pmatrix}$$

$$\hat{g}_{\uparrow(4)}(\omega_n) = \begin{pmatrix} \frac{1}{i\omega_n - \lambda_{41}} & 0 & 0\,0 \\ 0 & \frac{1}{i\omega_n - \lambda_{4\tilde{1}}} & 0\,0 \\ 0 & 0 & 0\,0 \\ 0 & 0 & 0\,0 \end{pmatrix}, \quad \hat{g}_{\downarrow(4)}(\omega_n) = \begin{pmatrix} 0\,0 & 0 & 0 \\ 0\,0 & 0 & 0 \\ 0\,0 & \frac{1}{i\omega_n - \lambda_{24}} & 0 \\ 0\,0 & 0 & \frac{1}{i\omega_n - \lambda_{\tilde{2}4}} \end{pmatrix}$$

$$\hat{g}_{\uparrow(\tilde{4})}(\omega_n) = \begin{pmatrix} \frac{1}{i\omega_n-\lambda_{\tilde{4}\tilde{1}}} & 0 & 0\,0 \\ 0 & \frac{1}{i\omega_n-\lambda_{\tilde{4}1}} & 0\,0 \\ 0 & 0 & 0\,0 \\ 0 & 0 & 0\,0 \end{pmatrix},\ \hat{g}_{\downarrow(\tilde{4})}(\omega_n) = \begin{pmatrix} 0\,0 & 0 & 0 \\ 0\,0 & 0 & 0 \\ 0\,0 & \frac{1}{i\omega_n-\lambda_{\tilde{2}\tilde{4}}} & 0 \\ 0\,0 & 0 & \frac{1}{i\omega_n-\lambda_{2\tilde{4}}} \end{pmatrix}$$

$$\hat{g}_{\uparrow(2)}(\omega_n) = \begin{pmatrix} 0\,0 & 0 & 0 \\ 0\,0 & 0 & 0 \\ 0\,0 & \frac{1}{i\omega_n-\lambda_{23}} & 0 \\ 0\,0 & 0 & \frac{1}{i\omega_n-\lambda_{2\tilde{3}}} \end{pmatrix},\ \hat{g}_{\downarrow(2)}(\omega_n) = \begin{pmatrix} 0\,0 & 0 & 0 \\ 0\,0 & 0 & 0 \\ 0\,0 & \frac{1}{i\omega_n-\lambda_{24}} & 0 \\ 0\,0 & 0 & \frac{1}{i\omega_n-\lambda_{2\tilde{4}}} \end{pmatrix}$$

$$\hat{g}_{\uparrow(\tilde{2})}(\omega_n) = \begin{pmatrix} 0\,0 & 0 & 0 \\ 0\,0 & 0 & 0 \\ 0\,0 & \frac{1}{i\omega_n-\lambda_{\tilde{2}\tilde{3}}} & 0 \\ 0\,0 & 0 & \frac{1}{i\omega_n-\lambda_{\tilde{2}3}} \end{pmatrix},\ \hat{g}_{\downarrow(\tilde{2})}(\omega_n) = \begin{pmatrix} 0\,0 & 0 & 0 \\ 0\,0 & 0 & 0 \\ 0\,0 & \frac{1}{i\omega_n-\lambda_{\tilde{2}\tilde{4}}} & 0 \\ 0\,0 & 0 & \frac{1}{i\omega_n-\lambda_{\tilde{2}4}} \end{pmatrix}$$

$$\hat{g}_{\uparrow(3)}(\omega_n) = \begin{pmatrix} 0\,0 & 0 & 0 \\ 0\,0 & 0 & 0 \\ 0\,0 & \frac{1}{i\omega_n-\lambda_{23}} & 0 \\ 0\,0 & 0 & \frac{1}{i\omega_n-\lambda_{\tilde{2}3}} \end{pmatrix},\ \hat{g}_{\downarrow(3)}(\omega_n) = \begin{pmatrix} \frac{1}{i\omega_n-\lambda_{31}} & 0 & 0\,0 \\ 0 & \frac{1}{i\omega_n-\lambda_{3\tilde{1}}} & 0\,0 \\ 0 & 0 & 0\,0 \\ 0 & 0 & 0\,0 \end{pmatrix}$$

$$\hat{g}_{\uparrow(\tilde{3})}(\omega_n) = \begin{pmatrix} 0\,0 & 0 & 0 \\ 0\,0 & 0 & 0 \\ 0\,0 & \frac{1}{i\omega_n-\lambda_{\tilde{2}\tilde{3}}} & 0 \\ 0\,0 & 0 & \frac{1}{i\omega_n-\lambda_{2\tilde{3}}} \end{pmatrix},\ \hat{g}_{\downarrow(\tilde{3})}(\omega_n) = \begin{pmatrix} \frac{1}{i\omega_n-\lambda_{\tilde{3}\tilde{1}}} & 0 & 0\,0 \\ 0 & \frac{1}{i\omega_n-\lambda_{\tilde{3}1}} & 0\,0 \\ 0 & 0 & 0\,0 \\ 0 & 0 & 0\,0 \end{pmatrix}$$

B. Samples of perturbation theory results

Analytical view of first order of perturbation theory for grand canonical potential for subspace $|1\rangle$:

$$\begin{gathered} t_{22}(\omega_n)t_{11}(\omega_\nu)(g_n^{\tilde{4}1}g_\nu^{41}g_\nu^{41} + g_n^{\tilde{4}1}g_n^{\tilde{4}1}g_\nu^{41} - g_\nu^{41}g_\nu^{41}g_{n-\nu}^{1\tilde{1}} + g_n^{\tilde{4}1}g_n^{\tilde{4}1}g_{n-\nu}^{\tilde{1}1})+ \\ t_{11}(\omega_n)t_{22}(\omega_\nu)(g_n^{41}g_\nu^{\tilde{4}1}g_\nu^{\tilde{4}1} + g_n^{41}g_n^{41}g_\nu^{\tilde{4}1} - g_\nu^{\tilde{4}1}g_\nu^{\tilde{4}1}g_{n-\nu}^{1\tilde{1}} + g_n^{41}g_n^{41}g_{n-\nu}^{\tilde{1}1})+ \\ t_{11}(\omega_n)t_{11}(\omega_\nu)(g_n^{41}g_\nu^{41})+ \\ t_{22}(\omega_n)t_{22}(\omega_\nu)(g_n^{\tilde{4}1}g_\nu^{\tilde{4}1})+ \\ t_{12}(\omega_n)t_{12}(\omega_\nu)(g_\nu^{41}g_\nu^{\tilde{4}1}g_{n-\nu}^{1\tilde{1}} - g_n^{41}g_n^{\tilde{4}1}g_{n-\nu}^{\tilde{1}1} + g_n^{41}g_\nu^{\tilde{4}1}g_0^{\tilde{1}1} - g_n^{\tilde{4}1}g_\nu^{41}g_0^{1\tilde{1}})+ \\ t_{21}(\omega_n)t_{21}(\omega_\nu)(g_\nu^{41}g_\nu^{\tilde{4}1}g_{n-\nu}^{1\tilde{1}} - g_n^{41}g_n^{\tilde{4}1}g_{n-\nu}^{\tilde{1}1} + g_n^{\tilde{4}1}g_\nu^{41}g_0^{\tilde{1}1} - g_n^{41}g_\nu^{\tilde{4}1}g_0^{1\tilde{1}})+ \\ t_{12}(\omega_n)t_{21}(\omega_\nu)(g_n^{41}g_\nu^{\tilde{4}1} - g_n^{41}g_\nu^{41}g_\nu^{\tilde{4}1} - g_n^{\tilde{4}1}g_n^{\tilde{4}1}g_\nu^{\tilde{4}1} - g_n^{41}g_\nu^{41}g_0^{\tilde{1}1} + g_\nu^{\tilde{4}1}g_\nu^{\tilde{4}1}g_0^{1\tilde{1}})+ \\ t_{21}(\omega_n)t_{12}(\omega_\nu)(g_n^{41}g_\nu^{\tilde{4}1} - g_n^{\tilde{4}1}g_\nu^{41}g_\nu^{\tilde{4}1} - g_n^{41}g_n^{\tilde{4}1}g_\nu^{41} - g_n^{\tilde{4}1}g_\nu^{41}g_0^{\tilde{1}1} + g_\nu^{41}g_\nu^{41}g_0^{1\tilde{1}}), \end{gathered}$$

where $g_n^{pq} \equiv g^{pq}(\omega_n)$.

Contribution to average values of Hubbard operators in the first order of perturbation theory from subspace $|1\rangle$:

$$\begin{aligned} \langle X^{11}\rangle^{(1)} &= (t_\uparrow^{11}g_n^{41}g_n^{41} + t_\uparrow^{22}g_n^{\tilde{4}1}g_n^{\tilde{4}1})\langle X^{11}\rangle_0 \\ &\quad + t_\uparrow^{11}g_n^{41}g_n^{41}\langle X^{44}\rangle_0 + t_\uparrow^{22}g_n^{\tilde{4}1}g_n^{\tilde{4}1}\langle X^{\tilde{4}\tilde{4}}\rangle_0, \\ \langle X^{1\tilde{1}}\rangle^{(1)} &= (t_\uparrow^{21}g_n^{\tilde{4}1}g_0^{1\tilde{1}} - t_\uparrow^{12}g_n^{41}g_0^{1\tilde{1}})\langle X^{11}\rangle_0 \\ &\quad + t_\uparrow^{21}g_n^{41}g_n^{4\tilde{1}}\langle X^{\tilde{4}\tilde{4}}\rangle_0 - t_\uparrow^{12}g_n^{41}g_n^{4\tilde{1}}\langle X^{44}\rangle_0 \\ &\quad - (t_\uparrow^{21}g_n^{4\tilde{1}}g_0^{1\tilde{1}} - t_\uparrow^{12}g_n^{4\tilde{1}}g_0^{1\tilde{1}})\langle X^{\tilde{1}\tilde{1}}\rangle_0, \\ \langle X^{\tilde{1}1}\rangle^{(1)} &= -(t_\uparrow^{21}g_n^{41}g_0^{1\tilde{1}} - t_\uparrow^{12}g_n^{\tilde{4}1}g_0^{1\tilde{1}})\langle X^{11}\rangle_0 \\ &\quad - t_\uparrow^{21}g_n^{41}g_n^{4\tilde{1}}\langle X^{44}\rangle_0 + t_\uparrow^{12}g_n^{\tilde{4}1}g_n^{4\tilde{1}}\langle X^{\tilde{4}\tilde{4}}\rangle_0 \\ &\quad + (t_\uparrow^{21}g_n^{4\tilde{1}}g_0^{1\tilde{1}} - t_\uparrow^{12}g_n^{4\tilde{1}}g_0^{1\tilde{1}})\langle X^{\tilde{1}\tilde{1}}\rangle_0, \\ \langle X^{\tilde{1}\tilde{1}}\rangle^{(1)} &= (t_\uparrow^{11}g_n^{\tilde{4}1}g_n^{\tilde{4}1} + t_\uparrow^{22}g_n^{4\tilde{1}}g_n^{4\tilde{1}})\langle X^{\tilde{1}\tilde{1}}\rangle_0 \\ &\quad + t_\uparrow^{11}g_n^{\tilde{4}1}g_n^{\tilde{4}1}\langle X^{\tilde{4}\tilde{4}}\rangle_0 + t_\uparrow^{22}g_n^{4\tilde{1}}g_n^{4\tilde{1}}\langle X^{44}\rangle_0, \\ \langle X^{44}\rangle^{(1)} &= -(t_\uparrow^{11}g_n^{41}g_n^{41} + t_\uparrow^{22}g_n^{4\tilde{1}}g_n^{4\tilde{1}})\langle X^{44}\rangle_0 \\ &\quad - t_\uparrow^{11}g_n^{41}g_n^{41}\langle X^{11}\rangle_0 - t_\uparrow^{22}g_n^{4\tilde{1}}g_n^{4\tilde{1}}\langle X^{\tilde{1}\tilde{1}}\rangle_0, \\ \langle X^{4\tilde{4}}\rangle^{(1)} &= (t_\uparrow^{21}g_n^{41}g_0^{4\tilde{4}} - t_\uparrow^{12}g_n^{4\tilde{1}}g_0^{4\tilde{4}})\langle X^{44}\rangle_0 \\ &\quad - t_\uparrow^{21}g_n^{41}g_n^{4\tilde{1}}\langle X^{11}\rangle_0 + t_\uparrow^{12}g_n^{4\tilde{1}}g_n^{4\tilde{1}}\langle X^{\tilde{1}\tilde{1}}\rangle_0 \\ &\quad - (t_\uparrow^{21}g_n^{4\tilde{1}}g_0^{4\tilde{4}} - t_\uparrow^{12}g_n^{4\tilde{1}}g_0^{4\tilde{4}})\langle X^{\tilde{4}\tilde{4}}\rangle_0, \\ \langle X^{\tilde{4}4}\rangle^{(1)} &= (t_\uparrow^{21}g_n^{\tilde{4}1}g_0^{4\tilde{4}} - t_\uparrow^{12}g_n^{\tilde{4}1}g_0^{4\tilde{4}})\langle X^{\tilde{4}\tilde{4}}\rangle_0 \\ &\quad + t_\uparrow^{21}g_n^{\tilde{4}1}g_n^{4\tilde{1}}\langle X^{\tilde{1}\tilde{1}}\rangle_0 - t_\uparrow^{12}g_n^{41}g_n^{4\tilde{1}}\langle X^{11}\rangle_0 \\ &\quad - (t_\uparrow^{21}g_n^{4\tilde{1}}g_0^{4\tilde{4}} - t_\uparrow^{12}g_n^{41}g_0^{4\tilde{4}})\langle X^{44}\rangle_0, \\ \langle X^{\tilde{4}\tilde{4}}\rangle^{(1)} &= -(t_\uparrow^{11}g_n^{\tilde{4}1}g_n^{\tilde{4}1} + t_\uparrow^{22}g_n^{\tilde{4}1}g_n^{\tilde{4}1})\langle X^{\tilde{4}\tilde{4}}\rangle_0 \\ &\quad - t_\uparrow^{11}g_n^{\tilde{4}1}g_n^{\tilde{4}1}\langle X^{\tilde{1}\tilde{1}}\rangle_0 - t_\uparrow^{22}g_n^{\tilde{4}1}g_n^{\tilde{4}1}\langle X^{11}\rangle_0. \end{aligned}$$

C. Summation over wave vectors in the matrix form

After introducing some density of states $\rho(t)$ we can write:

$$\hat{G}_{imp,\sigma}(\omega) = \int dt\rho(t)(\hat{\Xi}_\sigma^{-1}(\omega) - \hat{\alpha}_\sigma t)^{-1},$$

where $\hat{\alpha}_\sigma = \gamma^T \otimes \gamma$.

Rank of the matrix $\hat{\alpha}_\sigma$ is 1 so:

$$\det(\hat{\Xi}_\sigma^{-1}(\omega) - \hat{\alpha}_\sigma t) = Kt + \det(\hat{\Xi}_\sigma^{-1}(\omega)) \equiv Kt + b,$$

where

$$K = -\begin{vmatrix} \alpha^{11} & \alpha^{12} & \alpha^{13} & \alpha^{14} \\ (\hat{\Xi}_\sigma^{-1})^{21} & (\hat{\Xi}_\sigma^{-1})^{22} & (\hat{\Xi}_\sigma^{-1})^{23} & (\hat{\Xi}_\sigma^{-1})^{24} \\ (\hat{\Xi}_\sigma^{-1})^{31} & (\hat{\Xi}_\sigma^{-1})^{32} & (\hat{\Xi}_\sigma^{-1})^{33} & (\hat{\Xi}_\sigma^{-1})^{34} \\ (\hat{\Xi}_\sigma^{-1})^{41} & (\hat{\Xi}_\sigma^{-1})^{42} & (\hat{\Xi}_\sigma^{-1})^{43} & (\hat{\Xi}_\sigma^{-1})^{44} \end{vmatrix}$$

$$- \begin{vmatrix} (\hat{\Xi}_\sigma^{-1})^{11} & (\hat{\Xi}_\sigma^{-1})^{12} & (\hat{\Xi}_\sigma^{-1})^{13} & (\hat{\Xi}_\sigma^{-1})^{14} \\ \alpha^{21} & \alpha^{22} & \alpha^{23} & \alpha^{24} \\ (\hat{\Xi}_\sigma^{-1})^{31} & (\hat{\Xi}_\sigma^{-1})^{32} & (\hat{\Xi}_\sigma^{-1})^{33} & (\hat{\Xi}_\sigma^{-1})^{34} \\ (\hat{\Xi}_\sigma^{-1})^{41} & (\hat{\Xi}_\sigma^{-1})^{42} & (\hat{\Xi}_\sigma^{-1})^{43} & (\hat{\Xi}_\sigma^{-1})^{44} \end{vmatrix}$$

$$- \begin{vmatrix} (\hat{\Xi}_\sigma^{-1})^{11} & (\hat{\Xi}_\sigma^{-1})^{12} & (\hat{\Xi}_\sigma^{-1})^{13} & (\hat{\Xi}_\sigma^{-1})^{14} \\ (\hat{\Xi}_\sigma^{-1})^{21} & (\hat{\Xi}_\sigma^{-1})^{22} & (\hat{\Xi}_\sigma^{-1})^{23} & (\hat{\Xi}_\sigma^{-1})^{24} \\ \alpha^{31} & \alpha^{32} & \alpha^{33} & \alpha^{34} \\ (\hat{\Xi}_\sigma^{-1})^{41} & (\hat{\Xi}_\sigma^{-1})^{42} & (\hat{\Xi}_\sigma^{-1})^{43} & (\hat{\Xi}_\sigma^{-1})^{44} \end{vmatrix}$$

$$- \begin{vmatrix} (\hat{\Xi}_\sigma^{-1})^{11} & (\hat{\Xi}_\sigma^{-1})^{12} & (\hat{\Xi}_\sigma^{-1})^{13} & (\hat{\Xi}_\sigma^{-1})^{14} \\ (\hat{\Xi}_\sigma^{-1})^{21} & (\hat{\Xi}_\sigma^{-1})^{22} & (\hat{\Xi}_\sigma^{-1})^{23} & (\hat{\Xi}_\sigma^{-1})^{24} \\ (\hat{\Xi}_\sigma^{-1})^{31} & (\hat{\Xi}_\sigma^{-1})^{32} & (\hat{\Xi}_\sigma^{-1})^{33} & (\hat{\Xi}_\sigma^{-1})^{34} \\ \alpha^{41} & \alpha^{42} & \alpha^{43} & \alpha^{44} \end{vmatrix}.$$

Algebraic adjunct Δ_{ij} of matrix $(\hat{\Xi}_\sigma^{-1}(\omega) - \hat{\alpha}_\sigma t)$ with indices i, j is equal to:

$$\Delta_{ij} = \frac{\partial \det(\hat{\Xi}_\sigma^{-1}(\omega) - \hat{\alpha}_\sigma t)}{\partial(\hat{\Xi}_\sigma^{-1})^{ij}} = \frac{\partial K}{\partial(\hat{\Xi}_\sigma^{-1})^{ij}} t + \frac{\partial \det(\hat{\Xi}_\sigma^{-1})}{\partial(\hat{\Xi}_\sigma^{-1})^{ij}} \equiv \delta K_{ij} t + \delta b_{ij}\,.$$

It is obvious that

$$\delta b_{ij} = \frac{\partial \det(\hat{\Xi}_\sigma^{-1})}{\partial(\hat{\Xi}_\sigma^{-1})^{ij}} = (-1)^{i+j} \cdot \mathrm{minor}((\hat{\Xi}_\sigma^{-1}), i, j).$$

Thus, elements of inverted matrix are:

$$((\hat{\Xi}_\sigma^{-1} - \hat{\alpha}_\sigma t)^{ij} = \frac{\Delta_{ji}}{\det(\hat{\Xi}_\sigma^{-1} - \hat{\alpha}_\sigma t)},$$

and after some algebraic transformations we get

$$(\hat{\Xi}_\sigma^{-1} - \hat{\alpha}_\sigma t)^{ij} = \frac{\delta K_{ji}}{K} + \frac{1}{K}\left(\frac{\delta b_{ji} - \frac{\delta K_{ji} b}{K}}{t - (-\frac{\delta K_{ji} b}{K})}\right).$$

So, finally we have:

$$(\hat{G}_{imp,\sigma})^{ij} = \int \rho(t) \left(C_1^{ij} + \frac{C_2^{ij}}{t - t_0^{ij}} \right) dt,$$

where

$$\begin{array}{l} C_1^{ij} = \frac{\delta K_{ji}}{K}, \\ C_2^{ij} = \frac{\delta b_{ji}}{K} - \frac{\delta K_{ji} b}{K^2}, \\ t_0^{ij} = -\frac{\delta K_{ji} b}{K}, \end{array}$$

and after the integration:

$$\begin{array}{l} (\hat{G}_{imp,\sigma})^{ij} = C_1^{ij} + \\ + i C_2^{ij} \cdot \mathbf{sign}\left(\mathbf{Im}\left(t_0^{ij}\right)\right) \sqrt{\pi} e^{-(t_0^{ij})^2} \mathrm{erfc}\left(-i \cdot \mathbf{sign}\left(\mathbf{Im}\left(t_0^{ij}\right)\right) t_0^{ij}\right). \end{array}$$

D. Algorithm for calculating $\Omega_{(p)}(\{w_l\})$

First, we select initial condition for $J_\sigma(\omega)$:

$$J_\sigma^0(\omega) = iW,$$

where W is initial band width. Then the following iteration method is used:

1. $$G_{\sigma(p)} = \left(1 - \left(\gamma_\sigma \hat{g}_{\sigma(p)} \gamma_\sigma^T\right) J_\sigma\right)^{-1} \left(\gamma_\sigma \hat{g}_{\sigma(p)} \gamma_\sigma^T\right) J_\sigma,$$

2. $$G_\sigma = \sum_p w_p G_{\sigma(p)},$$

3. $$\Xi_\sigma^{-1} = G_\sigma^{-1} + J_\sigma,$$

4. $$G_\sigma = \int dt \rho(t) \left[\Xi_\sigma^{-1} - t\right]^{-1},$$

   where ρ is Gaussian density of states:

   $$\rho(t) = \frac{1}{\sqrt{\pi}} \exp\left(-t^2\right), \quad W = 1,$$

5. $$J_\sigma = \Xi_\sigma^{-1} - (G_\sigma)^{-1}.$$

Then, using obtained coherent potential J_σ we can calculate grand canonical potentials for subspaces:

$$\Omega_{(p)} = \lambda_p - \frac{1}{\beta}\int d\omega n_+(\omega)\,\mathrm{Im}\ln\left[1 - \left(\gamma_\sigma \hat{g}_{\sigma(p)}(\omega - i\delta)\gamma_\sigma^T\right) J_\sigma(\omega - i\delta)\right].$$

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Електронний спектр та термодинамічні властивості псевдоспін-електронної моделі тунельним розщепленням рівнів

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