

Metal-insulator transition in a doubly orbitally degenerate model with correlated hopping

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In the present paper, we propose a doubly orbitally degenerate narrow-band model with correlated hopping. The peculiarity of the model is taking into account the matrix element of electron-electron interaction, which describes intersite hoppings of electrons. In particular, this leads to the concentration dependence of the effective hopping integral. The cases of the strong and weak Hund's coupling are considered. By means of a generalized mean-field approximation the single-particle Green function and quasiparticle energy spectrum are calculated. Metal-insulator transition is studied in the model at different integer values of the electron concentration. With the help of the obtained energy spectrum, we find energy gap width and criteria of metal-insulator transition.

I. INTRODUCTION

The electron-electron interaction-driven metal-insulator transition (MIT) has fascinated theorists and experimentalists for many years. This transition is named after Sir Nevill Mott, being one of the pioneers who laid down the foundations of our physical understanding of this phenomenon.^{1,2} Despite a large amount of papers devoted to study of this transition (e.g., see a review³) the construction of consistent theory of MIT is still far from carrying out and constitutes one of the most challenging problems in condensed matter physics.

The simplest model describing MIT in materials with narrow energy bands is the Hubbard model.⁴ This model describes a single nondegenerate band of electrons with the local Coulomb interaction. The model Hamiltonian contains two energy parameters: the matrix element t_0 being the hopping integral of an electron from one site to another (t_0 is not dependent on occupation of sites involved in the hopping process) and the parameter U being the intraatomic Coulomb repulsion of two electrons of the opposite spins. This model is studied intensively (for recent reviews see Refs. 5 and 6).

Theoretical analyses, on the one hand, and available experimental data, on the other hand, point out the necessity of the Hubbard model generalization. As a rule this generalization is performed by two means: taking into account the orbital degeneration or correlated hopping (in the present paper we do not consider the generalization of the Hubbard model by taking into account the inter-atomic Coulomb and exchange interactions).

A model of nondegenerate band has to be generalized by taking into account the orbital degeneration being a characteristic of the transition-metal compounds, which exhibit MIT. First the degenerate Hubbard model was introduced for description of transition metal compounds in papers of Roth,⁷ Kugel' and Khomskii,⁸ Cyrot and Lyon-Caen.⁹ In these works, in particular, the importance of intra-atomic exchange interaction J , which stabilizes the localized magnetic moments in accordance with the Hund's rule was investigated.

The intensive study of MIT in the degenerate Hubbard model has begun only in few recent years by use of the slave

boson method,¹⁰⁻¹³ the variational method,¹⁴ the limit of infinite dimension.¹⁵

The results of works¹⁰⁻¹⁵ show the possibility of the metal-insulator transition in the doubly degenerate Hubbard model. However the criteria of the transition obtained in the noted works are substantially different. In particular, at $n = 1, J = 0$ (here in all the cases $T = 0$ K and the rectangular density of states are considered) in Refs. 11 and 12 the criterion of MIT is $U/w = 4.95$, in Ref. 14 – $U/w = 5.18$, in Ref. 15 – $U/w = 3.0$; at $n = 1, J = 0.1$ in Ref. 10 – $U/w = 3.04$; at $n = 2, J = 0$ in Refs. 11,12 – $U/w = 6.0$, in Ref. 10 $U/w = 4.0$, in Ref. 14 – $U/w = 9.0$, in Ref. 15 – $U/w = 3.7$. In addition in Ref. 10 at $n = 1$ MIT of first order is found, but in Refs. 12 and 14 – MIT of second order. Consequently a further investigation of MIT in narrow-band models with orbital degeneration is necessary.

Another way of the Hubbard model generalization which allows to describe the essential peculiarities of transition metal compounds is taking into account the correlated hopping. The necessity of taking into consideration correlated hopping is caused by two reasons. Firstly, theoretical analysis¹⁶ points out the inapplicability of the Hubbard model for the description of real strongly correlated electron systems, in some compounds (e.g., see the estimation in Refs. 17–21) the matrix element of electron-electron interaction describing correlated hopping is of the same order that the hopping integral or on-site Coulomb repulsion. Secondly, using the idea of correlated hopping and caused by it the electron-hole asymmetry we can interpret the peculiarities of some physical properties of narrow-band materials.²²⁻²⁸

Now two ways are commonly used to generalize the single-band Hubbard model by taking into account correlated hopping. One of them has been proposed in Ref. 16. Hirsch showed that in contrast to the hopping integral of the Hubbard model (which is not dependent on occupation of sites involved in the hopping process) this integral of a generalized Hubbard model had to depend on occupation of sites involved in the hopping process. Hamiltonian of the generalized in such a way Hubbard model is written as

$$H = - \sum_{ij\sigma} t_{ij}^{\sigma} a_{i\sigma}^{\dagger} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1.1)$$

$$t_{ij}^\sigma = t_{AA}(1 - n_{i\bar{\sigma}})(1 - n_{j\bar{\sigma}}) + t_{AB}(n_{i\bar{\sigma}} + n_{j\bar{\sigma}} - 2n_{i\bar{\sigma}}n_{j\bar{\sigma}}) + t_{BB}n_{i\bar{\sigma}}n_{j\bar{\sigma}}. \quad (1.2)$$

In recent few years Hamiltonian (1.1) is widely used to study MIT in narrow energy bands.²⁹⁻³¹

In Refs. 17 and 27 the necessity of the Hubbard model generalization by taking into account the matrix element of electron-electron interaction describing intersite hoppings of electrons had been pointed out. The Hamiltonian of the generalized Hubbard model with correlated hopping is

$$H = -\mu \sum_{i\sigma} a_{i\sigma}^+ a_{i\sigma} + t(n) \sum_{ij\sigma}' a_{i\sigma}^+ a_{j\sigma} + X \sum_{ij\sigma}' (a_{i\sigma}^+ a_{j\sigma} n_{i\bar{\sigma}} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1.3)$$

with

$$t(n) = t_0 + n \sum_{\substack{k \neq j \\ k \neq i}} J(ikjk) \quad (1.4)$$

being the effective hopping integral of electrons between nearest-neighbor sites of lattice, $X = J(iijj)$; $n = N_e/N$ is the electron concentration (N_e is the number of electrons, N is the number of lattice sites),

$$J(ikjk) = \int \int \varphi^*(\mathbf{r} - \mathbf{R}_i) \varphi(\mathbf{r} - \mathbf{R}_j) \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \times |\varphi(\mathbf{r}' - \mathbf{R}_k)|^2 d\mathbf{r} d\mathbf{r}', \quad (1.5)$$

$\varphi(\mathbf{r} - \mathbf{R}_i)$ is the Wannier function, the prime at the sums signifies that $i \neq j$.

In the model described by Hamiltonian (1.3) an electron hopping from one site to another is correlated both by the occupation of the sites involved in the hopping process (with the hopping integral X) and the occupation of the nearest-neighbor sites [with the matrix element $J(ikjk)$ at $k \neq i$, $k \neq j$] which we take into account in the Hartree-Fock approximation [Eq. (1.4)]. The peculiarity of model (1.3) is the concentration dependence of the hopping integral $t(n)$ in contrast to similar models.

MIT in a generalized Hubbard model with correlated hopping has been studied in a number of recent works.²⁹⁻³⁸ In particular, at half-filling and $t_0 = -X$ (or $t_{AB} = 0$) some exact results have been found.^{29,32-34} In a simple cubic lattice with coordination number z MIT occurs at

$$U_c = z(|t_{AA} + t_{BB}|) = 2z|t_0|. \quad (1.6)$$

If $U > U_c$ the ground state of system is a paramagnetic Mott-Hubbard insulator with the concentration of doubly occupied sites $d = 0$, the ground state energy is equal to zero.

For an arbitrary $t_0 \neq -X$ (or $t_{AB} \neq 0$) the finding of MIT criterion and the description of this phenomenon in a generalized Hubbard model with correlated hopping still remain an open problem. One of the steps to solve this task is recent papers^{30,31,35-38} where criteria of MIT, ground state energy,

concentration of doubly occupied sites have been found. In Refs. 30,31 and 35-37 the authors have obtained the following criterion of MIT:

$$U_c = z(|t_{AA}| + |t_{BB}|) = z(|t_0| + |t_0 + 2X|) \quad (1.7)$$

in agreement with the Mott's general physical ideas.² By means of the slave bosons method³⁹ it has been found in Ref. 38 that MIT occurs at $U_c = 4z|t + X|$; however here there is a problem of discrepancy of this result with the exact MIT criterion (1.6).

Considering the above arguments on the necessity of the Hubbard model generalization by taking into account orbital degeneration, on the one hand, and correlated hopping, on the other hand, in the present paper we propose a doubly orbitally degenerate narrow-band model with correlated hopping. The structure of this paper is the following. Section II is devoted to the model formulation and model Hamiltonian construction, the representation of the Hamiltonian of a doubly orbitally degenerate model with correlated hopping in the electron and Hubbard operators is given. In Sec. III metal-insulator transition in the model at different integer values of the electron concentration is studied. The cases of the strong and weak Hund's coupling are considered. The absence of a natural small expansion parameter in the region near the MIT requires to find the nonperturbative approaches; in such a situation methods of mean-field type are useful. We shall use one of these methods, a variant of the generalized Hartree-Fock approximation,^{40,41} which has been proposed in Refs. 27 and 42. The approach gives the exact band and atomic limits in the single-band Hubbard model and describes MIT. The method reproduces (see Ref. 37) the exact results [criterion of MIT (1.6) and ground-state energy] for the case of a half-filled nondegenerate band in a generalized Hubbard model with correlated hopping at $t_0 = -X$. By means of the generalized mean-field approximation the single-particle Green function and quasiparticle energy spectrum are calculated. With the help of the obtained energy spectrum we find energy gap width and criteria of metal-insulator transition. Finally, Sec. IV is devoted to the conclusions and the comparison of our results with those of other authors.

II. MODEL HAMILTONIAN

On the analogy of an orbitally non-degenerate model^{17,27} we start from the following generalization of the Hubbard model for an orbitally degenerate band taking into account the matrix element of electron-electron interaction, which describes intersite hoppings of electrons (correlated hopping):

$$H = -\mu \sum_{i\gamma\sigma} a_{i\gamma\sigma}^+ a_{i\gamma\sigma} + \sum_{ij\gamma\sigma}' a_{i\gamma\sigma}^+ \times \left[t_{ij} + \sum_{k\gamma'} J(i\gamma k\gamma' j\gamma k\gamma') n_{k\gamma'} \right] a_{j\gamma\sigma} + U \sum_{i\gamma} n_{i\gamma\uparrow} n_{i\gamma\downarrow} + U' \sum_{i\sigma} n_{i\alpha\sigma} n_{i\beta\bar{\sigma}} + (U' - J) \sum_{i\sigma} n_{i\alpha\sigma} n_{i\beta\sigma}, \quad (2.1)$$

where μ is the chemical potential, $a_{i\gamma\sigma}^+$, $a_{i\gamma\sigma}$ are the creation and destruction operators of an electron of spin σ ($\sigma = \uparrow, \downarrow$; $\bar{\sigma}$ denotes spin projection, which is opposite to σ) on i -site and in orbital γ ($\gamma = \alpha, \beta$ denotes two possible values of orbital states), $n_{i\gamma\sigma} = a_{i\gamma\sigma}^+ a_{i\gamma\sigma}$ is the number operator of electrons of spin σ and in orbital γ on i -site, $n_{i\gamma} = n_{i\gamma\uparrow} + n_{i\gamma\downarrow}$; t_{ij} is the hopping integral of an electron from γ orbital of j site to γ orbital of i site (we neglect the electron hoppings between α and β orbitals). In real systems the electron hoppings between different orbitals can exist, in addition the hopping integrals are anisotropic for e_g orbitals. This may have an effect on the orbital and magnetic ordering.^{8,43,44} We, however, assume for simplicity $t_{ij}^{\alpha\beta} = t_{ij} \delta_{\alpha\beta}$. This assumption considerably simplifies the analysis of properties of the model under consideration and allows to describe the physics of the metal-insulator transition.

$$J(i\gamma k\gamma'j\gamma k\gamma') = \int \int \varphi_{\gamma}^*(\mathbf{r}-\mathbf{R}_i) \varphi_{\gamma}(\mathbf{r}-\mathbf{R}_j) \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \times |\varphi_{\gamma'}(\mathbf{r}'-\mathbf{R}_k)|^2 d\mathbf{r}d\mathbf{r}' \quad (2.2)$$

(φ_{γ} is the Wannier function), the prime at second sum in Eq. (2.1) signifies that $i \neq j$,

$$U = \int \int |\varphi_{\gamma}(\mathbf{r}-\mathbf{R}_i)|^2 \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} |\varphi_{\gamma}(\mathbf{r}'-\mathbf{R}_i)|^2 d\mathbf{r}d\mathbf{r}' \quad (2.3)$$

is the intra-atomic Coulomb repulsion of two electrons of the opposite spins at the same orbital (we assume that it has the same value at α and β orbitals),

$$U' = \int \int |\varphi_{\alpha}(\mathbf{r}-\mathbf{R}_i)|^2 \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} |\varphi_{\beta}(\mathbf{r}'-\mathbf{R}_i)|^2 d\mathbf{r}d\mathbf{r}' \quad (2.4)$$

is the intra-atomic Coulomb repulsion of two electrons of the opposite spins at the different orbitals,

$$J = \int \int \varphi_{\alpha}^*(\mathbf{r}-\mathbf{R}_i) \varphi_{\beta}(\mathbf{r}-\mathbf{R}_i) \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \varphi_{\beta}^*(\mathbf{r}'-\mathbf{R}_i) \times \varphi_{\alpha}(\mathbf{r}'-\mathbf{R}_i) d\mathbf{r}d\mathbf{r}' \quad (2.5)$$

is the intra-atomic exchange interaction energy which stabilizes the Hund's states forming the atomic magnetic moments. The parameters U , U' , J are connected by the relation⁴⁵

$$U' = U - 2J. \quad (2.6)$$

In Hamiltonian (2.1) we rewrite the sum $\sum'_{ij\gamma\gamma'\sigma} J(i\gamma k\gamma'j\gamma k\gamma') a_{i\gamma\sigma}^+ n_{k\gamma'} a_{j\gamma\sigma}$ in the form

$$\begin{aligned} & \sum'_{ij\gamma\sigma} (J(i\gamma i\gamma j\gamma i\gamma) a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{i\gamma\bar{\sigma}} + \text{H.c.}) \\ & + \sum'_{ij\gamma\sigma} (J(i\gamma i\bar{\gamma} j\gamma i\bar{\gamma}) a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{i\bar{\gamma}} + \text{H.c.}) \\ & + \sum'_{ij\gamma\gamma'\sigma} \sum_{\substack{k \neq i \\ k \neq j}} J(i\gamma k\gamma'j\gamma k\gamma') a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{k\gamma'} \end{aligned} \quad (2.7)$$

($\bar{\gamma} = \beta$ if $\gamma = \alpha$, and $\bar{\gamma} = \alpha$ when $\gamma = \beta$).

The first and third terms of Eq. (2.7) generalize correlated hopping introduced for an orbitally nondegenerate model (e.g., see Ref. 27). The second term of expression (2.7) describes correlated hopping of electrons being the peculiarity of orbitally degenerate systems only (it is absent in a single-band case). Among this type of processes one can separate out three essentially different (from the energy point of view) hoppings (X_i^{kl} -representation allows to have done this easily).

The first and second sums of Eq. (2.7) describe the hoppings of electrons, which are correlated by electron occupation of sites involved in the hopping process. The third sum describes the hoppings of an electron between $|i\gamma\sigma\rangle$ and $|j\gamma\sigma\rangle$ states, which are dependent on the occupation number n_k of other ($k \neq i$, $k \neq j$) sites. Let us take into account the influence of occupation of these sites in the Hartree-Fock approximation

$$\begin{aligned} & \sum'_{ij\gamma\gamma'\sigma} \sum_{\substack{k \neq i \\ k \neq j}} J(i\gamma k\gamma'j\gamma k\gamma') a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{k\gamma'} \\ & \approx n \sum'_{ij\gamma\sigma} T_1(ij) a_{i\gamma\sigma}^+ a_{j\gamma\sigma}, \end{aligned} \quad (2.8)$$

where $n = \langle n_{i\alpha} + n_{i\beta} \rangle$ is the average number of electrons per site,

$$T_1(ij) = \sum_{\substack{k \neq i \\ k \neq j}} J(i\gamma k\gamma'j\gamma k\gamma') \quad (2.9)$$

[we suppose $J(i\gamma k\alpha j\gamma k\alpha) = J(i\gamma k\beta j\gamma k\beta)$ and $T_1(ij)$ have the same value for both α and β orbitals]. Assuming that α - and β -states are equivalent, denote:

$$J(i\gamma i\bar{\gamma} j\gamma i\bar{\gamma}) = t'_{\alpha\alpha}(ij) = t'_{\beta\beta}(ij) = t'_{ij}, \quad (2.10)$$

$$J(i\gamma i\gamma j\gamma i\gamma) = t''_{\alpha\alpha}(ij) = t''_{\beta\beta}(ij) = t''_{ij}. \quad (2.11)$$

So we can rewrite Hamiltonian (2.1) in the following form:

$$\begin{aligned} H = & -\mu \sum_{i\gamma\sigma} a_{i\gamma\sigma}^+ a_{i\gamma\sigma} + \sum'_{ij\gamma\sigma} t_{ij}(n) a_{i\gamma\sigma}^+ a_{j\gamma\sigma} \\ & + \sum'_{ij\gamma\sigma} (t'_{ij} a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{i\bar{\gamma}} + \text{H.c.}) \\ & + \sum'_{ij\gamma\sigma} (t''_{ij} a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{i\gamma\bar{\sigma}} + \text{H.c.}) + U \sum_{i\gamma} n_{i\gamma\uparrow} n_{i\gamma\downarrow} \\ & + U' \sum_{i\sigma} n_{i\alpha\sigma} n_{i\beta\bar{\sigma}} + (U' - J) \sum_{i\sigma} n_{i\alpha\sigma} n_{i\beta\sigma}, \end{aligned} \quad (2.12)$$

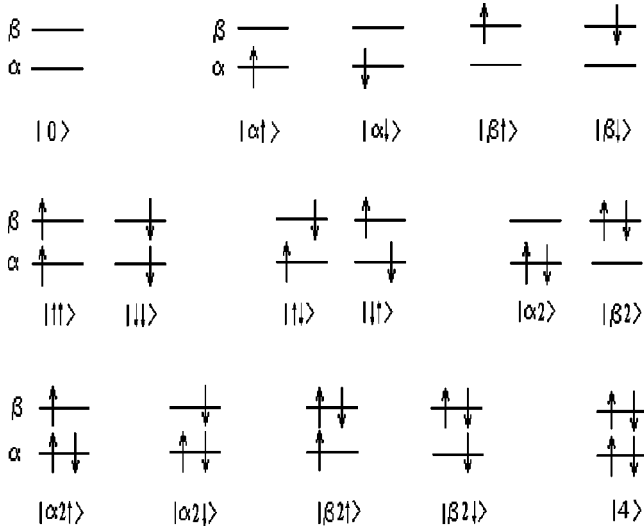


FIG. 1. The possible configurations of the lattice sites.

with the effective hopping integral $t_{ij}(n) = t_{ij} + nT_1(ij)$ being the concentration-dependent in consequence of taking into account correlated hopping $T_1(ij)$.

The distinction of Hamiltonian (2.12) from models of narrow-band materials with orbital degeneracy is taking into account the matrix element $J(i\gamma k\gamma'j\gamma k\gamma')$ caused by electron-electron interaction. This leads to the electron-hole asymmetry (which is analogous one to the case of a nondegenerate band^{26,27}) and the dependence of hopping integral on the average number of electrons per site. Thus, the narrow-band model that are described by Hamiltonian (2.12) shows much better physics than the Hubbard model with doubly orbital degeneracy.

In the model described by Hamiltonian (2.12) each site of the lattice can be in one of 16 states (see Fig. 1).

Let us pass to the configurational representation of Hamiltonian (2.12). Use the representation of the operators of creation and destruction of electron through X_i^{kl} -operators of transition of site i from the state l to the state k :

$$\begin{aligned}
 a_{i\alpha\uparrow}^+ &= X_i^{\alpha\uparrow,0} + X_i^{\uparrow\uparrow,\beta\uparrow} + X_i^{\uparrow\downarrow,\beta\downarrow} + X_i^{\alpha 2,\alpha\uparrow} + X_i^{\alpha 2\downarrow,\downarrow\downarrow} + X_i^{\alpha 2\uparrow,\uparrow\uparrow} \\
 &\quad + X_i^{\beta 2\uparrow,\beta 2} + X_i^{4,\beta 2\downarrow}, \\
 a_{i\alpha\downarrow}^+ &= X_i^{\alpha\downarrow,0} + X_i^{\downarrow\downarrow,\beta\downarrow} + X_i^{\downarrow\uparrow,\beta\uparrow} - X_i^{\alpha 2,\alpha\uparrow} - X_i^{\alpha 2\downarrow,\uparrow\downarrow} - X_i^{\alpha 2\uparrow,\uparrow\uparrow} \\
 &\quad + X_i^{\beta 2\downarrow,\beta 2} - X_i^{4,\beta 2\uparrow}, \\
 a_{i\beta\uparrow}^+ &= X_i^{\beta\uparrow,0} - X_i^{\uparrow\uparrow,\alpha\uparrow} - X_i^{\downarrow\uparrow,\alpha\downarrow} + X_i^{\beta 2,\beta\downarrow} - X_i^{\beta 2\downarrow,\downarrow\downarrow} - X_i^{\beta 2\uparrow,\uparrow\uparrow} \\
 &\quad + X_i^{\alpha 2\uparrow,\alpha 2} + X_i^{4,\alpha 2\downarrow}, \\
 a_{i\beta\downarrow}^+ &= X_i^{\beta\downarrow,0} - X_i^{\downarrow\downarrow,\alpha\downarrow} - X_i^{\downarrow\uparrow,\alpha\uparrow} - X_i^{\beta 2,\beta\uparrow} + X_i^{\alpha 2\downarrow,\alpha 2} + X_i^{\beta 2\uparrow,\uparrow\uparrow} \\
 &\quad + X_i^{\beta 2\downarrow,\downarrow\downarrow} - X_i^{4,\alpha 2\uparrow}.
 \end{aligned} \tag{2.13}$$

Such choice of representation with taking into account the commutational rules

$$\begin{aligned}
 \{X_i^{p,l}; X_j^{k,l}\} &= \delta_{ij}(\delta_{lk}X_i^{p,t} + \delta_{lp}X_i^{k,l}), \\
 [X_i^{p,l}; X_j^{k,t}] &= \delta_{ij}(\delta_{lk}X_i^{p,t} - \delta_{lp}X_i^{k,l}),
 \end{aligned} \tag{2.14}$$

where the anticommutator $(\{A;B\})$ has to be taken only if both operators are fermionic, i.e., change the particle number by one (e.g., $X_i^{\gamma\sigma,0}$ or $X_i^{\gamma 2\sigma,4}$), and the constraint

$$\sum_p X_i^p = 1, \tag{2.15}$$

where $X_i^p = X_i^{p,l}X_i^{l,p}$ is the operator of number of $|p\rangle$ states on the site i ensures the fulfillment of the anticommutation relations for a operators.

The model Hamiltonian in the configurational representation has the form:

$$\begin{aligned}
 H &= -\mu \left[\sum_{i\sigma} X_i^{\gamma\sigma} + 2 \sum_{i\sigma} (X_i^{\sigma\sigma} + X_i^{\sigma\bar{\sigma}}) + 2 \sum_{i\gamma} X_i^{\gamma 2} \right. \\
 &\quad \left. + 3 \sum_{i\gamma\sigma} X_i^{\gamma 2\sigma} + 4 \sum_i X_i^4 \right] + (U' - J) \sum_{i\sigma} X_i^{\sigma\sigma} + U' \sum_{i\sigma} X_i^{\sigma\bar{\sigma}} \\
 &\quad + U \sum_{i\gamma} X_i^{\gamma 2} + (U + 2U' - J) \sum_{i\gamma\sigma} X_i^{\gamma 2\sigma} \\
 &\quad + 2(U + 2U' - J) \sum_i X_i^4 + H_t,
 \end{aligned} \tag{2.16}$$

where the kinetic part of the Hamiltonian is

$$H_t = \sum_{n,m} H_{nm} \tag{2.17}$$

with $n, m = \{0 - \gamma\sigma, \gamma\sigma - \sigma\sigma, \gamma\sigma - \sigma\bar{\sigma}, \gamma\sigma - \gamma 2, \sigma\sigma - \gamma 2\sigma, \sigma\bar{\sigma} - \gamma 2\sigma, \gamma 2 - \gamma 2\sigma, \gamma 2\sigma - 4\}$.

The Hamiltonians H_{nm} contain the processes which form the energy subbands (analogues of the Hubbard subbands) and the processes of the hybridization of these subbands. In Fig. 2 the transitions between the states of the sites, which form the corresponding subbands are shown.

The different hopping integrals t_{ij}^{nm} correspond to the transitions within the different subbands H_{nn} or between the different subbands H_{nm} ($n \neq m$)

$$t_{ij}^{nm} = t_{ij} + (\tau^n + \tau^m), \tag{2.18}$$

where

$$\begin{aligned}
 \tau^{0 - \gamma\sigma} &= 0, & \tau^{\sigma\sigma - \gamma 2\sigma} &= t'_{ij} + t''_{ij}, \\
 \tau^{\gamma\sigma - \sigma\sigma} &= t'_{ij}, & \tau^{\sigma\bar{\sigma} - \gamma 2\sigma} &= t'_{ij} + t''_{ij}, \\
 \tau^{\gamma\sigma - \sigma\bar{\sigma}} &= t'_{ij}, & \tau^{\gamma 2 - \gamma 2\sigma} &= 2t'_{ij}, \\
 \tau^{\gamma\sigma - \gamma 2} &= t''_{ij}, & \tau^{\gamma 2\sigma - 4} &= 2t'_{ij} + t''_{ij}.
 \end{aligned} \tag{2.19}$$

The mutual placement and the overlapping of the noted subbands depend on the relations between the values of intra-atomic Coulomb repulsion parameters U, U' , intra-atomic exchange interaction parameter J and the widths of subbands.

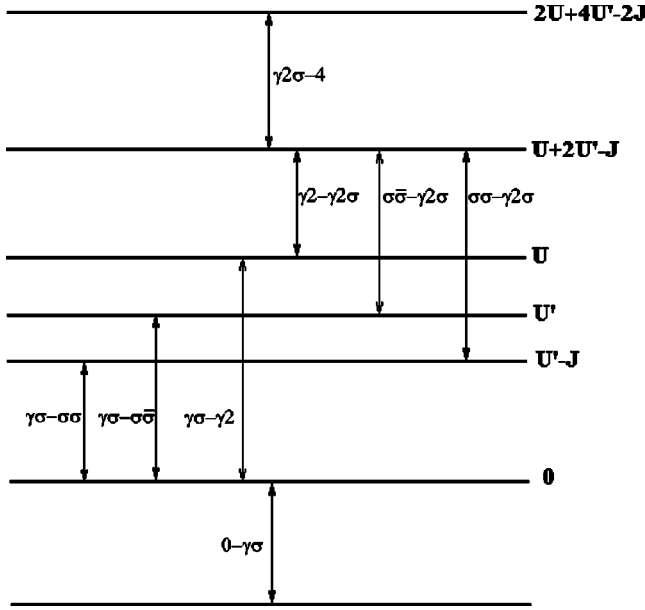


FIG. 2. Energy levels corresponding to the possible electron configurations of sites and the transitions between them.

III. METAL-INSULATOR TRANSITION

At integer values of electron concentration $n = 1, 2, 3$ in the model described by the Hamiltonian (2.16) MIT can occur. The possible metal-insulator transitions at some integer values of the mean electron number per site will be considered below.

A. Metal-insulator transition at electron concentration $n = 1$

1. The strong Hund's coupling case

Let us consider the case of the strong intra-atomic Coulomb interaction $U' \gg t_{ij}$ and the strong Hund's coupling $U' \gg U' - J$ (values U' and J are of the same order). These conditions allow us to neglect the states of site when there are more than two electrons on the site and the "non-Hund's" doubly occupied states $|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\alpha 2\rangle, |\beta 2\rangle$ (the analogous conditions are used for an investigation of magnetic properties of the Hubbard model with twofold orbital degeneration in Refs. 45–47). Thus lattice sites can be in one of seven possible states: a hole (a non-occupied by electron site) $|0\rangle$; a single occupied by electron site $|\alpha\uparrow\rangle, |\alpha\downarrow\rangle, |\beta\uparrow\rangle, |\beta\downarrow\rangle$; the Hund's doublon or site with two electrons on the different orbitals with the same spins $|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle$.

Let us pass to the configurational representation of the Hamiltonian. Electron operators in terms of the transition operators $X_i^{k,l}$ of site i from the state $|l\rangle$ to the state $|k\rangle$ are expressed by the formulas:

$$\begin{aligned}
 a_{i\alpha\uparrow}^+ &= X_i^{\alpha\uparrow,0} + X_i^{\uparrow\uparrow,\beta\uparrow}, & a_{i\alpha\uparrow} &= X_i^{0,\alpha\uparrow} + X_i^{\beta\uparrow,\uparrow\uparrow}, \\
 a_{i\alpha\downarrow}^+ &= X_i^{\alpha\downarrow,0} + X_i^{\downarrow\downarrow,\beta\downarrow}, & a_{i\alpha\downarrow} &= X_i^{0,\alpha\downarrow} + X_i^{\beta\downarrow,\downarrow\downarrow}, \\
 a_{i\beta\uparrow}^+ &= X_i^{\beta\uparrow,0} - X_i^{\uparrow\uparrow,\alpha\uparrow}, & a_{i\beta\uparrow} &= X_i^{0,\beta\uparrow} - X_i^{\alpha\uparrow,\uparrow\uparrow}, \\
 a_{i\beta\downarrow}^+ &= X_i^{\beta\downarrow,0} - X_i^{\downarrow\downarrow,\alpha\downarrow}, & a_{i\beta\downarrow} &= X_i^{0,\beta\downarrow} - X_i^{\alpha\downarrow,\downarrow\downarrow},
 \end{aligned} \tag{3.1}$$

(in these formulas we have taken into account only seven possible states). It should be emphasized that one has to consider all the possible site states in order to get the correct anticommutation rules for electron operators.

Let us calculate the quasiparticle energy spectrum of the model neglecting the correlated hopping $t'_{ij} = t''_{ij} = 0$, $t_{ij}(n) = t_{ij}$. We write the Hamiltonian in the form:

$$\begin{aligned}
 H &= -\mu \sum_{i\sigma} (X_i^{\alpha\sigma} + X_i^{\beta\sigma} + 2X_i^{\sigma\sigma}) + \sum'_{ij\gamma\sigma} t_{ij} (X_i^{\gamma\sigma,0} X_j^{0,\gamma\sigma} \\
 &+ X_i^{\sigma\sigma,\gamma\sigma} X_j^{\gamma\sigma,\sigma\sigma}) + (U' - J) \sum_{i\sigma} X_i^{\sigma\sigma} + H_{\alpha\beta}, \tag{3.2}
 \end{aligned}$$

where

$$\begin{aligned}
 H_{\alpha\beta} &= \sum'_{ij} t_{ij} (-X_i^{\uparrow\uparrow,\alpha\uparrow} X_j^{0,\beta\uparrow} + X_i^{\uparrow\uparrow,\beta\uparrow} X_j^{0,\alpha\uparrow} + X_i^{\downarrow\downarrow,\beta\downarrow} X_j^{0,\alpha\downarrow} \\
 &- X_i^{\downarrow\downarrow,\alpha\downarrow} X_j^{0,\beta\downarrow} + \text{H.c.}). \tag{3.3}
 \end{aligned}$$

For calculation of the quasiparticle energy spectrum and polar state concentration $c \equiv \langle X_i^0 \rangle$ — holes, $d_{\uparrow} \equiv \langle X_i^{\uparrow\uparrow} \rangle$, $d_{\downarrow} \equiv \langle X_i^{\downarrow\downarrow} \rangle$ being the Hund's doublons we use the method of the retarded Green functions. For the Green function

$$G_{pp'}^{(1)}(E) = \langle \langle X_p^{\alpha\uparrow,0} | X_{p'}^{0,\alpha\uparrow} \rangle \rangle \tag{3.4}$$

we have the equation

$$\begin{aligned}
 (E - \mu) \langle \langle X_p^{\alpha\uparrow,0} | X_{p'}^{0,\alpha\uparrow} \rangle \rangle &= \frac{\delta_{pp'}}{2\pi} \langle X_p^0 + X_p^{\alpha\uparrow} \rangle + \langle \langle [X_p^{\alpha\uparrow,0}, H_0] \\
 &+ [X_p^{\alpha\uparrow,0}, H_{\alpha\beta}] | X_{p'}^{0,\alpha\uparrow} \rangle \rangle, \tag{3.5}
 \end{aligned}$$

where

$$H_0 = \sum'_{ij\gamma\sigma} t_{ij} (X_i^{\gamma\sigma,0} X_j^{0,\gamma\sigma} + X_i^{\sigma\sigma,\gamma\sigma} X_j^{\gamma\sigma,\sigma\sigma}). \tag{3.6}$$

To break off the sequence of equations for Green functions we apply a variant⁴² of the generalized mean field approximation^{40,41}

$$[X_p^{\alpha\uparrow,0}, H_0] = \sum'_{j} \epsilon(pj) X_j^{\alpha\uparrow,0}, \tag{3.7}$$

$$[X_p^{\alpha\uparrow,0}, H_{\alpha\beta}] = \sum'_{j} \epsilon_1(pj) X_j^{\uparrow\uparrow,\beta\uparrow},$$

where $\epsilon(pj)$, $\epsilon_1(pj)$ are the nonoperator expressions, the method of its calculation will be given below. The representation (3.7) of commutators in Eq. (3.5) is defined by the operator structure of H_0 and $H_{\alpha\beta}$.

Using the approximation (3.7) Eq. (3.5) for the Green function $G_{pp'}^{(1)}(E)$ can be written as

$$\begin{aligned}
(E - \mu) \langle \langle X_p^{\alpha\uparrow,0} | X_{p'}^{0,\alpha\uparrow} \rangle \rangle \\
= \frac{\delta_{pp'}}{2\pi} \langle X_p^0 + X_p^{\alpha\uparrow} \rangle + \sum_j' \epsilon(pj) \langle \langle X_j^{\alpha\uparrow,0} | X_{p'}^{0,\alpha\uparrow} \rangle \rangle \\
+ \sum_j' \epsilon_1(pj) \langle \langle X_j^{\uparrow\uparrow,\beta\uparrow} | X_{p'}^{0,\alpha\uparrow} \rangle \rangle. \quad (3.8)
\end{aligned}$$

For the Green function

$$G_{pp'}^{(2)}(E) = \langle \langle X_p^{\uparrow\uparrow,\beta\uparrow} | X_{p'}^{0,\alpha\uparrow} \rangle \rangle \quad (3.9)$$

we write the analogous equation

$$\begin{aligned}
(E - \mu + U' - J) \langle \langle X_p^{\uparrow\uparrow,\beta\uparrow} | X_{p'}^{0,\alpha\uparrow} \rangle \rangle \\
= \sum_j' \tilde{\epsilon}(pj) \langle \langle X_j^{\uparrow\uparrow,\beta\uparrow} | X_{p'}^{0,\alpha\uparrow} \rangle \rangle + \sum_j' \epsilon_2(pj) \\
\times \langle \langle X_j^{\alpha\uparrow,0} | X_{p'}^{0,\alpha\uparrow} \rangle \rangle, \quad (3.10)
\end{aligned}$$

where the non-operator expressions $\tilde{\epsilon}$, ϵ_2 are defined by the formulas

$$[X_p^{\uparrow\uparrow,\beta\uparrow}, H_0] = \sum_j' \tilde{\epsilon}(pj) X_j^{\uparrow\uparrow,\beta\uparrow}, \quad (3.11)$$

$$[X_p^{\uparrow\uparrow,\beta\uparrow}, H_{\alpha\beta}] = \sum_j' \epsilon_2(pj) X_j^{\alpha\uparrow,0}.$$

Thus, we obtain the closed system of equations for functions $G_{pp'}^{(1)}(E)$ and $G_{pp'}^{(2)}(E)$.

To calculate $\epsilon(pj)$, $\epsilon_1(pj)$, $\tilde{\epsilon}(pj)$, $\epsilon_2(pj)$ we use the procedure proposed in paper.⁴² The values of $\epsilon(pj)$, $\epsilon_1(pj)$, $\tilde{\epsilon}(pj)$, $\epsilon_2(pj)$ we find by anticommutation of Eqs.(3.7) and (3.11) with the operators $X_{p'}^{0,\alpha\uparrow}$ and $X_{p'}^{\beta\uparrow,\uparrow\uparrow}$, respectively

$$\begin{aligned}
(X_p^0 + X_p^{\alpha\uparrow}) \epsilon(pp') &= \{X_p^{0,\alpha\uparrow}; [X_p^{\alpha\uparrow,0}, H_0]\}, \\
(X_p^{\beta\uparrow} + X_p^{\uparrow\uparrow}) \epsilon_1(pp') &= \{X_p^{\beta\uparrow,\uparrow\uparrow}; [X_p^{\alpha\uparrow,0}, H_{\alpha\beta}]\}, \\
(X_p^{\beta\uparrow} + X_p^{\uparrow\uparrow}) \tilde{\epsilon}(pp') &= \{X_p^{\beta\uparrow,\uparrow\uparrow}; [X_p^{\uparrow\uparrow,\beta\uparrow}, H_0]\}, \\
(X_p^0 + X_p^{\alpha\uparrow}) \epsilon_2(pp') &= \{X_p^{0,\alpha\uparrow}; [X_p^{\uparrow\uparrow,\beta\uparrow}, H_{\alpha\beta}]\}. \quad (3.12)
\end{aligned}$$

We rewrite X_i^{kl} -operator in the form $X_i^{k,l} = \alpha_{ik}^+ \alpha_{il}$, where α_{ik}^+ , α_{il} are the operators of creation and destruction for $|k\rangle$ - and $|l\rangle$ -states on i -site respectively (with the constraint $\sum_k \alpha_{ik}^+ \alpha_{ik} = 1$); thus $X_i^0 = \alpha_{i0}^+ \alpha_{i0}$, $X_i^{\sigma\sigma} = \alpha_{i\sigma\sigma}^+ \alpha_{i\sigma\sigma}$, $X_i^{\gamma\sigma} = \alpha_{i\gamma\sigma}^+ \alpha_{i\gamma\sigma}$. Let us substitute α -operators by c -numbers (here there is a partial equivalence with the slave boson method³⁹). At $n=1$ in a paramagnetic state

$$\begin{aligned}
d \equiv d_{\uparrow} = d_{\downarrow} = c/2, \quad \langle X_i^{\alpha\uparrow} \rangle = 0.25 - d, \\
\alpha_{i0}^+ = \alpha_{i0} = c^{1/2}; \quad \alpha_{i\sigma\sigma}^+ = \alpha_{i\sigma\sigma} = d^{1/2}; \quad (3.13) \\
\alpha_{i\gamma\sigma}^+ = \alpha_{i\gamma\sigma} = (0.25 - d)^{1/2}.
\end{aligned}$$

The proposed approximation is based on the following physical idea. When the lower and upper Hubbard subbands overlap weakly (the case of a paramagnetic Mott-Hubbard semimetal) $|0\rangle$ and $|\sigma\sigma\rangle$ states almost do not influence on $|\gamma\sigma\rangle$ states then $|\gamma\sigma\rangle$ subsystem can be considered as a quasiclassical subsystem (an analogue of the thermodynamic reservoir). In this case one can substitute α operators through c numbers. We extend this ideology to determination of $\epsilon(pj)$, $\epsilon_1(pj)$, $\tilde{\epsilon}(pj)$, $\epsilon_2(pj)$. Thus we substitute the creation and destruction operators of $|0\rangle$, $|\sigma\sigma\rangle$, and $|\gamma\sigma\rangle$ states through respective quasiclassical expressions. Actually, the proposed procedure is equivalent to a separation of the charge and spin degrees of freedom.

Then we obtain the formulas in \mathbf{k} representation

$$\begin{aligned}
\epsilon(\mathbf{k}) &= \frac{-0.5c^2 + 0.5c - 0.25}{0.25 + 0.5c} t_{\mathbf{k}}, \quad \epsilon_1(\mathbf{k}) = (1.5c + c^2) t_{\mathbf{k}}, \\
\tilde{\epsilon}(\mathbf{k}) &= (c^2 + c - 0.5) t_{\mathbf{k}}, \quad \epsilon_2(\mathbf{k}) = \frac{0.25c^2 + 0.375c}{0.25 + 0.5c} t_{\mathbf{k}}. \quad (3.14)
\end{aligned}$$

From system of Eqs. (3.8) and (3.10) we have

$$G_{\mathbf{k}}^{(1)}(E) = \frac{0.5c + 0.25}{2\pi} \frac{E - \mu + U' - J - \tilde{\epsilon}(\mathbf{k})}{[E + E_1(\mathbf{k})][E + E_2(\mathbf{k})]}, \quad (3.15)$$

$$G_{\mathbf{k}}^{(2)}(E) = \frac{0.5c + 0.25}{2\pi} \frac{\epsilon_2(\mathbf{k})}{[E + E_1(\mathbf{k})][E + E_2(\mathbf{k})]}, \quad (3.16)$$

where the expressions

$$\begin{aligned}
E_{1,2}(\mathbf{k}) &= -\mu - \frac{\epsilon(\mathbf{k}) - \tilde{\epsilon}(\mathbf{k}) + (U' - J)}{2} \\
&\mp \frac{1}{2} \{ [\epsilon(\mathbf{k}) + \tilde{\epsilon}(\mathbf{k}) - (U' - J)]^2 + 4\epsilon(\mathbf{k})(U' - J) \\
&+ 4[\epsilon_1(\mathbf{k})\epsilon_2(\mathbf{k}) - \epsilon(\mathbf{k})\tilde{\epsilon}(\mathbf{k})] \}^{1/2} \quad (3.17)
\end{aligned}$$

are the quasiparticle energy spectrum. $E_2(\mathbf{k})$ describes the electron spectrum in the $0-\alpha\sigma$ subband (an analogue of the lower Hubbard subband), $E_1(\mathbf{k})$ describes the electron spectrum in the $\alpha\sigma-\sigma\sigma$ subband (an analogue of the upper Hubbard subband). The computation of the quasiparticle energy spectrum in the $0-\beta\sigma$ and $\beta\sigma-\sigma\sigma$ subbands gives the same Eq. (3.17).

The energy gap width (difference of energies between bottom of the upper and top of the lower bands) is

$$\Delta E = E_2(-w) - E_1(w). \quad (3.18)$$

The peculiarity of the obtained energy spectrum and energy gap width is their dependence on the hole concentration c . With decrease of temperature or rise of the parameter $(U-J)/(2w)$ the holes concentration decrease smoothly.

The energy gap width ΔE as a function of the parameters $(U'-J)/(2w)$ and $(kT)/(2w)$ is presented in Figs. 3 and 4, respectively. With a change of the parameter $(U'-J)/(2w)$ system undergoes the transition from an insulating to a metallic state (negative values of the energy gap

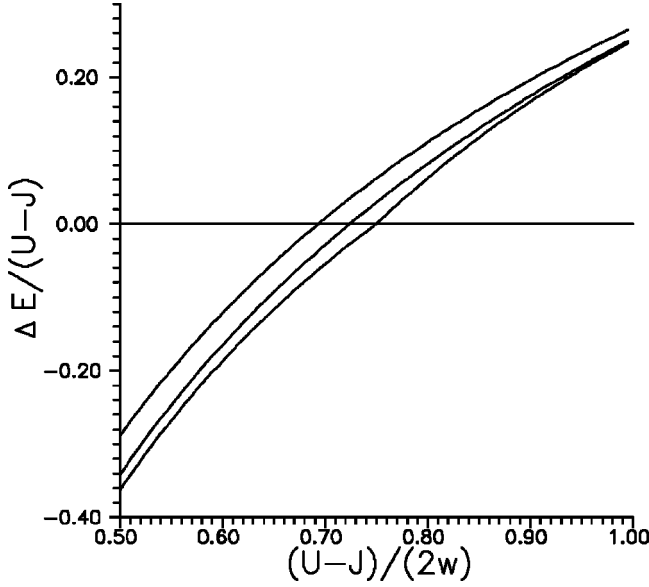


FIG. 3. The dependence of energy gap width $\Delta E/(U-J)$ on the parameter $(U'-J)/(2w)$: the upper curve $-(kT)/(2w)=0.1$; the middle curve $-(kT)/(2w)=0.05$; the lower curve $-(kT)/(2w)=0$.

width correspond to the overlapping of the Hubbard subbands). In the model under consideration at $T=0$ K insulator-metal transition at $n=1$ occurs when $(U'-J)/(2w)=0.75$ (Fig. 3, the lower curve) [in the single-band Hubbard model the respective parameter is $U/(2w)=1$].⁴²

The transition from a metallic to an insulating state with increase of temperature at given value of the parameter $(U'-J)/(2w)$ is also possible (Fig. 4). It can be explained by the fact that energy gap width ΔE (3.18) increases at increasing temperature T which is caused by the rise of polar states concentration at constant w , $(U'-J)$.

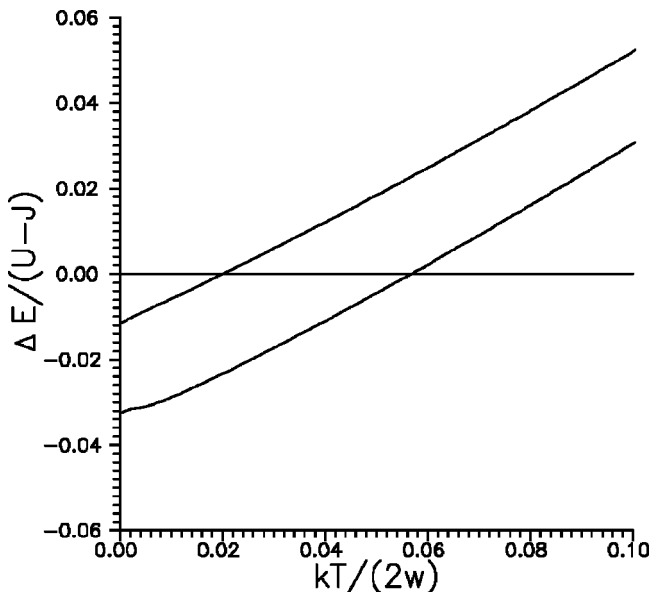


FIG. 4. The dependence of energy gap width $\Delta E/(U-J)$ on the parameter $(kT)/(2w)$: the upper curve $-(U'-J)/(2w)=0.74$; the lower curve $-(U'-J)/(2w)=0.72$.

2. The limit of the weak Hund's coupling

Let us consider the MIT at electron concentration $n=1$. If the exchange interaction is small comparatively to the Coulomb interaction $J \ll U$ then we can take J into account in the mean-field approximation (see, e.g., Ref. 10). The corresponding terms of the Hamiltonian (2.12) can be written as

$$\begin{aligned}
 & -2J \sum_{i\sigma} n_{i\alpha\sigma} n_{i\beta\bar{\sigma}} - 3J \sum_{i\sigma} n_{i\alpha\sigma} n_{i\beta\sigma} \\
 & = -2J \sum_{i\sigma} (\langle n_{i\alpha\sigma} \rangle n_{i\beta\bar{\sigma}} + n_{i\alpha\sigma} \langle n_{i\beta\bar{\sigma}} \rangle) \\
 & \quad - 3J \sum_{i\sigma} (\langle n_{i\alpha\sigma} \rangle n_{i\beta\sigma} + n_{i\alpha\sigma} \langle n_{i\beta\sigma} \rangle) \\
 & = -5J \langle n_{i\gamma\sigma} \rangle \sum_{i\gamma\sigma} n_{i\gamma\sigma}. \tag{3.19}
 \end{aligned}$$

The Hamiltonian (2.12) takes the form

$$\begin{aligned}
 H = & -\tilde{\mu} \sum_{i\gamma\sigma} a_{i\gamma\sigma}^+ a_{i\gamma\sigma} + \sum'_{ij\gamma\sigma} t_{ij}(n) a_{i\gamma\sigma}^+ a_{j\gamma\sigma} \\
 & + \sum'_{ij\gamma\sigma} (t'_{ij} a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{i\bar{\gamma}} + \text{H.c.}) \\
 & + \sum'_{ij\gamma\sigma} (t''_{ij} a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{i\gamma\bar{\sigma}} + \text{H.c.}) \\
 & + U \sum_{i\sigma\gamma} (n_{i\gamma\sigma} n_{i\gamma\bar{\sigma}} + n_{i\gamma\sigma} n_{i\bar{\gamma}\bar{\sigma}} + n_{i\gamma\sigma} n_{i\bar{\gamma}\sigma}), \tag{3.20}
 \end{aligned}$$

where $\tilde{\mu} = \mu + 5J \langle n_{i\gamma\sigma} \rangle$.

Considering MIT at the electron concentration n we can take into account in the Hamiltonian only the states of site with $n-1$, n , $n+1$ electrons (the analogous simplification has been used in Refs. 11 and 13). In the vicinity of the transition point at the electron concentration $n=1$ the concentrations of sites occupied by three and four electrons are small. Neglecting the small amounts of these sites we can write the electron operators in the form:

$$\begin{aligned}
 a_{i\alpha\uparrow}^+ & = X_i^{\alpha\uparrow,0} + X_i^{\uparrow\uparrow,\beta\uparrow} + X_i^{\uparrow\downarrow,\beta\downarrow} + X_i^{\alpha 2,\alpha\uparrow}, \\
 a_{i\alpha\downarrow}^+ & = X_i^{\alpha\downarrow,0} + X_i^{\downarrow\downarrow,\beta\downarrow} + X_i^{\downarrow\uparrow,\beta\uparrow} - X_i^{\alpha 2,\alpha\uparrow}, \\
 a_{i\beta\uparrow}^+ & = X_i^{\beta\uparrow,0} - X_i^{\uparrow\uparrow,\alpha\uparrow} - X_i^{\downarrow\uparrow,\alpha\downarrow} + X_i^{\beta 2,\beta\downarrow}, \\
 a_{i\beta\downarrow}^+ & = X_i^{\beta\downarrow,0} - X_i^{\downarrow\downarrow,\alpha\downarrow} - X_i^{\uparrow\downarrow,\alpha\uparrow} - X_i^{\beta 2,\beta\downarrow}. \tag{3.21}
 \end{aligned}$$

Hamiltonian (3.20) in the configurational representation takes the form:

$$\begin{aligned}
 H = & -\tilde{\mu} \left[\sum_{i\gamma\sigma} X_i^{\gamma\sigma} + 2 \sum_{i\sigma} (X_i^{\sigma\sigma} + X_i^{\sigma\bar{\sigma}}) + 2 \sum_{i\gamma} X_i^{\gamma 2} \right] \\
 & + U \left(\sum_{i\sigma} X_i^{\sigma\sigma} + \sum_{i\sigma} X_i^{\sigma\bar{\sigma}} + \sum_{i\gamma} X_i^{\gamma 2} \right) + H_1 + H_2, \tag{3.22}
 \end{aligned}$$

where the kinetic part of the Hamiltonian is

$$\begin{aligned}
H_1 = & \sum_{i,j} \left(t_{ij} \sum_{\gamma\sigma} X_i^{\gamma\sigma,0} X_j^{0,\gamma\sigma} + (t_{ij} + 2t'_{ij}) \sum_{\gamma\sigma} X_i^{\gamma^2,\gamma\sigma} X_j^{\gamma\sigma,\gamma^2} \right. \\
& + (t_{ij} + 2t'_{ij}) \left\{ \sum_{\gamma\sigma} X_i^{\sigma\sigma,\gamma\sigma} X_j^{\gamma\sigma,\sigma\sigma} + \sum_{\sigma} [X_i^{\sigma\bar{\sigma},\alpha\sigma} X_j^{\alpha\sigma,\sigma\bar{\sigma}} \right. \\
& + X_i^{\sigma\bar{\sigma},\beta\bar{\sigma}} X_j^{\beta\bar{\sigma},\sigma\bar{\sigma}} + (X_i^{\sigma\sigma,\alpha\sigma} X_j^{\alpha\bar{\sigma},\sigma\bar{\sigma}} + X_i^{\sigma\sigma,\beta\sigma} X_j^{\beta\bar{\sigma},\sigma\bar{\sigma}} \\
& \left. \left. + \text{H.c.}) \right\} + (t_{ij} + t'_{ij} + t''_{ij}) \left[\sum_{\gamma\sigma} \eta_{\sigma} \eta_{\bar{\gamma}} X_i^{\sigma\sigma,\gamma\sigma} X_j^{\bar{\gamma}\bar{\sigma},\bar{\gamma}^2} \right. \\
& \left. \left. + \sum_{\sigma} \eta_{\sigma} (X_i^{\sigma\bar{\sigma},\beta\bar{\sigma}} X_j^{\alpha\bar{\sigma},\alpha^2} + X_i^{\sigma\bar{\sigma},\alpha\sigma} X_j^{\beta\sigma,\beta^2}) + \text{H.c.} \right] \right), \quad (3.23)
\end{aligned}$$

$$\begin{aligned}
H_2 = & \sum_{i,j} \left\{ (t_{ij} + t'_{ij}) \left[\sum_{\gamma\sigma} (\eta_{\gamma} X_i^{\gamma\sigma,0} X_j^{\bar{\gamma}\sigma,\sigma\sigma} + \text{H.c.}) \right. \right. \\
& \left. \left. + \sum_{\sigma} (X_i^{\alpha\sigma,0} X_j^{\beta\bar{\sigma},\sigma\bar{\sigma}} - X_i^{\beta\sigma,0} X_j^{\alpha\bar{\sigma},\sigma\bar{\sigma}} + \text{H.c.}) \right] \right. \\
& \left. + (t_{ij} + t''_{ij}) \sum_{\gamma\sigma} (\eta_{\sigma} X_i^{\gamma\sigma,0} X_j^{\bar{\gamma}\sigma,\gamma^2} + \text{H.c.}) \right\}, \quad (3.24)
\end{aligned}$$

where $\eta_{\uparrow} = \eta_{\alpha} = 1$, $\eta_{\downarrow} = \eta_{\beta} = -1$.

The processes that form energy subbands are included in the Hamiltonian H_1 , the processes of hybridization of these subbands are included in the Hamiltonian H_2 .

The single-particle Green function can be written as

$$\begin{aligned}
\langle\langle a_{p\alpha\uparrow} | a_{p'\alpha\uparrow}^+ \rangle\rangle = & \langle\langle X_p^{0,\alpha\uparrow} | X_{p'}^{\alpha\uparrow,0} \rangle\rangle + \langle\langle X_p^{0,\alpha\uparrow} | Y_{p'}^+ \rangle\rangle \\
& + \langle\langle Y_p | X_{p'}^{\alpha\uparrow,0} \rangle\rangle + \langle\langle Y_p | Y_{p'}^+ \rangle\rangle. \quad (3.25)
\end{aligned}$$

Here we have introduced the following notation: $Y_p = X_p^{\alpha\downarrow,\alpha^2} + X_p^{\beta\uparrow,\uparrow\uparrow} + X_p^{\beta\downarrow,\uparrow\downarrow}$. The functions $\langle\langle X_p^{0,\alpha\uparrow} | X_{p'}^{\alpha\uparrow,0} \rangle\rangle$ and $\langle\langle X_p^{0,\alpha\uparrow} | Y_{p'}^+ \rangle\rangle$ satisfy the equations:

$$\begin{aligned}
(E + \tilde{\mu}) \langle\langle X_p^{0,\alpha\uparrow} | X_{p'}^{\alpha\uparrow,0} \rangle\rangle = & \frac{\langle X_p^0 + X_{p'}^{\alpha\uparrow} \rangle}{2\pi} \delta_{ij} \\
& + \langle\langle [X_p^{0,\alpha\uparrow}; H_1 + H_2] | X_{p'}^{\alpha\uparrow,0} \rangle\rangle, \\
(E + \tilde{\mu} - U) \langle\langle Y_p | X_{p'}^{\alpha\uparrow,0} \rangle\rangle = & \langle\langle [Y_p; H_1 + H_2] | X_{p'}^{\alpha\uparrow,0} \rangle\rangle. \quad (3.26)
\end{aligned}$$

For calculation of these functions we use the generalized mean-field approximation.⁴² Let us take the commutators in Eq. (3.26) in the form:

$$\begin{aligned}
[X_p^{0,\alpha\uparrow}, H_1] = & \sum_j' \epsilon(pj) X_j^{0,\alpha\uparrow}, \\
[X_p^{0,\alpha\uparrow}, H_2] = & \sum_j' \tilde{\epsilon}(pj) Y_j, \quad (3.27)
\end{aligned}$$

$$[Y_p, H_1] = \sum_j' \zeta(pj) Y_j, \quad [Y_p, H_2] = \sum_j' \tilde{\zeta}(pj) X_j^{0,\alpha\uparrow},$$

where $\epsilon(pj), \tilde{\epsilon}(pj), \zeta(pj), \tilde{\zeta}(pj)$ are the nonoperator expressions.

After transition to \mathbf{k} representation the system of Eqs. (3.26) taking into account (3.27) has the solutions:

$$\langle\langle X_p^{0,\alpha\uparrow} | X_{p'}^{\alpha\uparrow,0} \rangle\rangle_{\mathbf{k}} = \frac{\langle X_p^0 + X_{p'}^{\alpha\uparrow} \rangle}{2\pi} \frac{E + \tilde{\mu} - U - \zeta(\mathbf{k})}{[E - E_1(\mathbf{k})][E - E_2(\mathbf{k})]}, \quad (3.28)$$

$$\langle\langle Y_p | X_{p'}^{\alpha\uparrow,0} \rangle\rangle_{\mathbf{k}} = \frac{\langle X_p^0 + X_{p'}^{\alpha\uparrow} \rangle}{2\pi} \frac{\tilde{\zeta}(\mathbf{k})}{[E - E_1(\mathbf{k})][E - E_2(\mathbf{k})]}.$$

Here, $E_{1,2}(\mathbf{k})$ is the quasiparticle energy spectrum:

$$\begin{aligned}
E_{1,2}(\mathbf{k}) = & -\tilde{\mu} + \frac{U}{2} + \frac{\epsilon(\mathbf{k}) + \zeta(\mathbf{k})}{2} \\
& \mp \frac{1}{2} \{ [U - \epsilon(\mathbf{k}) + \zeta(\mathbf{k})]^2 + 4\tilde{\epsilon}(\mathbf{k})\tilde{\zeta}(\mathbf{k}) \}^{1/2}. \quad (3.29)
\end{aligned}$$

The same expression for the quasiparticle energy spectrum we obtain from the functions $\langle\langle X_p^{0,\alpha\uparrow} | Y_{p'}^+ \rangle\rangle_{\mathbf{k}}$ and $\langle\langle Y_p | Y_{p'}^+ \rangle\rangle_{\mathbf{k}}$. The values of $\epsilon(pj), \tilde{\epsilon}(pj), \zeta(pj), \tilde{\zeta}(pj)$ we find by anticommutation of Eq. (3.27) with the operators $X_{p'}^{\alpha\uparrow,0}$ and $Y_{p'}^+$:

$$\begin{aligned}
(X_p^0 + X_{p'}^{\alpha\uparrow}) \epsilon(pp') = & \{ X_{p'}^{\alpha\uparrow,0}; [X_p^{0,\alpha\uparrow}, H_1] \}, \\
(X_p^{\alpha\downarrow} + X_p^{\beta\uparrow} + X_p^{\beta\downarrow} + X_p^{\uparrow\uparrow} + X_p^{\uparrow\downarrow} + X_p^{\alpha^2}) \tilde{\epsilon}(pp') = & \{ Y_{p'}^+; [X_p^{0,\alpha\uparrow}, H_2] \}, \\
(X_p^{\alpha\downarrow} + X_p^{\beta\uparrow} + X_p^{\beta\downarrow} + X_p^{\uparrow\uparrow} + X_p^{\uparrow\downarrow} + X_p^{\alpha^2}) \zeta(pp') = & \{ Y_{p'}^+; [Y_p, H_1] \}, \\
(X_p^0 + X_{p'}^{\alpha\uparrow}) \tilde{\zeta}(pp') = & \{ X_{p'}^{\alpha\uparrow,0}; [Y_p, H_2] \}. \quad (3.30)
\end{aligned}$$

By use of the mean-field approximation analogously to the above, in the case of $t'_k = t''_k$ we obtain

$$\begin{aligned}
\epsilon(\mathbf{k}) = & t_{\mathbf{k}} \left[(c+b) + \frac{3b^2}{c+b} \right] - 3\tilde{t}_{\mathbf{k}} \frac{6d^2}{c+b}, \\
\tilde{\epsilon}(\mathbf{k}) = & \frac{t_{\mathbf{k}} + \tilde{t}_{\mathbf{k}}}{2} \left[(c+b) - \frac{b^2}{d+b} + \frac{6d^2}{d+b} \right], \quad (3.31)
\end{aligned}$$

$$\zeta(\mathbf{k}) = -t_{\mathbf{k}} \frac{6d^2}{d+b} + \tilde{t}_{\mathbf{k}} \left[3(d+b) + \frac{b^2}{d+b} + \frac{8d^2}{3(d+b)} \right],$$

$$\tilde{\zeta}(\mathbf{k}) = \frac{t_{\mathbf{k}} + \tilde{t}_{\mathbf{k}}}{2} \left[(d+b) - \frac{b^2}{c+b} + \frac{6d^2}{c+b} \right],$$

here c, b, d are the concentrations of the holes and sites occupied by one, two electrons, respectively, connected by the relations

$$c = 6d, \quad b = \frac{1}{4} - 3d; \quad (3.32)$$

and

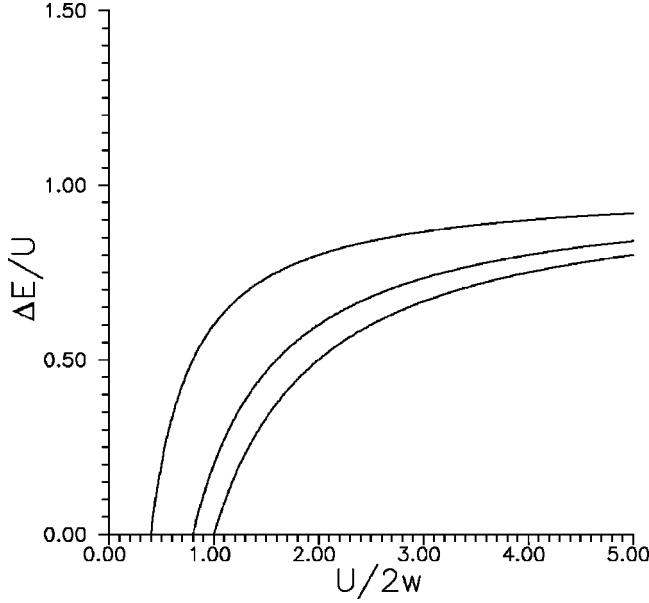


FIG. 5. The dependence of energy gap width $\Delta E/U$ on the parameter $U/(2w)$ for $n=1$ at different values of the parameter $\kappa = t'_{ij}/t_{ij}$: the lower curve $-\kappa=0$; the middle curve $-\kappa=0.2$; the upper curve $-\kappa=0.6$.

$$\tilde{t}_{\mathbf{k}} = t_{\mathbf{k}} + 2t'_{\mathbf{k}}. \quad (3.33)$$

In the point of transition, when the concentrations of the holes and doublons are equal to zero, the energies of the electrons within the subbands are

$$E_1(\mathbf{k}) = -\tilde{\mu} + t_{\mathbf{k}}, \quad (3.34)$$

$$E_2(\mathbf{k}) = -\tilde{\mu} + U + \tilde{t}_{\mathbf{k}}.$$

The energy gap in this case is

$$\Delta E = U - w - \tilde{w} = 0, \quad (3.35)$$

where $w = z|t_{ij}|$, $\tilde{w} = z|\tilde{t}_{ij}|$. From the Eq. (3.35) we obtain the criterion of MIT

$$U = w + \tilde{w}. \quad (3.36)$$

In the partial case $t'_{\mathbf{k}} = t''_{\mathbf{k}} = 0$ (in this case $t_{\mathbf{k}} = \tilde{t}_{\mathbf{k}}$) we have

$$\frac{U}{2w} = 1. \quad (3.37)$$

In Fig. 5 the energy gap for different values of the correlated hopping at $T=0$ is plotted. With the increase of the correlated hopping at the fixed value of parameter $U/2w$ the en-

ergy gap width increases and the region of values of $U/2w$ at which the system is in a metallic state, decreases.

B. The limit of the weak Hund's coupling at electron concentration $n=2$

Let us consider the MIT at electron concentration $n=2$. In the vicinity of the transition point in the case of two electrons per atom the concentrations of holes and sites occupied by four electrons are small. Neglecting the small amounts of these sites we can write the electron operators in the form:

$$a_{i\alpha\uparrow}^+ = X_i^{\uparrow\uparrow,\beta\uparrow} + X_i^{\uparrow\downarrow,\beta\downarrow} + X_i^{\alpha 2,\alpha\downarrow} + X_i^{\alpha 2\downarrow,\downarrow\downarrow} + X_i^{\alpha 2\uparrow,\downarrow\uparrow} + X_i^{\beta 2\uparrow,\beta 2},$$

$$a_{i\alpha\downarrow}^+ = X_i^{\downarrow\downarrow,\beta\downarrow} + X_i^{\downarrow\uparrow,\beta\uparrow} - X_i^{\alpha 2,\alpha\uparrow} - X_i^{\alpha 2\downarrow,\uparrow\downarrow} - X_i^{\alpha 2\uparrow,\uparrow\uparrow} + X_i^{\beta 2\downarrow,\beta 2}, \quad (3.38)$$

$$a_{i\beta\uparrow}^+ = -X_i^{\uparrow\uparrow,\alpha\uparrow} - X_i^{\downarrow\uparrow,\alpha\downarrow} + X_i^{\beta 2,\beta\downarrow} - X_i^{\beta 2\downarrow,\downarrow\downarrow} - X_i^{\beta 2\uparrow,\downarrow\uparrow} + X_i^{\alpha 2\uparrow,\alpha 2},$$

$$a_{i\beta\downarrow}^+ = -X_i^{\downarrow\downarrow,\alpha\downarrow} - X_i^{\downarrow\uparrow,\alpha\uparrow} - X_i^{\beta 2,\beta\uparrow} + X_i^{\alpha 2\downarrow,\alpha 2} + X_i^{\beta 2\uparrow,\uparrow\uparrow} + X_i^{\beta 2\downarrow,\downarrow\uparrow}.$$

Let us rewrite the Hamiltonian (3.20) in the configurational representation at electron concentration $n=2$. For the small values of the intra-atomic exchange interaction ($J \ll U$) we take J into account in the mean-field approximation (3.19). The Hamiltonian takes the form

$$H = -\tilde{\mu} \left[\sum_{i\gamma\sigma} X_i^{\gamma\sigma} + 2 \sum_{i\sigma} (X_i^{\sigma\sigma} + X_i^{\sigma\bar{\sigma}}) + 2 \sum_{i\gamma} X_i^{\gamma 2} + 3 \sum_{i\gamma\sigma} X_i^{\gamma 2\sigma} \right] + U \left(\sum_{i\sigma} X_i^{\sigma\sigma} + \sum_{i\sigma} X_i^{\sigma\bar{\sigma}} + \sum_{i\gamma} X_i^{\gamma 2} + 3 \sum_{i\gamma\sigma} X_i^{\gamma 2\sigma} \right) + H_1 + H_2, \quad (3.39)$$

where the kinetic part of the Hamiltonian is

$$\begin{aligned}
H_1 = & \sum_{i,j} \left((t_{ij} + 2t''_{ij}) \sum_{\gamma\sigma} X_i^{\gamma^2, \gamma\sigma} X_j^{\gamma\sigma, \gamma^2} + (t_{ij} + 2t'_{ij}) \left\{ \sum_{\gamma\sigma} X_i^{\sigma\sigma, \gamma\sigma} X_j^{\gamma\sigma, \sigma\sigma} + \sum_{\sigma} [X_i^{\sigma\bar{\sigma}, \alpha\sigma} X_j^{\alpha\sigma, \sigma\bar{\sigma}} + X_i^{\sigma\bar{\sigma}, \beta\sigma} X_j^{\beta\sigma, \sigma\bar{\sigma}} \right. \right. \\
& + (X_i^{\sigma\sigma, \alpha\sigma} X_j^{\alpha\bar{\sigma}, \sigma\bar{\sigma}} + X_i^{\sigma\sigma, \beta\sigma} X_j^{\beta\bar{\sigma}, \sigma\bar{\sigma}} + \text{H.c.}) \left. \left. \right\} + (t_{ij} + t'_{ij} + t''_{ij}) \left[\sum_{\gamma\sigma} \eta_{\sigma} \eta_{\bar{\gamma}} X_i^{\sigma\sigma, \gamma\sigma} X_j^{\bar{\gamma}\bar{\sigma}, \bar{\gamma}^2} + \sum_{\sigma} \eta_{\sigma} (X_i^{\sigma\bar{\sigma}, \beta\sigma} X_j^{\alpha\bar{\sigma}, \alpha^2} \right. \right. \\
& + X_i^{\sigma\bar{\sigma}, \alpha\sigma} X_j^{\beta\sigma, \beta^2}) + \text{H.c.} \left. \left. \right] + (t_{ij} + 2t'_{ij} + 2t''_{ij}) \left[\sum_{\gamma\sigma} X_i^{\gamma^2\sigma, \sigma\sigma} X_j^{\sigma\sigma, \gamma^2\sigma} + \sum_{\sigma} (X_i^{\alpha^2\sigma, \sigma\sigma} X_j^{\sigma\bar{\sigma}, \alpha^2\sigma} + X_i^{\beta^2\sigma, \sigma\sigma} X_j^{\sigma\bar{\sigma}, \beta^2\sigma}) \right] \right. \\
& + (t_{ij} + 4t'_{ij}) \sum_{\gamma\sigma} X_i^{\gamma^2\sigma, \gamma^2} X_j^{\gamma^2, \gamma^2\sigma} + (t_{ij} + 2t'_{ij} + 2t''_{ij}) \sum_{\sigma} (X_i^{\alpha^2\sigma, \sigma\sigma} X_j^{\sigma\bar{\sigma}, \alpha^2\sigma} + X_i^{\beta^2\sigma, \sigma\sigma} X_j^{\sigma\bar{\sigma}, \beta^2\sigma} + \text{H.c.}) \\
& + (t_{ij} + 3t'_{ij} + t''_{ij}) \sum_{\gamma\sigma} (\eta_{\sigma} \eta_{\bar{\gamma}} X_i^{\gamma^2\sigma, \sigma\sigma} X_j^{\bar{\gamma}^2, \bar{\gamma}^2\sigma} + \text{H.c.}) + (t_{ij} + 3t'_{ij} + t''_{ij}) \\
& \left. \times \sum_{\sigma} \eta_{\sigma} (X_i^{\alpha^2\sigma, \sigma\sigma} X_j^{\beta^2, \beta^2\sigma} - X_i^{\beta^2\sigma, \sigma\sigma} X_j^{\alpha^2, \alpha^2\sigma} + \text{H.c.}) \right), \tag{3.40}
\end{aligned}$$

$$\begin{aligned}
H_2 = & \sum_{i,j} \left((t_{ij} + 2t'_{ij} + t''_{ij}) \left\{ \sum_{\gamma\sigma} (\eta_{\sigma} X_i^{\sigma\sigma, \gamma\sigma} X_j^{\sigma\bar{\sigma}, \bar{\gamma}^2\bar{\sigma}} + \eta_{\bar{\sigma}} X_i^{\gamma^2, \gamma\sigma} X_j^{\bar{\gamma}^2, \bar{\gamma}^2\bar{\sigma}}) + \sum_{\sigma} [\eta_{\sigma} (X_i^{\sigma\sigma, \beta\sigma} X_j^{\sigma\bar{\sigma}, \alpha^2\sigma} + X_i^{\sigma\sigma, \alpha\sigma} X_j^{\sigma\bar{\sigma}, \beta^2\sigma} \right. \right. \\
& + X_i^{\sigma\bar{\sigma}, \beta\sigma} X_j^{\sigma\bar{\sigma}, \alpha^2\sigma} + X_i^{\sigma\bar{\sigma}, \beta\sigma} X_j^{\sigma\bar{\sigma}, \alpha^2\sigma}) + \eta_{\bar{\sigma}} (X_i^{\sigma\bar{\sigma}, \alpha\sigma} X_j^{\sigma\bar{\sigma}, \beta^2\sigma} - X_i^{\sigma\bar{\sigma}, \alpha\sigma} X_j^{\sigma\bar{\sigma}, \beta^2\sigma}) \left. \left. \right\} + (t_{ij} + 3t'_{ij}) \left[\sum_{\gamma\sigma} \eta_{\bar{\sigma}} X_i^{\sigma\sigma, \gamma\sigma} X_j^{\gamma^2, \gamma^2\sigma} \right. \right. \\
& + \sum_{\sigma} (X_i^{\sigma\bar{\sigma}, \beta\sigma} X_j^{\beta^2, \beta^2\sigma} - X_i^{\sigma\bar{\sigma}, \alpha\sigma} X_j^{\alpha^2, \alpha^2\sigma}) \left. \left. \right] + (t_{ij} + t'_{ij} + 2t''_{ij}) \left[\sum_{\gamma\sigma} \eta_{\gamma} X_i^{\gamma^2, \gamma\sigma} X_j^{\sigma\sigma, \gamma^2\sigma} + \sum_{\sigma} (X_i^{\alpha^2, \alpha\sigma} X_j^{\sigma\bar{\sigma}, \alpha^2\sigma} \right. \right. \\
& \left. \left. - X_i^{\beta^2, \beta\sigma} X_j^{\sigma\bar{\sigma}, \beta^2\sigma}) \right] + \text{H.c.} \right).
\end{aligned}$$

The processes that form energy subbands are included in the Hamiltonian H_1 , the processes of hybridization of these subbands are included in the Hamiltonian H_2 .

Let us write the single-particle Green function as

$$\begin{aligned}
\langle\langle a_{p\alpha\uparrow} | a_{p',\alpha\uparrow}^+ \rangle\rangle = & \langle\langle Y_p | Y_{p'}^+ \rangle\rangle + \langle\langle Z_p | Y_{p'}^+ \rangle\rangle + \langle\langle Y_p | Z_{p'}^+ \rangle\rangle \\
& + \langle\langle Z_p | Z_{p'}^+ \rangle\rangle. \tag{3.41}
\end{aligned}$$

Here the following notations have been introduced:

$$\begin{aligned}
Y_p = & X_p^{\alpha^1, \alpha^2} + X_p^{\beta^1, \uparrow\uparrow} + X_p^{\beta^1, \uparrow\downarrow}, \\
Z_p = & X_p^{\downarrow\downarrow, \alpha^2\downarrow} + X_p^{\downarrow\uparrow, \alpha^2\uparrow} + X_p^{\beta^2, \beta^2\uparrow}.
\end{aligned}$$

The functions $\langle\langle Y_p | Y_{p'}^+ \rangle\rangle$ and $\langle\langle Z_p | Y_{p'}^+ \rangle\rangle$ satisfy the equations:

$$(E + \tilde{\mu} - U) \langle\langle Y_p | Y_{p'}^+ \rangle\rangle = \frac{A}{2\pi} \delta_{ij} + \langle\langle [Y_p; H_1 + H_2] | Y_{p'}^+ \rangle\rangle, \tag{3.42}$$

$$(E + \tilde{\mu} - 2U) \langle\langle Z_p | Y_{p'}^+ \rangle\rangle = \langle\langle [Z_p; H_1 + H_2] | Y_{p'}^+ \rangle\rangle,$$

where $A = \langle X_p^{\alpha^1} + X_p^{\beta^1} + X_p^{\beta^1} + X_p^{\uparrow\uparrow} + X_p^{\uparrow\downarrow} + X_p^{\alpha^2} \rangle$. On the analogy of the previous section we use the generalized mean-field approximation to calculate these functions. Let us take the commutators in Eq. (3.42) in the form

$$[Y_p, H_1] = \sum_j' \epsilon(pj) Y_j, \quad [Y_p, H_2] = \sum_j' \tilde{\epsilon}(pj) Z_j, \tag{3.43}$$

$$[Z_p, H_1] = \sum_j' \zeta(pj) Z_j, \quad [Z_p, H_2] = \sum_j' \tilde{\zeta}(pj) Y_j,$$

where $\epsilon(pj), \tilde{\epsilon}(pj), \zeta(pj), \tilde{\zeta}(pj)$ are the nonoperator expressions, which we calculate using method of paper.⁴²

After transition to \mathbf{k} representation the system of Eqs. (3.42) taking into account Eq. (3.43) has the solutions

$$\langle\langle Y_p | Y_{p'}^+ \rangle\rangle_{\mathbf{k}} = \frac{A}{2\pi} \frac{E + \tilde{\mu} - 2U - \zeta(\mathbf{k})}{[E - E_1(\mathbf{k})][E - E_2(\mathbf{k})]}, \tag{3.44}$$

$$\langle\langle Z_p | Y_{p'}^+ \rangle\rangle_{\mathbf{k}} = \frac{A}{2\pi} \frac{\tilde{\zeta}(\mathbf{k})}{[E - E_1(\mathbf{k})][E - E_2(\mathbf{k})]}.$$

Here, $E_{1,2}(\mathbf{k})$ is the quasiparticle energy spectrum

$$E_{1,2}(\mathbf{k}) = -\tilde{\mu} + \frac{3U}{2} + \frac{\epsilon(\mathbf{k}) + \zeta(\mathbf{k})}{2}$$

$$\mp \frac{1}{2} \{ [U - \epsilon(\mathbf{k}) + \zeta(\mathbf{k})]^2 + 4\tilde{\epsilon}(\mathbf{k})\tilde{\zeta}(\mathbf{k}) \}^{1/2}.$$

The same expression for the quasiparticle energy spectrum we obtain from the functions $\langle\langle Y_p | Z_{p'}^+ \rangle\rangle_{\mathbf{k}}$ and $\langle\langle Z_p | Z_{p'}^+ \rangle\rangle_{\mathbf{k}}$. The values of $\epsilon(pp'), \tilde{\epsilon}(pp'), \zeta(pp'), \tilde{\zeta}(pp')$ we find by anticommutation of Eq. (3.43) with the operators $Y_{p'}^+$ and $Z_{p'}^+$

$$\begin{aligned}
& (X_p^{\alpha\downarrow} + X_p^{\beta\uparrow} + X_p^{\beta\downarrow} + X_p^{\uparrow\uparrow} + X_p^{\uparrow\downarrow} + X_p^{\alpha 2}) \epsilon(pp') \\
&= \{Y_{p'}^+, [Y_p, H_1]\}, \\
& (X_p^{\downarrow\downarrow} + X_p^{\downarrow\uparrow} + X_p^{\beta 2} + X_p^{\alpha 2\uparrow} + X_p^{\alpha 2\downarrow} + X_p^{\beta 2\uparrow}) \tilde{\epsilon}(pp') \\
&= \{Z_{p'}^+, [Y_p, H_2]\}, \\
& (X_p^{\downarrow\downarrow} + X_p^{\downarrow\uparrow} + X_p^{\beta 2} + X_p^{\alpha 2\uparrow} + X_p^{\alpha 2\downarrow} + X_p^{\beta 2\uparrow}) \zeta(pp') \\
&= \{Z_{p'}^+, [Z_p, H_1]\}, \\
& (X_p^{\alpha\downarrow} + X_p^{\beta\uparrow} + X_p^{\beta\downarrow} + X_p^{\uparrow\uparrow} + X_p^{\uparrow\downarrow} + X_p^{\alpha 2}) \tilde{\zeta}(pp') \\
&= \{Y_{p'}^+, [Z_p, H_2]\}.
\end{aligned} \tag{3.46}$$

By use of the mean-field approximation analogously to the above, in the case of $t'_k = t''_k$ we obtain

$$\begin{aligned}
\epsilon(\mathbf{k}) &= \tilde{t}_{\mathbf{k}} \left[3(d+b) + \frac{b^2}{d+b} + \frac{8d^2}{3(d+b)} \right] - t_{\mathbf{k}}^* \frac{8b^2}{3(d+b)}, \\
\tilde{\epsilon}(\mathbf{k}) &= \frac{\tilde{t}_{\mathbf{k}} + t_{\mathbf{k}}^*}{2} \left[3(d+b) - \frac{8d^2}{3(d+b)} + \frac{7b^2}{3(d+b)} \right],
\end{aligned} \tag{3.47}$$

$$\zeta(\mathbf{k}) = -\tilde{t}_{\mathbf{k}} \frac{8b^2}{3(d+b)} + t_{\mathbf{k}}^* \left[3(d+b) + \frac{b^2}{d+b} + \frac{8d^2}{3(d+b)} \right],$$

$$\tilde{\zeta}(\mathbf{k}) = \frac{\tilde{t}_{\mathbf{k}} + t_{\mathbf{k}}^*}{2} \left[3(d+b) - \frac{8d^2}{3(d+b)} + \frac{7b^2}{3(d+b)} \right],$$

with

$$\tilde{t}_{\mathbf{k}} = t_{\mathbf{k}} + 2t'_{\mathbf{k}}, \tag{3.48}$$

$$t_{\mathbf{k}}^* = t_{\mathbf{k}} + 4t'_{\mathbf{k}};$$

here b is the concentration of the sites occupied by one (or three) electrons, d is the concentration of the doubly occupied sites, connected by the relation

$$b = \frac{1-8d}{6}. \tag{3.49}$$

In the point of transition, when the concentrations of the singly and triply occupied sites are equal to zero, the quasiparticle energy spectrum is

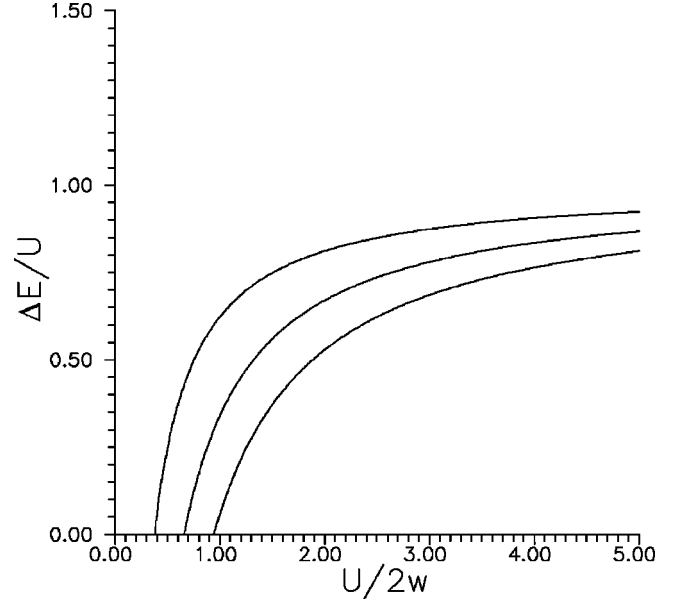


FIG. 6. The dependence of energy gap width $\Delta E/U$ on the parameter $U/(2w)$ for $n=2$ at different values of the parameter $\kappa = t'_{ij}/t_{ij}$: the lower curve— $\kappa=0$; the middle curve— $\kappa=0.1$; the upper curve— $\kappa=0.2$.

$$\begin{aligned}
E_{1,2}(\mathbf{k}) &= -\tilde{\mu} + \frac{3U}{2} + \frac{17}{18} \frac{t_{\mathbf{k}}^* + \tilde{t}_{\mathbf{k}}}{2} \\
&+ \frac{1}{2} \left\{ \left[U + \frac{17}{18} \frac{t_{\mathbf{k}}^* - \tilde{t}_{\mathbf{k}}}{2} \right]^2 + \left[\frac{t_{\mathbf{k}}^* + \tilde{t}_{\mathbf{k}}}{18} \right]^2 \right\}^{1/2}.
\end{aligned} \tag{3.50}$$

Using the quasiparticle energy spectrum (3.50) we find the energy gap width. In the point of MIT the energy gap is equal to zero. From this condition we find the criterion of MIT. In the partial case of $t'_k = t''_k = 0$ (in this case $t_{\mathbf{k}}^* = \tilde{t}_{\mathbf{k}}$) we find

$$\frac{U}{2w} = 2 \sqrt{\frac{2}{3}}. \tag{3.51}$$

In Fig. 6 the energy gap for different values of the correlated hopping at $T=0$ is plotted. With the increase of the correlated hopping at the fixed value of parameter $U/2w$ the energy gap width increases faster than at $n=1$ and the region of values of $U/2w$ at which the system is in the metallic state, decreases, analogously to the case $n=1$.

C. The limit of the weak Hund's coupling at electron concentration $n=3$

Let us consider the MIT at electron concentration $n=3$. In the vicinity of the transition point in the case of three electrons per atom the concentrations of holes and sites occupied by one electron are small. Neglecting the small amounts of these sites we can write the electron operators in the form:

$$a_{i\alpha}^+ = +X_i^{\alpha 2\downarrow, \downarrow\downarrow} + X_i^{\alpha 2\uparrow, \uparrow\uparrow} + X_i^{\beta 2\uparrow, \beta 2} + X_i^{\beta 2\downarrow},$$

$$\begin{aligned}
a_{i\alpha\downarrow}^+ &= -X_i^{\alpha 2\downarrow, \uparrow\downarrow} - X_i^{\alpha 2\uparrow, \uparrow\uparrow} + X_i^{\beta 2\downarrow, \beta 2} - X_i^{4, \beta 2\uparrow}, \\
a_{i\beta\uparrow}^+ &= -X_i^{\beta 2\downarrow, \downarrow\downarrow} - X_i^{\beta 2\uparrow, \uparrow\downarrow} + X_i^{\alpha 2\uparrow, \alpha 2} + X_i^{4, \alpha 2\downarrow}, \\
a_{i\beta\downarrow}^+ &= +X_i^{\alpha 2\downarrow, \alpha 2} + X_i^{\beta 2\uparrow, \uparrow\uparrow} + X_i^{\beta 2\downarrow, \downarrow\uparrow} - X_i^{4, \alpha 2\uparrow}.
\end{aligned} \quad (3.52)$$

Let us rewrite the Hamiltonian (3.20) in the configurational representation at electron concentration $n=3$. For the small values of the intra-atomic exchange interaction ($J \ll U$) we take J into account in the mean field approximation (3.19). The Hamiltonian takes the form

$$\begin{aligned}
H = -\tilde{\mu} & \left[2 \sum_{i\sigma} (X_i^{\sigma\sigma} + X_i^{\sigma\bar{\sigma}}) + 2 \sum_{i\gamma} X_i^{\gamma 2} + 3 \sum_{i\gamma\sigma} X_i^{\gamma 2\sigma} \right. \\
& + 4 \sum_i X_i^4 \left. \right] + U \left(\sum_{i\sigma} X_i^{\sigma\sigma} + \sum_{i\sigma} X_i^{\sigma\bar{\sigma}} + \sum_{i\gamma} X_i^{\gamma 2} \right. \\
& \left. + 3 \sum_{i\gamma\sigma} X_i^{\gamma 2\sigma} + 6 X_i^4 \right) + H_1 + H_2, \quad (3.53)
\end{aligned}$$

where the kinetic part of the Hamiltonian

$$\begin{aligned}
H_1 = \sum_{i,j} & \left\{ (t_{ij} + 2t'_{ij} + 2t''_{ij}) \left[\sum_{\gamma\sigma} X_i^{\gamma 2\sigma, \sigma\sigma} X_j^{\sigma\sigma, \gamma 2\sigma} + \sum_{\sigma} (X_i^{\alpha 2\sigma, \bar{\sigma}\sigma} X_j^{\bar{\sigma}\sigma, \alpha 2\sigma} + X_i^{\beta 2\sigma, \sigma\bar{\sigma}} X_j^{\sigma\bar{\sigma}, \beta 2\sigma} + \text{H.c.}) \right] \right. \\
& + (t_{ij} + 4t'_{ij}) \sum_{\gamma\sigma} X_i^{\gamma 2\sigma, \gamma 2} X_j^{\gamma 2, \gamma 2\sigma} + (t_{ij} + 2t'_{ij} + 2t''_{ij}) \sum_{\sigma} (X_i^{\alpha 2\sigma, \sigma\sigma} X_j^{\sigma\bar{\sigma}, \alpha 2\bar{\sigma}} + X_i^{\beta 2\sigma, \sigma\sigma} X_j^{\sigma\bar{\sigma}, \beta 2\bar{\sigma}} + \text{H.c.}) \\
& + (t_{ij} + 3t'_{ij} + t''_{ij}) \sum_{\gamma\sigma} (\eta_{\bar{\sigma}} \eta_{\gamma} X_i^{\gamma 2\sigma, \sigma\sigma} X_j^{\bar{\gamma} 2, \bar{\gamma} 2\bar{\sigma}} + \text{H.c.}) + (t_{ij} + 3t'_{ij} + t''_{ij}) \sum_{\sigma} \eta_{\sigma} (X_i^{\alpha 2\sigma, \bar{\sigma}\sigma} X_j^{\beta 2, \beta 2\sigma} - X_i^{\beta 2\sigma, \sigma\bar{\sigma}} X_j^{\alpha 2, \alpha 2\sigma} + \text{H.c.}) \\
& \left. + (t_{ij} + 4t'_{ij} + 2t''_{ij}) X_i^{4, \gamma 2\sigma} X_j^{\gamma 2\sigma, 4} \right\}, \\
H_2 = \sum_{i,j} & \left\{ (t_{ij} + 3t'_{ij} + 2t''_{ij}) \sum_{\gamma\sigma} \left[\eta_{\gamma} X_i^{\gamma 2\sigma, \sigma\sigma} X_j^{\bar{\gamma} 2\sigma, 4} + \sum_{\sigma} (X_i^{\alpha 2\sigma, \bar{\sigma}\sigma} X_j^{\beta 2\bar{\sigma}, 4} - X_i^{\beta 2\sigma, \sigma\bar{\sigma}} X_j^{\alpha 2\bar{\sigma}, 4}) \right] \right. \\
& \left. + (t_{ij} + 3t'_{ij}) \sum_{\gamma\sigma} \eta_{\sigma} X_i^{\gamma 2\sigma, \gamma 2} X_j^{\gamma 2\bar{\sigma}, 4} + \text{H.c.} \right\}.
\end{aligned}$$

The processes that form energy subbands are included in the Hamiltonian H_1 , the processes of hybridization of these subbands are included in the Hamiltonian H_2 .

Let us write the single-particle Green function as:

$$\begin{aligned}
\langle\langle a_{p\alpha\uparrow} | a_{p'\alpha\uparrow}^+ \rangle\rangle &= \langle\langle X_p^{\beta 2\downarrow, 4} | X_{p'}^{4, \beta 2\downarrow} \rangle\rangle + \langle\langle X_p^{\beta 2\downarrow, 4} | Z_{p'}^+ \rangle\rangle \\
&+ \langle\langle Z_p | X_{p'}^{4, \beta 2\downarrow} \rangle\rangle + \langle\langle Z_p | Z_{p'}^+ \rangle\rangle. \quad (3.54)
\end{aligned}$$

Here the following notations have been introduced: $Z_p = X_p^{\downarrow\downarrow, \alpha 2\downarrow} + X_p^{\downarrow\uparrow, \alpha 2\uparrow} + X_p^{\beta 2, \beta 2\uparrow}$. The functions $\langle\langle X_p^{\beta 2\downarrow, 4} | X_{p'}^{4, \beta 2\downarrow} \rangle\rangle$ and $\langle\langle Z_p | X_{p'}^{4, \beta 2\downarrow} \rangle\rangle$ satisfy the equations:

$$\begin{aligned}
(E + \tilde{\mu} - 3U) \langle\langle X_p^{\beta 2\downarrow, 4} | X_{p'}^{4, \beta 2\downarrow} \rangle\rangle &= \frac{\langle X_p^{\beta 2\downarrow} + X_p^4 \rangle}{2\pi} \delta_{ij} + \langle\langle [X_p^{\beta 2\downarrow, 4}; H_1 + H_2] | X_{p'}^{4, \beta 2\downarrow} \rangle\rangle, \\
(E + \tilde{\mu} - 2U) \langle\langle Z_p | X_{p'}^{4, \beta 2\downarrow} \rangle\rangle &= \langle\langle [Z_p; H_1 + H_2] | X_{p'}^{\alpha\uparrow, 0} \rangle\rangle. \quad (3.55)
\end{aligned}$$

On the analogy of the previous sections we use the generalized mean-field approximation to calculate these functions. Let us take the commutators in (3.55) in the form:

$$[X_p^{\beta 2\downarrow, 4}, H_1] = \sum_j' \epsilon(pj) X_j^{\beta 2\downarrow, 4},$$

$$[X_p^{\beta 2\downarrow, 4}, H_2] = \sum_j' \tilde{\epsilon}(pj) Z_j, \quad (3.56)$$

$$[Z_p, H_1] = \sum_j' \zeta(pj) Z_j, \quad [Z_p, H_2] = \sum_j' \tilde{\zeta}(pj) X_j^{\beta 2\downarrow, 4},$$

where $\epsilon(pj), \tilde{\epsilon}(pj), \zeta(pj), \tilde{\zeta}(pj)$ are the non-operator expressions.

After transition to \mathbf{k} representation the system of Eqs. (3.55) taking into account Eq. (3.56) has the solutions:

$$\begin{aligned}
\langle\langle X_p^{\beta 2\downarrow, 4} | X_{p'}^{4, \beta 2\downarrow} \rangle\rangle_{\mathbf{k}} &= \frac{\langle X_p^{\beta 2\downarrow} + X_p^4 \rangle}{2\pi} \frac{E + \tilde{\mu} - 2U - \zeta(\mathbf{k})}{[E - E_1(\mathbf{k})][E - E_2(\mathbf{k})]}, \\
\langle\langle Z_p | X_{p'}^{4, \beta 2\downarrow} \rangle\rangle_{\mathbf{k}} &= \frac{\langle X_p^{\beta 2\downarrow} + X_p^4 \rangle}{2\pi} \frac{\tilde{\zeta}(\mathbf{k})}{[E - E_1(\mathbf{k})][E - E_2(\mathbf{k})]}. \quad (3.57)
\end{aligned}$$

Here $E_{1,2}(\mathbf{k})$ is the quasiparticle energy spectrum:

$$E_{1,2}(\mathbf{k}) = -\tilde{\mu} + \frac{5U}{2} + \frac{\epsilon(\mathbf{k}) + \zeta(\mathbf{k})}{2} \mp \frac{1}{2} \{ [U - \epsilon(\mathbf{k}) + \zeta(\mathbf{k})]^2 + 4\tilde{\epsilon}(\mathbf{k})\tilde{\zeta}(\mathbf{k}) \}^{1/2}. \quad (3.58)$$

The same expression for the quasiparticle energy spectrum we obtain from the functions $\langle\langle X_p^{\beta 2\downarrow,4} | Z_p^+ \rangle\rangle$, $\langle\langle Z_p | Z_p^+ \rangle\rangle$.

The values of $\epsilon(pp')$, $\tilde{\epsilon}(pp')$, $\zeta(pp')$, $\tilde{\zeta}(pp')$ we find by anti-commutation of Eq. (3.56) with the operators $X_p^{4,\beta 2\downarrow}$ and Z_p^+ ,

$$\begin{aligned} (X_p^{\beta 2\downarrow} + X_p^4)\epsilon(pp') &= \{X_p^{4,\beta 2\downarrow}; [X_p^{\beta 2\downarrow,4}, H_1]\}, \\ (X_p^{\downarrow\downarrow} + X_p^{\downarrow\uparrow} + X_p^{\beta 2} + X_p^{\alpha 2\uparrow} + X_p^{\alpha 2\downarrow} + X_p^{\beta 2\uparrow})\tilde{\epsilon}(pp') &= \{Z_p^+; [X_p^{0,\alpha\uparrow}, H_2]\}, \end{aligned} \quad (3.59)$$

$$\begin{aligned} (X_p^{\downarrow\downarrow} + X_p^{\downarrow\uparrow} + X_p^{\beta 2} + X_p^{\alpha 2\uparrow} + X_p^{\alpha 2\downarrow} + X_p^{\beta 2\uparrow})\zeta(pp') &= \{Z_p^+; [Z_p, H_1]\}, \\ (X_p^{\beta 2\downarrow} + X_p^4)\tilde{\zeta}(pp') &= \{X_p^{\alpha\uparrow,0}; [Z_p, H_2]\}. \end{aligned}$$

By use of the mean-field approximation analogously to the above, in the case $t'_k = t''_k$ we obtain

$$\begin{aligned} \epsilon(\mathbf{k}) &= t_{\mathbf{k}}^* \left[(t+f) + \frac{3t^2}{t+f} \right] - 3t_{\mathbf{k}}^* \frac{3df}{t+f}, \\ \tilde{\epsilon}(\mathbf{k}) &= \frac{t_{\mathbf{k}}^* + t_{\mathbf{k}}^*}{2} \left[(t+f) - \frac{t^2}{d+t} + \frac{df}{d+t} \right], \\ \zeta(\mathbf{k}) &= -t_{\mathbf{k}}^* \frac{df}{d+t} + t_{\mathbf{k}}^* \left[3(d+t) + \frac{t^2}{d+t} + \frac{4d^2}{(d+t)} \right], \\ \tilde{\zeta}(\mathbf{k}) &= \frac{t_{\mathbf{k}}^* + t_{\mathbf{k}}^*}{2} \left[(d+t) - \frac{t^2}{t+f} + \frac{3df}{t+f} \right], \end{aligned} \quad (3.60)$$

here

$$\begin{aligned} t_{\mathbf{k}}^* &= t_{\mathbf{k}} + 4t'_{\mathbf{k}}, \\ t_{\mathbf{k}}^* &= t_{\mathbf{k}} + 6t'_{\mathbf{k}}; \end{aligned} \quad (3.61)$$

d , t , f are the concentrations of the sites occupied by two, three and four electrons, respectively, connected by the relations:

$$f = 6d, \quad t = \frac{1}{4} - 3d. \quad (3.62)$$

In the point of transition, when the concentrations of the holes and single electrons are equal to zero, the energies of the electrons within the subbands are

$$\begin{aligned} E_1(\mathbf{k}) &= -\tilde{\mu} + 2U + t_{\mathbf{k}}^*, \\ E_2(\mathbf{k}) &= -\tilde{\mu} + 3U + t_{\mathbf{k}}^*. \end{aligned} \quad (3.63)$$

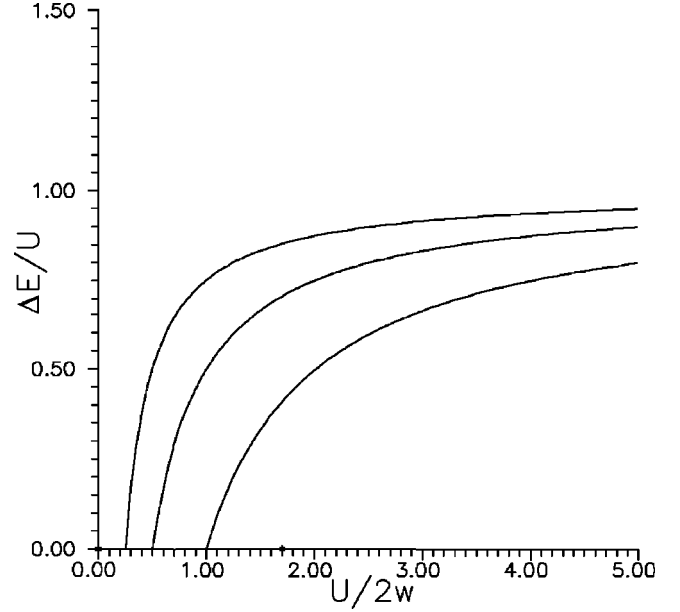


FIG. 7. The dependence of energy gap width $\Delta E/U$ on the parameter $U/(2w)$ for $n=3$ at different values of the parameter $\kappa = t'_{ij}/t_{ij}$: the lower curve $-\kappa=0$; the middle curve $-\kappa=0.1$; the upper curve $-\kappa=0.15$.

The energy gap in this case is

$$\Delta E = U - w^* - w^* = 0, \quad (3.64)$$

where $w^* = z|t_{ij}^*|$, $w^* = z|t_{ij}^*|$.

From Eq. (3.64) we obtain the criterion of the MIT at the electron concentration $n=3$:

$$U = w^* + w^*. \quad (3.65)$$

In the partial case $t'_k = t''_k = 0$ (in this case $t_{\mathbf{k}} = \tilde{t}_{\mathbf{k}}$) we have

$$\frac{U}{2w} = 1. \quad (3.66)$$

This result coincides with the corresponding critical value at the electron concentration $n=1$ in the consequence of the electron-hole symmetry of the model without the correlated hopping.

In Fig. 7 the energy gap for different values of the correlated hopping at $T=0$ is plotted. With the increase of the correlated hopping at the fixed value of parameter $U/2w$ the energy gap width increases faster than at $n=1$, $n=2$; and the region of values of $U/2w$ at which the system is in a metallic state, decreases.

IV. DISCUSSIONS AND CONCLUSIONS

In the present paper we have proposed a doubly orbitally degenerate narrow-band model with correlated hopping. The peculiarity of the model is taking into account the matrix element of electron-electron interaction, which describes intersite hoppings of electrons. In particular, this leads to the concentration dependence of the hopping integrals. Using the representation of Hamiltonian of a doubly orbitally degenerate model with correlated hopping in terms of the Hubbard operators the cases of the strong and weak Hund's coupling

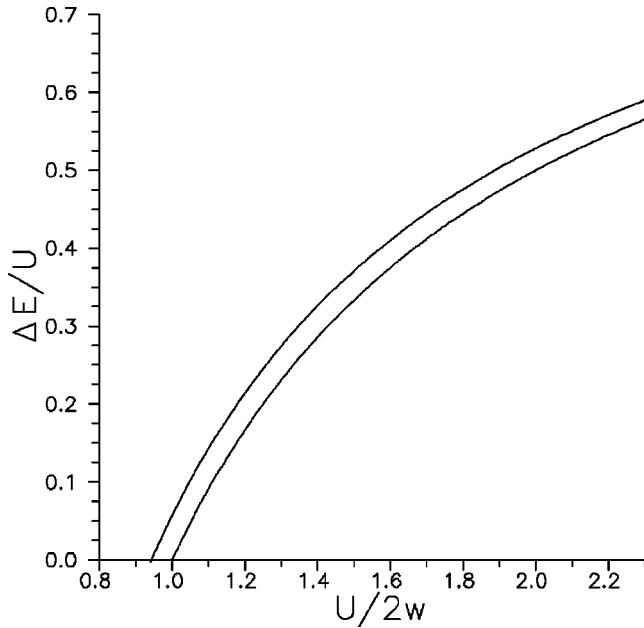


FIG. 8. The dependence of energy gap width $\Delta E/U$ on the parameter $U/(2w)$ in the absence of correlated hopping ($t'_k = t''_k = 0$): the lower curve— $n=1$, $n=3$; the upper curve— $n=2$.

have been considered. By means of a generalized mean-field approximation we have calculated the single-particle Green function and quasiparticle energy spectrum. Metal-insulator transition has been studied in the model at different integer values of the electron concentration. With the help of the obtained energy spectrum we have found energy gap width and criteria of metal-insulator transition.

The peculiarities of the expressions for quasiparticle energy spectrum and energy gap are dependences on the concentration of polar states (holes, doublons at $n=1$; single electron and triple occupied sites at $n=2$; doublons and sites occupied by four electrons at $n=3$), on the hopping integrals (thus on external pressure). At given values of U and hopping integrals (constant external pressure) the concentration dependence of ΔE allows to study MIT under the action of external influences. In particular, $\Delta E(T)$ -dependence can lead to the transition from a metallic state to an insulating state with the increase of temperature (see Fig. 4); the described transition is observed, in particular, in the $(V_{1-x}Cr_x)_2O_3$ compound^{2,48} and the $NiS_{2-x}Se_x$ system.^{49,50} The similar dependence of energy gap width can be observed at change of the polar states concentration under the action of photoeffect or magnetic field. The strong magnetic field can lead, for example, to the decrease of polar state concentration (see Ref. 26) initiating the transition from a paramagnetic insulator state to a paramagnetic metal state. Contrariwise, the increase of polar state concentration under the action of light stimulates the metal-insulator transition, analogously to the influence of temperature change. At the increase of bandwidth (for example, under the action of external pressure or composition changes) the insulator-to-metal transition can occur.

The results allow to study the influence of the correlated hopping and orbital degeneracy on MIT. The dependences of energy gap width on the parameter $U/2w$ in absence of the correlated hopping ($t'_k = t''_k = 0$) at different electron concen-

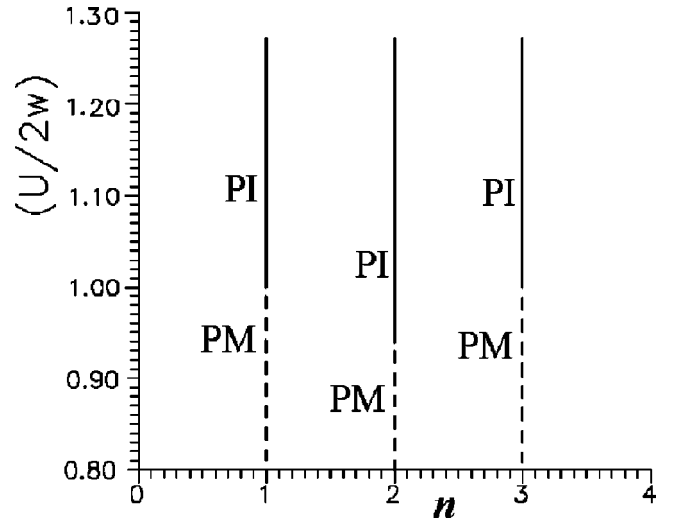


FIG. 9. The electron vs interaction phase diagram showing the paramagnetic metal and paramagnetic insulator in absence of correlated hopping.

trations are given in Fig. 8. One can see that in the case $n=2$ the MIT occurs at smaller value of $U/2w$ than at $n=1$. This result is in qualitative accordance with the results of work,¹⁰ in distinction from Refs. 13 and 15. Using the critical values of the parameter $U/(2w)$ at which MIT occurs for different integer electron concentrations (see Fig. 9) we can interpret the fact that in the series of disulphides MS_2 the CoS_2 (one electron within e_g band corresponding to $n=1$) and CuS_2 compounds (three electrons within e_g band corresponding $n=3$) are metals, and the NiS_2 compound (two electrons within e_g band corresponding $n=2$) is an insulator. Really, for $0.94 \leq U/2w \leq 1$ at the electron concentration $n=2$ system described by the present model is an insulator, whereas for the same values of the parameter $U/2w$ at the electron concentrations $n=1, 3$ system is a metal (according with the calculations of Ref. 51 the ratios $U/2w$ in these

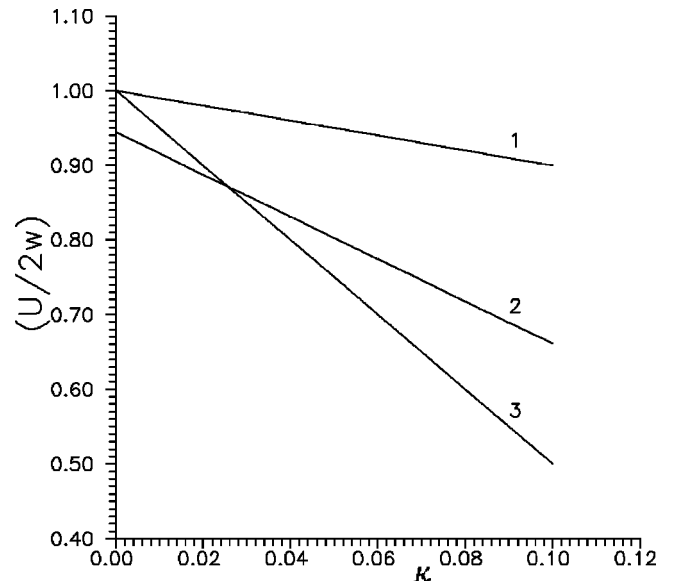


FIG. 10. The dependence of critical value $(U/2w)_c$ on the parameter of correlated hopping $\kappa = t'_{ij}/t_{ij}$: the curve 1 - $n=1$; the curve 2 - $n=2$; the curve 3 - $n=3$.

compounds have close values).

We have found that in the case of the strong Hund's coupling at $n=1$ metal-insulator transition occurs at smaller value of the parameter $[(U-J)/2w]_c=0.75$ than in the case of the weak Hund's coupling $[(U-J)/2w]_c=1$.

When the magnetically ordered states are taken into account the phase diagram of the considered model (Fig. 9) can be changed. In particular, with increase of correlation strength the transition from paramagnetic to magnetically ordered state^{8,9} (antiferromagnetic insulator or ferromagnetic insulator) can occur, similarly to the magnetic transition found in Ref. 12 by use of slave-boson method for the doubly degenerate Hubbard model.

At nonzero values of correlated hopping the point of MIT moves towards the values of parameter $U/2w$ (Figs. 5–7) at which system is a metal in proportion to correlated hopping value (Fig. 10). From Fig. 10 one can see that $(U/2w)_c$ decreases with increasing correlated hopping, and what is more at $n=2$ with the increase of the correlated hopping parameter κ the value $(U/2w)_c$ decreases faster than at the electron concentration $n=1$, and at $n=3$ the value $(U/2w)_c$ decreases faster than at $n=1, n=2$. The non-equivalence of the cases $n=1$ and $n=3$ is a manifestation of the electron-hole asymmetry which is a characteristic of the models with correlated hopping.

Thus both orbital degeneracy and correlated hopping are the factors favoring the transition of system to an insulating state in the case of half filling with the increase of intra-atomic Coulomb repulsion in comparison with the single-band Hubbard model (in this connection see Refs. 35 and 37).

In the present paper considering MIT we have neglected the correlated hopping T_1 . Taking into account T_1 leads to the concentration dependence of the hopping integrals and as a result to decreasing U_c . This effect shows itself the more the larger is the value of electron concentration n . A more detailed analysis of the correlated hopping T_1 influence will be given in subsequent papers.

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