Metal-insulator transition in a generalized Hubbard model with correlated hopping at half-filling

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Abstract

In the present paper metal-insulator transition is studied in a generalized Hubbard model with correlated hopping at half-filling and zero temperature. Single-particle Green function and energy spectrum of electron system are calculated. The expressions for energy gap width and the concentration of polar states (holes or doublons) are obtained. The conditions for metallic and insulating states are found.

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1 Introduction

In the present paper we consider a generalized Hubbard model including correlated hopping [1, 2]. In such a model the hopping integrals, which describe hoppings of holes and doublons are different. These hopping integrals also are distinguished from the hopping integral which is connected with the processes of paired creation and destruction of holes and doublons. In recent years the similar models have been studied intensively [3] - [15]. In particular, some of these models [3, 4, 6, 7, 8] have been solved exactly under the condition that the number of doubly occupied sites is conserved.

The important puzzle arising in an investigation of the generalized models is metal-insulator transition problem. In papers [4, 10] a new mean-field approximation (MFA) which leads to the correct description of metal-insulator transition (MIT) has been proposed. In the present paper we use this MFA to study MIT in a generalized Hubbard model with correlated hopping at half-filling and zero temperature. In Sec. 2 we introduce the Hamiltonian of narrow-band model. The decoupling scheme of Green functions is described in Sec. 3. Also single-particle Green function and energy spectrum of electron system are calculated. In Sec. 4 the expression for energy gap width is found. With the help of this formula and the obtained expression for the concentration of polar states MIT is studied. Finally, Sec. 5 is devoted to the
2 Hamiltonian of narrow-band model

Theoretical analysis, on the one hand, and available experimental data, on the other hand, point out the necessity of the Hubbard model generalization by taking into account interelectron interactions describing intersite hoppings of electrons (correlated hopping). The characteristic property of these correlated hopping integrals is the dependence on the occupation of sites by electrons.

So, we start from the following generalization of the Hubbard model including correlated hopping:

\[
H = -\mu \sum_{i\sigma} a_{i\sigma}^+ a_{i\sigma} + \sum_{ij\sigma} a_{i\sigma}^+ \left( t_0 + \sum_{k} J(ijk) n_k \right) a_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow},
\]

(2.1)

where \(a_{i\sigma}^+, a_{i\sigma}\) are the operators of creation and destruction for the electrons with spin \(\sigma (\sigma = \uparrow, \downarrow)\) on \(i\)-site, \(n_{i\sigma} = a_{i\sigma}^+ a_{i\sigma}\), \(n_i = n_{i\uparrow} + n_{i\downarrow}\); \(\mu\) is the chemical potential; \(U\) is the intra-atomic Coulomb repulsion; \(t_0\) is the matrix element which describe the hoppings of electrons between nearest-neighbor sites of lattice in consequence of electron-ion interaction.

\[
J(ijk) = \int \int \phi^*(r - R_i) \phi(r - R_j) \frac{e^2}{|r - r'|} |\phi(r' - R_k)|^2 drdr',
\]

(2.2)

\((\phi\text{-function is the Wannier function})\). The prime at second sum in Eq. (2.1) signifies that \(i \neq j\).

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

\[
\sum'_{ij\sigma} \sum_{k \neq i, k \neq j} J(ijk) a_{i\sigma}^+ n_k a_{j\sigma} + \sum'_{ij\sigma} \left( J(iii) a_{i\sigma}^+ a_{j\sigma} n_{i\sigma} + \text{h.c.} \right)
\]

(2.3)

(\(\bar{\sigma}\) denotes the spin projection which is opposite to \(\sigma\)), here we have used that \(J(iiji) = J(jiiii) = J(iiij)\) in consequence of the matrix elements symmetry. Let us suppose (as in the papers) that

\[
\sum'_{ij\sigma} \sum_{k \neq i, k \neq j} J(ijk) a_{i\sigma}^+ n_k a_{j\sigma} = T_1 \sum_{ij\sigma} a_{i\sigma}^+ a_{j\sigma}
\]

(2.4)

with \(T_1 = n \sum_{k \neq j} J(ijk)\) and \(n = \langle n_{i\uparrow} + n_{i\downarrow} \rangle\) (sites \(i\) and \(j\) are nearest neighbors); it should be noted that this supposition is exact in the homeopolar limit (\(n_i = 1\)).

Thus at half-filling \((n = 1)\) we can write Hamiltonian (2.1) in the form

\[
H = -\mu \sum_{i\sigma} a_{i\sigma}^+ a_{i\sigma} + t \sum'_{ij\sigma} a_{i\sigma}^+ a_{j\sigma} + T_2 \sum'_{ij\sigma} a_{i\sigma}^+ a_{j\sigma} n_{i\sigma} + \text{h.c.}
\]

\[
+ U \sum_{i} n_{i\uparrow} n_{i\downarrow},
\]

(2.5)

where \(t = t_0 + T_1\) and \(T_2 = J(iiij)\).
dependence of the hopping integral $t$. It is the distinction of the present model from similar models \[3, 4, 6, 7, 18, 19\]. In the case $n = 1$ taking into account the correlated hopping $T_1$ leads to the renormalization of the hopping integral $t_0$ only.

Rewrite Hamiltonian (2.5) in terms of $X_{kl}^{kl}$-Hubbard operators \[20\] using the formulae \[21\]

\[
 a^+_i \sigma = X^{0\sigma}_i, \quad a_i \sigma = X^{\sigma \sigma}_i, \\
 a_i^+ = X^{2\sigma}_i, \quad a_i = X^{\sigma 2}_i, \\
 a_i^\tau = X^{\tau \sigma}_i, \quad a_i = X^{\tau 2}_i + X^{0\sigma}_i,
\]

where $X_{kl}^{kl}$ is the transition-operator of $i$-site from state $|l\rangle$ to state $|k\rangle$; $|0\rangle$ denotes the site, which is not occupied by an electron (hole), $|\sigma\rangle \equiv a^+_i|0\rangle$ denotes the singly occupied (by an electron with spin $\sigma$) $i$-site, $|2\rangle \equiv a^+_i a_i|0\rangle$ denotes the doubly occupied (by two electrons with the opposite spins) $i$-site (doublon).

In terms of $X_{kl}^{kl}$-operators Hamiltonian (2.5) takes the following form:

\[
 H = H_0 + H_1 + H'_1, \tag{2.6}
\]

with

\[
 H_0 = -\mu \sum_i \left( X^{\uparrow}_i + X^{\downarrow}_i + 2X^{2\downarrow}_i \right) + U \sum_i X^{\uparrow 2}_i, \\
 H_1 = t \sum_{ij\sigma} X^{\sigma 0}_i X^{0\sigma}_j + i \sum_{ij\sigma} X^{2\sigma}_i X^{\sigma 2}_j, \\
 H'_1 = t' \sum_{ij\sigma} \left( \eta_i X^{\sigma 0}_i X^{\sigma 2}_j + h.c. \right),
\]

where $X_{kl}^{kl} = X_{kl}^{kl}X_{ik}^{lk}$ is the operator of the number of $|k\rangle$-states on $i$-site, $\eta_\uparrow = -1$, $\eta_\downarrow = 1$;

\[
 \tilde{t} = t + 2T_2, \quad t' = t + T_2. \tag{2.7}
\]

The single-particle Green function

\[
 C^\sigma_{pp'}(E) = \langle \langle a_{p\sigma} a_{p'\sigma}^+ \rangle \rangle \tag{2.8}
\]

in terms of Hubbard operators is written

\[
 C^\sigma_{pp'}(E) = \langle \langle X^{0\sigma}_p|X^{0\sigma}_{p'} \rangle \rangle + \eta_\sigma \langle \langle X^{0\sigma}_p|X^{2\sigma}_{p'} \rangle \rangle + \eta_\sigma \langle \langle X^{2\sigma}_p|X^{2\sigma}_{p'} \rangle \rangle + \langle \langle X^{2\sigma}_p|X^{0\sigma}_{p'} \rangle \rangle. \tag{2.9}
\]

$H_0$ describes the atomic limit of narrow-band models.

$H_1$ describes the translational hopping of holes and doublons. In the present model (in contrast to the narrow-band models of the Hubbard type) the hopping integrals of holes $t$ and doublons $\tilde{t}$ are different. It should be noted that in consequence of the difference of the hopping integrals, which describe translational hopping of current carriers within the lower (hole) band and upper (doublon) band, the energy width of the upper band can be much smaller and the effective mass of current carriers within this band can be much larger than in the lower band. Thus, within the proposed model the ideas of the “wide” and “narrow” subbands and the “light” and “heavy” current carriers are introduced (as the result of electron-electron interactions).
3 Energy spectrum of electron system: MFA

Here we use MFA proposed in papers [2, 16] to calculate the energy spectrum of electron system described by Hamiltonian (2.7).

The Green function \( \langle \langle X_p^{0\sigma} | X_{p'}^{\sigma 0} \rangle \rangle \) is given by the equation

\[
(E + \mu) \langle \langle X_p^{0\sigma} | X_{p'}^{\sigma 0} \rangle \rangle = \frac{\delta_{pp'}}{2\pi} \langle X_p^{\sigma} + X_{p'}^{\sigma 0} \rangle + \langle \langle X_p^{0\sigma}, H_1 \rangle \rangle | X_{p'}^{\sigma 0} \rangle \rangle, 
\]

(3.1)

with \([A, B] = AB - BA\),

\[
\left[ X_p^{0\sigma}, H_1 \right] = t \sum_j \left( (X_p^{\sigma} + X_p^{0})X_j^{0\sigma} + X_p^{\sigma}\sigma X_j^{0\sigma} \right) - i \sum_j X_{p}^{02} X_{j}^{2\sigma},
\]

(3.2)

\[
\left[ X_p^{0\sigma}, H'_1 \right] = \left[ \sum_j \epsilon(pj) X_j^{0\sigma}, \sum_j \epsilon'_1(pj) X_j^{\sigma 2} \right] = \left[ X_p^{0\sigma}, H_1' \right],
\]

(3.3)

To break off the sequence of Green function equations according to generalized Hartree-Fock approximation [22] we suppose that

\[
\left[ X_p^{0\sigma}, H_1 \right] = \sum_j \epsilon(pj) X_j^{0\sigma}, \quad \left[ X_p^{0\sigma}, H_1' \right] = \sum_j \epsilon'_1(pj) X_j^{\sigma 2},
\]

(3.4)

where \(\epsilon(pj)\) and \(\epsilon'_1(pj)\) are the non-operator expressions. The representation choice of the commutators in form (3.2) and (3.3) is prompted by the operator structure of these commutators which maps the energy non-equivalence of the hopping processes prescribed by \(H_1\) and \(H_1'\). Taking into account (3.4) we rewrite Eq. (3.1) in the form

\[
(E + \mu) \langle \langle X_p^{0\sigma} | X_{p'}^{\sigma 0} \rangle \rangle = \frac{\delta_{pp'}}{2\pi} \langle X_p^{\sigma} + X_{p'}^{\sigma 0} \rangle + \sum_j \epsilon(pj) \langle \langle X_j^{0\sigma} | X_{p'}^{\sigma 0} \rangle \rangle + \sum_j \epsilon'_1(pj) \langle \langle X_j^{\sigma 2} | X_{p'}^{\sigma 0} \rangle \rangle.
\]

(3.5)

After anticommutation of both sides of the first of formulae (3.4) with \(X_k^{\sigma 0}\) and the second formula with \(X_{k}^{2\sigma}\) we obtain

\[
\epsilon(pk)(X_k^{\sigma} + X_k^{0}) = t(X_k^{\sigma} + X_k^{0})(X_p^{\sigma} + X_p^{0}) + tX_k^{\sigma\sigma} X_p^{0\sigma} - \delta_{pk} t \sum_j X_k^{\sigma 0} X_j^{\sigma 0} + \delta_{pk} t \sum_j X_k^{2\sigma} X_j^{0\sigma},
\]

(3.6)

\[
\epsilon_1(pk)(X_k^{\sigma} + X_k^{2}) = -t'(X_k^{\sigma} + X_k^{0})(X_p^{\sigma} + X_p^{2}) + t'X_k^{\sigma\sigma} X_p^{\sigma\sigma} - \delta_{pk} t' \sum_j X_k^{\sigma 0} X_k^{\sigma 0} + \delta_{pk} t' \sum_j X_k^{2\sigma} X_k^{2\sigma}.
\]
Similarly, for the Green function $\langle\langle X^2_p | X^0_p \rangle\rangle$ we can write the equation

$$(E + \mu - U)\langle\langle X^2_p | X^0_p \rangle\rangle = \sum_j \tilde{\epsilon}(pj)\langle\langle X^2_j | X^0_p \rangle\rangle + \sum_j \epsilon_2(pj)\langle\langle X^0_j | X^0_p \rangle\rangle,$$  \hspace{1cm} (3.8)

where $\tilde{\epsilon}(pj)$ and $\epsilon_2(pj)$ are determined through the expressions which are analogous to (3.6) and (3.7). Thus we obtain the closed system of equations for the Green functions $\langle\langle X^0_p | X^0_p \rangle\rangle$ and $\langle\langle X^2_p | X^0_p \rangle\rangle$.

By neglecting correlated hopping and by averaging expressions (3.6) and (3.7) we obtain the approximations [17, 23, 24]; the defects of these approximations are well-known (see, for example Ref. [25]). Here we use the approach which has been proposed in the papers [3, 16].

To determine $\epsilon(pj)$, $\epsilon_1(pj)$ we rewrite $X^kl$-operator in Eqs. (3.6) and (3.7) in the form $X^kl = \alpha^k_\downarrow \alpha^l_\downarrow$, where $\alpha^k_\downarrow$, $\alpha^l_\downarrow$ are the operators of creation and destruction for $|k\rangle$- and $|l\rangle$-states on i-site respectively (the Schubin-Wonsowsky operators [27]); thus $X^i_0 = \alpha^+_i \alpha^{-i}_0$, $X^2_i = \alpha^+_i \alpha^{-i}_2$, $X^\sigma_i = \alpha^+_i \alpha^{-i}_\sigma$. Let us substitute $\alpha$-operators by c-numbers in Eqs. (3.6) and (3.7) (here there is a partial equivalence with slave boson method [28]).

$$\alpha^+_{i\sigma} = \alpha^{-i}_\sigma = \left(\frac{1 - 2d}{2}\right)^{1/2}, \hspace{1cm} \alpha^+_i = \alpha^{-i}_0 = \alpha^+_i = \alpha^{-i}_2 = d^{1/2} \hspace{1cm} (3.9)$$

(we consider a paramagnetic case, electron concentration on site $n = 1$); $d$ is the concentration of polar states (holes or doublons).

The proposed approximation is based on the following physical idea. Let us consider a paramagnetic Mott-Hubbard insulator at $T \neq 0$. Within the wide temperature interval ($k_B T \ll U$) the concentration of polar states is small ($d \ll 1$). An analogous consideration is valid for a paramagnetic Mott-Hubbard semimetal (hole and doublon subbands overlap weakly, $d \ll 1$). So, the change of states and polar excitations influences on $|\sigma\rangle$-states weakly. Thus we may consider $|\sigma\rangle$-states as the quasiclassical system and substitute the operators $\alpha^+_{i\sigma}$, $\alpha^{-i}_\sigma$ by c-numbers. In addition, when we find $\epsilon(pj)$, $\epsilon_1(pj)$ we substitute the creation and destruction operators of $|0\rangle$- and $|2\rangle$-states through the respective quasiclassical expressions. Actually the proposed approximation is equivalent to a separation of the charge and spin degrees of freedom. Note that the present approach is the most justifiable when $d \to 0$.

Thus in $k$-representation we obtain

$$\epsilon(k) = (1 - 2d + 2d^2)t_k - 2d^2\tilde{t}_k, \hspace{1cm} \epsilon_1(k) = -2dt'_k, \hspace{1cm} (3.10)$$

where $t_k$, $\tilde{t}_k$, $t'_k$ are the Fourier transforms of the hopping integral $t$, $\tilde{t}$, $t'$ respectively. Similarly, we find that

$$\tilde{\epsilon}(k) = (1 - 2d + 2d^2)\tilde{t}_k - 2d^2t'_k, \hspace{1cm} \epsilon_2(k) = -2dt'_k, \hspace{1cm} (3.11)$$

The Fourier transform of the Green function $\langle\langle X^0_p | X^0_p \rangle\rangle$ is found from the system of equations (3.5) and (3.8).
with
\[ E_{1,2}(k) = -\mu + \frac{(1 - 2d)(t_k + \tilde{t}_k) + U}{2} + \frac{1}{2} F_k, \] (3.13)
\[ F_k = \sqrt{\left[B(t_k - \tilde{t}_k) - U\right]^2 + (4dt'_k)^2}, \quad B = 1 - 2d + 4d^2. \] (3.14)

An analogous procedure is realized also in the equations for the other Green functions in Eq. (2.6).

Finally, in \( k \)-representation the single-particle Green function is
\[ G_k(E) = \frac{1}{2\pi} \left( \frac{A_k}{E - E_1(k)} + \frac{B_k}{E - E_2(k)} \right), \] (3.15)
\[ A_k = \frac{1}{2} - \frac{2dt'_k}{F_k}, \quad B_k = \frac{1}{2} + \frac{2dt'_k}{F_k}. \] (3.16)

Single-particle Green function (3.15) gives the exact atomic and band limits: if \( U = 0 \) and \( t_k = \tilde{t}_k = t'_k = t_0(k) \) (it means neglecting correlated hopping) then \( G_k(E) \) takes the band form \((d = 1/4 \text{ when } U = 0)\), if \( t_k = \tilde{t}_k = t'_k \rightarrow 0 \) then we obtain the exact atomic limit.

The peculiarities of obtained quasiparticle energy spectrum (3.13) of narrow-band system which is described by Hamiltonian (2.5) are the dependence on the concentration of polar states and the non-equivalence of the lower and upper Hubbard bands. This non-equivalence is caused by the difference of the hopping integrals \( t, \tilde{t}, t' \).

Quasiparticle energy spectrum (3.13) allows to study MIT in the proposed model.

4 Metal-insulator transition

With the help of energy spectrum of electrons (3.13) we find the expression for the energy gap width (difference of energies between bottom of the upper and top of the lower Hubbard bands):
\[ \Delta E = -(1 - 2d)(w + \tilde{w}) + \frac{1}{2}(Q_1 + Q_2), \] (4.1)
\[ Q_1 = \sqrt{[B(w - \tilde{w}) - U]^2 + (4dzt')^2}, \]
\[ Q_2 = \sqrt{[B(w - \tilde{w}) + U]^2 + (4dzt')^2}, \]
where \( w \) and \( \tilde{w} \) are the half-widths of the lower (hole) and upper (doublon) Hubbard bands respectively: \( w = z|t|, \quad \tilde{w} = z|\tilde{t}| \) (\( z \) is the number of nearest neighbors to a site).

The peculiarities of the expression for energy gap (4.1) are dependences on the concentration of polar states, on the widths of hole and doublon bands, on the hopping integral \( t' \) (thus on external pressure). At given \( U, t, \tilde{t}, t' \) (constant external pressure) the concentration dependence of \( \Delta E \) allows to study MIT under the action of external influences: temperature change, photoeffect and magnetic field. In particular, \( \Delta E(T) \) dependence may lead to the transition from a metallic state to an insulating state [29].
transition from the state of a paramagnetic metal to the paramagnetic insulator state in the \((V_{1-x}Cr_x)_{2}O_3\) compound [30, 31], in NiS\(_2\) [32] and in the NiS\(_2-x\)Se\(_x\) system [32, 33, 34] should be noted). Under the action of light or magnetic field the concentration of polar states can be changed; it leads to the fact that the energy gap width is changed also and MIT can occur.

Distinction of formulae (3.13)–(3.16), (4.1) from earlier obtained results (e.g., see reviews [31, 35, 36]) is the dependence on concentration of polar states. Let us find the expression for its calculation.

The concentration of polar states is given by the equation

\[
\langle X^2_i \rangle = \frac{1}{N} \sum_{k} \int_{-\infty}^{+\infty} J_k(E) dE = \frac{1}{2N} \sum_{k} \left( \frac{C_k}{\exp \frac{E_1(k)}{\theta} + 1} + \frac{D_k}{\exp \frac{E_2(k)}{\theta} + 1} \right),
\]

(4.2)

where

\[
C_k = \frac{1}{2} - \frac{B(t_k - \tilde{t}_k)}{2F_k} - \frac{U}{2F_k},
\]

\[
D_k = \frac{1}{2} + \frac{B(t_k - \tilde{t}_k)}{2F_k} + \frac{U}{2F_k},
\]

\[
\theta = k_B T, \quad k_B \text{ is the Boltzmann’s constant, } N \text{ is the number of sites, } J_k(E) \text{ is the spectral intensity of the Green function }
\]

\[
\langle \langle X^p_{\sigma} X^q_{\sigma'} \rangle \rangle_k = \frac{1}{4\pi} \left( \frac{C_k}{E - E_1(k)} + \frac{D_k}{E - E_2(k)} \right).
\]

(4.3)

At \(T = 0\) and the rectangular density of states

\[
\frac{1}{N} \sum_{k} \delta(E - \tilde{t}_k) = \frac{1}{2w} \theta(w^2 - E^2)
\]

\((\theta(x) = 1 \text{ if } x > 0, = 0 \text{ otherwise})\) from Eq. (4.2) we obtain that

\[
-\frac{B \tilde{t} - t}{\lambda} \left[ \varphi(\epsilon_0) - \varphi(-\epsilon_0) \right] + \frac{U}{\lambda \sqrt{\lambda}} \left( 1 - \frac{\lambda^2 (\tilde{t} - t)^2}{\varphi(\epsilon_0)} \right) \times
\]

\[
\ln \left| \frac{\sqrt{\lambda} \varphi(\epsilon_0) - \lambda \epsilon_0 - BU(\tilde{t} - t)}{\sqrt{\lambda} \varphi(-\epsilon_0) + \lambda \epsilon_0 - BU(\tilde{t} - t)} \right| = 8d - 2 \quad (U < w + \tilde{w})
\]

(4.4)

with

\[
\epsilon_0 = 2 \sqrt{\frac{\mu U - \mu^2}{(1 - 2d)^2(t + \tilde{t})^2 - \lambda}}, \quad \mu = \frac{(1 - 2d + 2d^2)w - 2d^2 \tilde{w}}{(1 - 2d)(w + \tilde{w})} U,
\]

\[
\varphi(\epsilon) = \left\{ \lambda \epsilon^2 - 2BU(\tilde{t} - t) + U^2 \right\}^{\frac{1}{2}}, \quad \lambda = B^2(\tilde{t} - t)^2 + (4dt')^2.
\]

For narrow-band semimetal \((d \ll 1)\) Eq. (4.4) takes the following form:
Fig. 1 shows the dependence of \( d \) on \( U/w \) which is obtained from Eq. (4.4). The parameters \( \tau_1 = T_1/|t_0| \), \( \tau_2 = T_2/|t_0| \) characterize the value of correlated hopping. One can see that a value of \( d \) depends on the parameters of correlated hopping \( \tau_1 \), \( \tau_2 \) (thus on \( \tilde{w}/|w| \)) weakly when \( U/w \) is close to zero. But with the increase of \( U/w \) the concentration of polar states becomes strongly dependent on the parameters \( \tau_1 \), \( \tau_2 \). It testifies on the fact that taking into account the correlated hopping is important to consider the metal-insulator transition problem.

Fig. 1 shows also that if \( U \geq w + \tilde{w} \) then the concentration of polar states \( d = 0 \). In the special case \( t + t' = t' = 0 \) this consequence is in accordance with the results of Refs. [6, 7, 11].

At \( T = 0 \) the energy gap width \( \Delta E \leq 0 \) (i.e. MIT occurs) when the condition

\[
U \leq w + \tilde{w}
\]

is satisfied (in agreement with general physical ideas [31]). For the special case \( t' = 0 \) condition (4.6) covers the exact results of Refs. [4, 6, 8].

Fig. 2 which is obtained from formula (4.1) using Eq. (4.4) shows that in a metallic state the overlapping of energy subbands decreases and in an insulating state the energy gap width increases with decrease of the parameter \( \tilde{w}/w \) (at given \( U/w \)).

In the Hubbard model energy gap width (4.1) takes the following form:

\[
\Delta E = -2w(1 - 2d) + \sqrt{U^2 + (4dw)^2},
\]

and the concentration of polar states (4.4) is

\[
d = \left( \frac{1}{4} + \frac{U}{32dw} \ln(1 - 4d) \right) \theta(2w - U).
\]

In the region of metal-insulator transition \( d = 1/4 - U/(8w) \); this dependence is in qualitative accordance with the result of Brinkman and Rice [37] obtained by use of Gutzwiller variational method [38], those of the general Gutzwiller-correlated wave functions in infinite dimensions [39] and the Kotliar-Ruckenstein slave bosons [28].

For \( U/2w \to 0 \) we obtain \( d = 1/4 + U/(8w) \ln(U/2w) \) (if we consider Coulomb repulsion as perturbation then \( d(U \to 0) = 1/4 - O(U) \)); in order to compare the obtained dependence (4.8) \( d \) on \( U/w \) in the Hubbard model with other approximate theories see e.g. [30]). \( \Delta E \leq 0 \) when the condition \( 2w \geq U \) is satisfied.

## 5 Conclusions

In the present paper Mott-Hubbard transition has been studied in a generalized Hubbard model with correlated hopping at half-filling using a mean-field approximation [4, 15].

We have obtained the expression to calculate the concentration of polar states. With the increase of the parameter \( \tilde{w}/w \) \((0 \leq \tilde{w}/w \leq 1)\) the concentration of polar states increases at given \( U/w \).

Quasiparticle energy spectrum has been calculated. With the help of this en-
non-equivalence of the upper and lower Hubbard bands. The increase of the parameter $\tilde{w}/w$ (at given $U/w$) leads to decreasing energy gap width. In consequence of it, in particular, MIT occurs when the condition $U/w = 1 + \tilde{w}/w$ is satisfied.

The cases $n \neq 1$ and $T \neq 0$, an application of the obtained results to the interpretation of the experimental data will be considered in the next papers.

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Figure 1: Concentration of polar states $d$ as a function of $U/w$: the upper curve corresponds to $\tau_1 = \tau_2 = 0$; the middle curve $\tau_1 = \tau_2 = 0.1$; the lower curve $\tau_1 = \tau_2 = 0.2$.

Figure 2: Energy gap width $\Delta E$ as a function of $U/w$. 

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