On chemical potential of a generalized Hubbard model with correlated hopping at half-filling

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Abstract
In the present paper we study chemical potential of a generalized Hubbard model with correlated hopping at half-filling using a generalized mean-field approximation. For the special case of the model the approach reproduces the exact results: metal-insulator transition, ground state energy. Chemical potential of generalized Hubbard model with correlated hopping as function of hopping integrals at zero temperature is found. It is shown that chemical potential of the model is temperature-dependent. The dependences of chemical potential of a generalized Hubbard model with correlated hopping on the model parameters are different in metallic and insulating phases leading to a kink at the point of metal-insulator transition in the ground state. With the increase of temperature the kink in the chemical potential curve disappears. The obtained results differ from those of the Hubbard model indicating the important role of correlated hopping.

1 Model Hamiltonian
One of the simplest model describing correlation effects in narrow energy bands is the Hubbard model [1]. 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 intra-atomic Coulomb repulsion of two electrons of the opposite spins. This model is studied intensively (for recent reviews see Refs. [2, 3]).

Theoretical analyses, 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 correlated hopping. This necessity is caused by two reasons. Firstly, theoretical analyses [4, 5] point 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. [4, 6–9]) the matrix element of electron-electron interaction describing correlated hopping is the same order that the hopping integral or on-site Coulomb repulsion. Secondly, using the concept of correlated hopping and caused by it the electron-hole asymmetry we can interpret the peculiarities of some physical properties of narrow-band materials [4, 10–16].
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 parameter 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

\[ H = - \sum_{ij\sigma} t_{ij}^\sigma a_{ij\sigma}^+ a_{ij\sigma} + U \sum_i n_{ii\uparrow} n_{ii\downarrow}, \]  

(1.1)

\[ t_{ij}^\sigma = t_{AA}(1 - n_{i\sigma})(1 - n_{j\sigma}) + t_{AB}(n_{i\sigma} + n_{j\sigma} - 2n_{i\sigma}n_{j\sigma}) + t_{BB}n_{i\sigma}n_{j\sigma}. \]  

(1.2)

In recent few years Hamiltonian (1.1) is widely used to study metal-insulator transition in narrow energy bands [7]-[13].

In Ref. [4, 15] 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

\[ H = H_0 + H_1 + H_1', \]  

(1.3)

\[ H_0 = -\mu \sum_i \left(X_i^\uparrow + X_i^\downarrow + 2X_i^2\right) + U \sum_i X_i^2, \]  

(1.4)

\[ H_1 = t(n) \sum_{ij\sigma} X_i^\sigma X_j^\sigma + \bar{t}(n) \sum_{ij\sigma} X_i^{2\sigma} X_j^{2\sigma}, \]  

(1.5)

\[ H_1' = t'(n) \sum_{ij\sigma} \left(\eta_{ij} X_i^{\sigma} X_j^{\sigma} + h.c.\right), \]  

(1.6)

where \( \mu \) is the chemical potential, \( X_i^{kl} = |k\rangle \langle l| \) is the Hubbard operator \([20]; |0\rangle \) denotes the state of site, which is not occupied by an electron (hole), \( |\sigma\rangle \) denotes the state of singly occupied (by an electron with spin \( \sigma \)) \( i \)-site, \( |2\rangle \) denotes the state of doubly occupied (by two electrons with the opposite spins) \( i \)-site (doublon).

\[ t(n) = t_0 + n \sum_{k \neq i \neq j} J(ikjk) = t_0 + nT_1 \]  

(1.7)

is the effective hopping integral of electrons between nearest-neighbor sites of lattice, \( n \) is the electron concentration, \( \eta_\uparrow = -1, \eta_\downarrow = 1, \)

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

(1.8)

\( \varphi(r - R_i) \) is the Wannier function,

\[ \bar{t}(n) = t(n) + 2T_2, \quad t'(n) = t(n) + T_2, \quad T_2 = J(iiij), \]  

(1.9)

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 \( T_2 \)) and the occupation of the nearest-neighbor sites (with the hopping integral \( T_1 \)) which we take into account in the Hartree-Fock approximation (Eq. (1.7)). The peculiarity of model (1.3) is the concentration dependence of the hopping integral \( t(n) \) in contrast to similar models. Below we shall consider the half-filling case,
Properties of generalized Hubbard model with correlated hopping, in particular metal-insulator transition (MIT) has been studied in a number of recent works \cite{17}-\cite{19, 21}-\cite{25}. At half-filling and \( t' = 0 \) (or \( t_{AB} = 0 \)) some exact results have been found \cite{17, 21}. In a simple cubic lattice with coordination number \( z \) MIT occurs at
\[
U_c = z(|t_{AA}| + t_{BB}|) = 2z|t_0|. \tag{1.10}
\]
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 \( t' \neq 0 \) (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 step to solve this task is recent papers \cite{18, 19, 22}-\cite{24} where criteria of MIT, ground state energy, concentration of doubly occupied sites have been found. In Refs. \cite{18, 19, 22}-\cite{24} the authors have obtained the following criterion of MIT:
\[
U_c = z(|t_{AA}| + |t_{BB}|) = z(|t| + |t'|) \tag{1.11}
\]
in agreement with the Mott’s general physical ideas \cite{26}. By means of the slave bosons method \cite{27} it has been found in Ref. \cite{25} that MIT occurs at \( U_c = 4z|t + T_2| \); however here there is a problem of discrepancy of this result with the exact MIT criterion \( (1.10) \).

The present paper is devoted to a further study of properties generalized Hubbard model with correlated hopping at half-filling, in particular investigation of the model chemical potential in the region of metal-insulator transition.

## 2 Results

The single-particle Green function in terms of the Hubbard operators reads as
\[
⟨⟨a_{p\sigma} a_{p'\sigma}^+⟩⟩ = ⟨⟨X_p^0σ|X_{p'}^{0\bar{σ}}⟩⟩ + η_{σ}⟨⟨X_p^0σ|X_{p'}^{2\bar{σ}}⟩⟩ + η_{\bar{σ}}⟨⟨X_p^{2σ}|X_{p'}^{0σ}⟩⟩ + ⟨⟨X_p^{2σ}|X_{p'}^{2\bar{σ}}⟩⟩. \tag{2.1}
\]
The Green function \( ⟨⟨X_p^{0σ}|X_{p'}^{0\bar{σ}}⟩⟩ \) is given by the equation
\[
(E + μ)⟨⟨X_p^{0σ}|X_{p'}^{0\bar{σ}}⟩⟩ = \frac{δ_{p'p}}{2π}⟨⟨X_p^σ + X_p^{0}\rangle⟩ + ⟨⟨X_p^0σ, H_1⟩⟩ |X_p^{0\bar{σ}}⟩⟩
+⟨⟨X_p^{0σ}, H_1^0⟩⟩ |X_p^{0\bar{σ}}⟩⟩, \tag{2.2}
\]
with \( [A, B] = AB - BA \). Using a variant \cite{28} of the generalized mean-field approximation \cite{27} we suppose that
\[
[X_p^{0σ}, H_1] = \sum_\epsilon (p\bar{σ})X_j^{0\bar{σ}}, \quad [X_p^{0\bar{σ}}, H_1^0] = \sum_\epsilon (p\bar{σ})X_j^{2\bar{σ}}, \tag{2.3}
\]
where \( \epsilon(p\bar{σ}) \) and \( \epsilon_1(p\bar{σ}) \) are the non-operator expressions. The procedure of \( \epsilon(p\bar{σ}) \) and \( \epsilon_1(p\bar{σ}) \) calculation is described in Ref. \cite{28} (here there is a partial equivalence with the slave boson method \cite{27}). Thus we obtain the closed system of equations for the Green functions \( ⟨⟨X_p^{0σ}|X_{p'}^{0\bar{σ}}⟩⟩ \) and \( ⟨⟨X_p^{2σ}|X_{p'}^{0\bar{σ}}⟩⟩ \). An analogous procedure is realized also in the equations for the other Green functions \cite{27}. \"
In this way, we find single-particle Green function and quasiparticle energy spectrum. For paramagnetic case in \( k \)-representation the spectrum is \[23\]:

\[
E_{1,2}(k) = -\mu + \frac{(1 - 2d)(t_k + \tilde{t}_k) + U}{2} \pm \frac{1}{2} F_k,
\]

\[
F_k = \sqrt{[B(t_k - \tilde{t}_k) - U]^2 + (4dt'_k)^2}, \quad B = 1 - 2d + 4d^2,
\]

where \( d \) is the doublon concentration which is found from the equation

\[
d = \langle X^2_i \rangle = \frac{1}{N} \sum \int_{-\infty}^{+\infty} J_k(E) dE
\]

\[
= \frac{1}{2N} \sum_k \left( \frac{A_k}{\exp \frac{E_1(k)}{\theta} + 1} + \frac{B_k}{\exp \frac{E_2(k)}{\theta} + 1} \right),
\]

with

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

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

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

\[
\langle \langle X_{p}^2 | X_{p'}^2 \rangle \rangle_k = \frac{1}{4\pi} \left( \frac{A_k}{E - E_1(k)} + \frac{B_k}{E - E_2(k)} \right).
\]

For the Hubbard model single-particle Green function \[24\] and spectrum \[24\] at \( t_0 = 0 \) have the exact atomic form, and at \( U = 0 \) describe the band result. For the case \( t' = 0 \) quasiparticle energy spectrum \[24\] reproduces (see Ref. \[24\]) the exact results \[17, 21\]: metal-insulator transition and ground state energy.

Chemical potential of the model is given by the equation \( \langle \langle X^0_i \rangle = \langle X^2_i \rangle \) :

\[
\sum \frac{A_k}{\exp \frac{E_1(k)}{\theta} + 1} + \frac{B_k}{\exp \frac{E_2(k)}{\theta} + 1}
\]

\[
= \sum \frac{B_k}{\exp \frac{-E_1(k)}{\theta} + 1} + \frac{A_k}{\exp \frac{-E_2(k)}{\theta} + 1}.
\]

From Eq. \( (2.10) \) at \( T = 0 \) we find chemical potential of generalized Hubbard model with correlated hopping in the region of metal-insulator transition as

\[
\mu = \frac{w}{w + \tilde{w}} U \quad (U \leq w + \tilde{w}),
\]

\[
\mu = \frac{U}{2} + \frac{w - \tilde{w}}{2} \quad (U > w + \tilde{w}),
\]

with \( w = z|t|, \quad \tilde{w} = z|\tilde{t}|. \)
consequence of the electron-hole symmetry which is a characteristic of the model in this case. Note that the value of $U_c = w + \tilde{w}$ corresponds to the metal-insulator transition point of generalized Hubbard model.

At arbitrary value of temperature from Eq. (2.10) we find the expression to calculate chemical potential:

$$
\int_{-w}^{w} \left[ \frac{1}{\exp \frac{E_2(\epsilon)}{\theta} + 1} - \frac{1}{\exp \frac{E_1(\epsilon)}{\theta} + 1} \right] d\epsilon = 0,
$$

where $E_1(\epsilon), E_2(\epsilon)$ is obtained from the respective formulae (2.4) for $E_1(k), E_2(k)$ as a result of the substitution $t_k \rightarrow \epsilon, \tilde{t}_k \rightarrow \tilde{\epsilon}, t'_k \rightarrow \tilde{t}' \epsilon$.

Fig. 1–3 where the dependences of chemical potential on the ratio $U/w$ and temperature are plotted show the fact that chemical potential of generalized Hubbard model with correlated hopping $\mu > U/2$ and only in the atomic limit chemical potential $\mu = U/2$. From Eqs. (2.11) and (2.12) one can see that chemical potential of generalized Hubbard model with correlated hopping depends on $U$, $w$, $\tilde{w}$. The dependences on these parameters are different in metallic and insulating phases, this leads to a kink at the point of MIT (see Fig. 1); $\tilde{t} = 0$ (i.e. $\tilde{w} = 0$) and $t' = 0.5t$ correspond to the values of correlated hopping parameters $\tau_1 = T_1/|t_0| = 0$ and $\tau_2 = T_2/|t_0| = 0.5$.

With the increase of temperature the kink in the chemical potential curve disappears (Fig. 2). The similar peculiarity in the evolution of free energy dependence on the parameter $U/w$ with temperature was noted by Mott [26].

From Fig. 3 one can see that in the model under consideration chemical potential is essentially dependent not only on the parameters $w$ and $\tilde{w}$ and also on temperature (in contrast to chemical potential of the Hubbard model), and what is more with the decrease of temperature chemical potential rapidly increases depending on the correlated hopping parameters $\tau_1, \tau_2$. In high temperature region in the generalized Hubbard model chemical potential tends to $U/2$ with the increase of temperature; really, at $T \rightarrow \infty$ the probabilities of an electron finding within the lower and upper Hubbard bands are equal.

In summary, in the present paper we have studied chemical potential of a generalized Hubbard model with correlated hopping at half-filling. Chemical potential of the model as function of the hopping integrals at zero temperature has been found. It has been shown that chemical potential of the model is temperature-dependent. The dependences of chemical potential of a generalized Hubbard model with correlated hopping on the model parameters are different in metallic and insulating phases leading to a kink at the point of metal-insulator transition in the ground state. With the increase of temperature the kink in the chemical potential curve disappears. The obtained result differ essentially from those of the Hubbard model that indicate the important role of the correlated hopping.

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Figure 1: The dependence of chemical potential $\mu$ of generalized Hubbard model with correlated hopping in the ground state: the upper curve corresponds to $\tau_1 = 0$, $\tau_2 = 0.5$; the middle curve – $\tau_1 = 0$, $\tau_2 = 0.3$; the lower curve – $\tau_1 = \tau_2 = 0$ (the Hubbard model). The asterisks denote the point of metal-insulator transition.

Figure 2: Evolution of the dependence of chemical potential $\mu$ of generalized Hubbard model ($\tau_1 = 0$, $\tau_2 = 0.5$) on $U/w$ with temperature $\theta = 0$, 0.1, 0.3, 1 respectively. The lowermost curve corresponds to the behaviour of chemical potential of the Hubbard model.

Figure 3: The temperature dependence of chemical potential $\mu$ of generalized Hubbard model with correlated hopping at $U/2w = 1$: the upper curve corresponds to $\tau_1 = \tau_2 = 0.3$; the lower curve – $\tau_1 = \tau_2 = 0.1$; the straight – $\tau_1 = \tau_2 = 0$ (the Hubbard model).
