Electron correlations in narrow energy bands: 
ground state energy and metal-insulator 
transition

L. Didukh, Yu. Skorenkyy  
Ternopil State Technical University, Department of Physics  
56 Rus’ka Str., Ternopil UA–282001, Ukraine  
E-mail: didukh@tu.edu.te.ua

Abstract

The electron correlations in narrow energy bands are examined in 
framework of the Hubbard model. The single-particle Green func-
tion and energy spectrum are obtained in paramagnetic state at half-
filling by means of new two-pole approximation. In the ground state 
analitical expressions for the energy gap, polar states concentra-
tion and energy of the system are found. Metal-insulator transitions in 
the model at change of bandwidth or temperature are investigated. 
The obtained results are used for interpretation of some experimental 
data in narrow-band materials. PACS 71.28.+d, 71.27.+a, 71.10.Fd,  
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1 Introduction

Among the observed in narrow-bands materials metal-insulator transi-
tions (MIT) the significant interest is attracted to the transitions from para-
magnetic metal state to paramagnetic insulator state at increase of temper-
aturce which exhibit the systems NiS$_{2-x}$Se$_x$ [1-3], (V$_{1-x}$Cr$_x$)$_2$O$_3$ [4, 5] and 
Y$_{1-x}$Ca$_x$TiO$_3$ [6, 7]; in these systems the paramagnetic insulator - paramag-
netic metal transitions under external pressure are observed also. There are
reasons to believe that noted transitions are the consequences of electron-electron interactions and can be described within the framework of Hubbard model [7].

Hubbard model is the simplest model describing MIT in materials with narrow energy bands. This model describes a single non-degenerate band of electrons with the local Coulomb interaction. The model Hamiltonian contains two energy parameters: the hopping integral of an electron from one site to another and the intraatomic Coulomb repulsion of two electrons of the opposite spins. This model is used intensively (for recent reviews see Refs. [1, 8]-[10]) in order to describe the peculiarities of physical properties of narrow-band materials; in this connection two-pole approaches are attractive. The two-pole approaches in the Hubbard model and the Hubbard bands conception (being the consequence of two-pole approximation) have been useful for understanding of the peculiarities of electric and magnetic properties of narrow-band materials [1, 10]. However within the framework of two-pole approaches there are series of issues, in particular the problem of metal-insulator transition description [1, 14]-[21].

In the present paper recently proposed two-pole approximation [11] is used to study effects of electron correlations in the Hubbard model. The single particle Green function and energy spectrum are obtained. In the ground state analitical dependences of energy gap, polar states (doublons or holes) concentration and energy of the system on model parameters are found. Dependences for energy gap, polar states concentration on temperature are calculated. The obtained results are compared with corresponding results of other approximations and are used for the interpretation of some experimental data. In particular, the observable transitions from an insulating state to a metallic one at increase of bandwidth, and from a metallic state to an insulating one at increasing temperature are explained.

2 Single-particle Green function and energy spectrum

The Hubbard Hamiltonian [1] in terms of transition-operators of i-site from state |l⟩ to state |k⟩ \( X_{kl}^l \) [12] is written as

\[
H = H_0 + H_1 + H_1';
\]  (1)
\[ H_0 = -\mu \sum_{i,\sigma} (X_\sigma^0 + X_\sigma^2) + U \sum_i X_i^2, \]  
\[ H_1 = \sum_{ij,\sigma,i \neq j} t_{ij} \left( X_i^{\sigma 0} X_j^{\bar{\sigma} 0} + X_i^{2\sigma} X_j^{2\bar{\sigma}} \right), \]  
\[ H_1' = \sum_{ij,\sigma,i \neq j} t_{ij} \left( X_i^{\sigma 0} X_j^{\bar{\sigma} 2} - X_i^{\sigma 0} X_j^{\bar{\sigma} 2} + \text{h.c.} \right), \]

where \( \mu \) is the chemical potential, \( U \) is the intra-atomic Coulomb repulsion, \( t_{ij} \) is the nearest-neighbor hopping integral, \( X_i^k \) is the operator of number of \(|k\rangle\)-states on \( i \)-site; \( \sigma \) denotes spin of an electron (\( \sigma = \downarrow, \uparrow \)) and \( \bar{\sigma} \) denotes the projection of electron spin opposite to \( \sigma \); \( H_0 \) describes system in the atomic limit, \( H_1 \) describes electron hoppings between single occupied sites and empty sites (holes) (the first sum in \( H_1 \) – processes forming “h-band”) and electron hoppings between doubly occupied sites (doublons) and single occupied sites (the second sum in \( H_1 \) – processes forming “d-band”). \( H_1' \) describes “hybridization” between the “h-band” and “d-band” (the processes of pair creation and annihilation of holes and doublons).

The single-particle Green function is written in \( X_i^{kl} \)-operators as

\[ \langle \langle a_p^\dagger | a_{s}^\dagger \rangle \rangle = \langle \langle X_p^{12} | X_s^{21} \rangle \rangle - \langle \langle X_p^{01} | X_s^{21} \rangle \rangle - \langle \langle X_p^{12} | X_s^{10} \rangle \rangle + \langle \langle X_p^{01} | X_s^{10} \rangle \rangle. \]  

The functions \( \langle \langle X_p^{12} | X_s^{21} \rangle \rangle \) and \( \langle \langle X_p^{01} | X_s^{21} \rangle \rangle \) satisfy the equations

\[ (E + \mu - U) \langle \langle X_p^{12} | X_s^{21} \rangle \rangle = \frac{\delta_{ps}}{2\pi} \langle X_p^{1+} + X_s^{2} \rangle + \langle \langle [X_p^{12}, H_1^\dagger]_\text{\_} | X_s^{21} \rangle \rangle, \]

\[ (E + \mu) \langle \langle X_p^{01} | X_s^{21} \rangle \rangle = \langle \langle [X_p^{01}, H_1]_\text{\_} | X_s^{21} \rangle \rangle + \langle \langle [X_p^{01}, H_1']_\text{\_} | X_s^{21} \rangle \rangle, \]

with \([A, B]_\text{\_} = AB - BA\). To obtain the closed system of equations we apply new two-pole approximation, proposed in work \([11]\). Suppose in Eq. (6) that

\[ [X_p^{01}, H_1]_\text{\_} = \sum_j \epsilon(pj) X_j^{01}, \]
\[ [X_p^{12}, H_1]_\text{\_} = \sum_j \bar{\epsilon}(pj) X_j^{12}, \]

where \( \epsilon(pj) \) and \( \bar{\epsilon}(pj) \) are non-operator expressions which we calculate using the method of work \([13]\). At electron concentration \( n=1 \) in a paramagnetic
state we have

\[ \epsilon(pj) = (1 - 2d)t_{pj}, \]
\[ \tilde{\epsilon}(pj) = (1 - 2d)t_{pj}, \]  

with \( d = \langle X_p^2 \rangle \) being the concentration of doublons.

Let us take into account the functions \( \langle \langle X_{p}^{12}, H_{1}^\prime \rangle \rangle \) and \( \langle \langle X_{p}^{0\dagger}, H_{1}^\prime \rangle \rangle \) in the mean-field approximation:

\[
\begin{align*}
\langle \langle X_{p}^{12}, H_{1}^\prime \rangle \rangle & = - \sum_{i,i\neq p} t_{ip} \langle \langle (X_{p}^{+} + X_{p}^{\dagger})X_{i}^{0\dagger} | X_{s}^{2\dagger} \rangle \rangle + \langle \langle X_{p}^{02} X_{i}^{2\dagger} | X_{s}^{2\dagger} \rangle \rangle, \\
\langle \langle X_{p}^{0\dagger}, H_{1}^\prime \rangle \rangle & = - \sum_{i,i\neq p} t_{ip} \langle \langle (X_{p}^{0} + X_{p}^{\dagger})X_{i}^{12} | X_{s}^{2\dagger} \rangle \rangle + \langle \langle X_{p}^{02} X_{i}^{12} | X_{s}^{2\dagger} \rangle \rangle.
\end{align*}
\]

in this way we neglect the processes describing the “inter-band” hoppings of electrons which are connected with spin turning over and “inter-band” hoppings with creation or annihilation of two electrons on the same site.

So we obtain the closed system of equations

\[
(E - \mu + U)\langle \langle X_{p}^{12} | X_{s}^{2\dagger} \rangle \rangle - \sum_{i} \tilde{\epsilon}(pi) \langle \langle X_{i}^{12} | X_{s}^{2\dagger} \rangle \rangle + \langle X_{p}^{+} + X_{p}^{\dagger} \rangle \sum_{i,i\neq p} t_{ip} \langle \langle X_{i}^{12} | X_{s}^{2\dagger} \rangle \rangle = \frac{\langle X_{p}^{2} + X_{p}^{\dagger} \rangle}{2\pi},
\]

\[
(E - \mu)\langle \langle X_{p}^{0\dagger} | X_{s}^{2\dagger} \rangle \rangle - \sum_{i} \epsilon(pi) \langle \langle X_{i}^{0\dagger} | X_{s}^{2\dagger} \rangle \rangle + \langle X_{p}^{0} + X_{p}^{\dagger} \rangle \sum_{i,i\neq p} t_{ip} \langle \langle X_{i}^{12} | X_{s}^{2\dagger} \rangle \rangle = 0.
\]

After the Fourier transformation we obtain solutions of system of Eqs. (10):

\[
\begin{align*}
\langle \langle X_{p}^{12} | X_{s}^{2\dagger} \rangle \rangle_{k} &= \frac{X_{p}^{2} + X_{p}^{\dagger}}{2\pi} \left( \frac{A_{k}^{1}}{E - E_{h}(k)} + \frac{B_{k}^{1}}{E - E_{d}(k)} \right), \\
A_{k}^{1} &= \frac{1}{2} \left( 1 - \frac{U - \epsilon(k) + \tilde{\epsilon}(k)}{E_{d}(k) - E_{h}(k)} \right), \quad B_{k}^{1} = 1 - A_{k}^{1},
\end{align*}
\]
\[ \langle (X^0_p | X^2_s) \rangle_k = \frac{\langle X^2_p + X^\downarrow_p \rangle \langle X^0_p + X^\uparrow_p \rangle}{2\pi} \times \frac{t(k)}{E_d(k) - E_h(k)} \left( \frac{1}{E} - \frac{1}{E - E_d(k)} \right). \] (12)

Here \( t(k) \) is the hopping integral in \( k \)-representation and

\[ E_h(k) = -\mu + \frac{U}{2} + \frac{\epsilon(k) + \bar{\epsilon}(k)}{2} - \frac{1}{2} \sqrt{[U - \epsilon(k) + \bar{\epsilon}(k)]^2 + \langle X^p_p + X^\downarrow_p \rangle \langle X^\downarrow_p + X^\uparrow_p \rangle (t(k))^2}, \] (13)

\[ E_d(k) = -\mu + \frac{U}{2} + \frac{\epsilon(k) + \bar{\epsilon}(k)}{2} + \frac{1}{2} \sqrt{[U - \epsilon(k) + \bar{\epsilon}(k)]^2 + \langle X^p_p + X^\uparrow_p \rangle \langle X^\downarrow_p + X^\uparrow_p \rangle (t(k))^2} \] (14)

are the energies of electron in lower (“hole”) and upper (“doublon”) subbands, respectively; \( \epsilon(k) \) and \( \bar{\epsilon}(k) \) are the Fourier components of \( \epsilon(pj) \) and \( \bar{\epsilon}(pj) \).

Analogous procedure gives for functions \( \langle (X^1_p | X^0_s) \rangle \) and \( \langle (X^0_p | X^1_s) \rangle \) the following expressions:

\[ \langle (X^1_p | X^0_s) \rangle_k = \langle (X^0_p | X^2_s) \rangle_k, \]

\[ \langle (X^0_p | X^1_s) \rangle_k = \frac{\langle X^0_p + X^\uparrow_p \rangle}{2\pi} \left( \frac{A_k^2}{E - E_h(k)} - \frac{B_k^2}{E - E_d(k)} \right), \] (15)

\[ A_k^2 = B_k^1, \quad B_k^2 = A_k^1. \]

Finally, in \( k \)-representation single-particle Green function (5) we obtain

\[ \langle (a_{p\uparrow} | a^{\downarrow}_{s\uparrow}) \rangle_k = \frac{1}{2\pi} \left( \frac{A_k}{E - E_h(k)} + \frac{B_k}{E - E_d(k)} \right), \] (16)

\[ A_k = \frac{1}{2} \left( 1 - \frac{(C_1 - C_2)(U - \epsilon(k) + \bar{\epsilon}(k)) + 4t(k)C_1C_2}{E_d(k) - E_h(k)} \right), \]

\[ B_k = 1 - A_k, \]

where \( C_1 = \langle X^0_p + X^\uparrow_p \rangle, \quad C_2 = \langle X^2_p + X^\downarrow_p \rangle. \)
In the important for an investigation of metal-insulator transition case $n = 1$ in a paramagnetic state ($\langle X^\uparrow_p \rangle = \langle X^\downarrow_p \rangle$) single-particle Green function (16) has the form

$\langle \langle a_p^\uparrow | a_s^\uparrow \rangle \rangle_k = \frac{1}{2\pi} \left( \frac{A_k}{E - E_h(k)} + \frac{B_k}{E - E_d(k)} \right)$, \hspace{1cm} (17)

$A_k = \frac{1}{2} \left( 1 - \frac{t(k)}{\sqrt{U^2 + (t(k))^2}} \right)$,

$B_k = 1 - A_k$,

where single-particle energy spectrum is

$E_h(k) = (1 - 2d)t(k) - \frac{1}{2}\sqrt{U^2 + (t(k))^2}$,

$E_d(k) = (1 - 2d)t(k) + \frac{1}{2}\sqrt{U^2 + (t(k))^2}$ \hspace{1cm} (18)

(here we took into account that $\mu = \frac{U}{2}$ for $n = 1$).

Single-particle Green function (17) and energy spectrum (18) are exact in the band and atomic limits. It is worthwhile to note, that in distinction from the results of two-pole approximations of Hubbard [7] and Ikeda, Larsen, Mattuck [14] the energy spectrum (18) depends on polar states concentration (thus on temperature). In distinction from approximations based on ideology of Roth [15] (in this connection see also Refs. [16]-[21]) the energy spectrum (18) describes metal-insulator transition. Energy spectrum which describes metal-insulator transition was earlier obtained in work [13]. Expressions (18) differs from the respective expressions in work [13] by presence of term $\sqrt{U^2 + t^2(k)}$ instead of $\sqrt{U^2 + 4d^2t^2(k)}$. This leads to the series of distinctions between results of this work and results of work [13] ($d(U/w)$-dependence, the condition of metal-insulator transition, etc); at the same time expression (18) depends on polar state concentration similarly to respective expression in work [13].
3 Energy gap and polar states concentration

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

$$\Delta E = E_d(-w) - E_h(w) = -2w(1 - 2d) + \sqrt{U^2 + w^2},$$

(19)

(where $w = z|t|$ is the halfwidth of uncorrelated electron band, $z$ is the number of nearest neighbors to a site). Expression (19) describes the vanishing of the energy gap in the spectrum of paramagnetic insulator at critical value $(\frac{U}{w})_c$ when the halfbandwidth $w$ increase (under pressure). Dependence of $\Delta E$ on temperature can lead to the transition from metallic to insulator state with increase of temperature (in this connection note the transition at increasing temperatures from the state of paramagnetic metal to the paramagnetic insulator state in the systems NiS$_{2-x}$Se$_x$, (V$_{1-x}$Cr$_x$)$_2$O$_3$ and Y$_{1-x}$Ca$_x$TiO$_3$).

For the calculation of polar states concentration we use function (11). At $T = 0$ and rectangular density of states the concentration of polar states is

$$d = \frac{1}{4} + \frac{U}{8w} \ln \left( \frac{1 - 4d}{3 - 4d} \right)$$

(20)

if $(\frac{U}{w}) \leq (\frac{U}{w})_c$ and

$$d = \frac{1}{4} + \frac{U}{8w} \ln \left( \frac{\sqrt{1 + \left(\frac{U}{w}\right)^2} + 1}{\sqrt{1 + \left(\frac{U}{w}\right)^2} - 1} \right)$$

(21)

if $(\frac{U}{w}) > (\frac{U}{w})_c$. At $T = 0$ we have $(\frac{U}{w})_c = 1.672$.

The dependence $d(\frac{U}{w})$ given by Eqs. (20)-(21) is plotted on Fig. 1. One can see that in the point $(\frac{U}{w})_c$ the slope of $d(\frac{U}{w})$—dependence changes; the concentration of doublons vanishes at $\frac{U}{w} \to \infty$. Our result for $d(\frac{U}{w})$ in region of MIT is in good agreement with result of papers [9, 23] obtained in the limit of infinite dimensions (Fig. 2). The parameter $U$ is normalized by averaged band energy in absence of correlation $\varepsilon_0$.

In Fig. 3 the dependences of polar states concentration on parameter $\frac{U}{w}$ at different temperatures are presented. Note the important difference (see Fig.4) of the dependence of $d$ on temperature from result of papers [9, 23]: we found that at any temperature polar states concentration increases
monotonically with increasing temperature at the fixed value of \( \frac{U}{w} \) when respective dependence in [3, 23] has a minimum.

The dependence of \( \frac{\Delta E}{U} \) on parameter \( \frac{U}{w} \) at zero temperature is plotted in Fig. 5. It is important to note that in the point of gap disappearance \( d \neq 0 \) in contrast to the previously obtained result [13]. At increasing \( \frac{U}{w} \) the energy gap width increases (the negative values of \( \Delta E \) correspond to the overlapping of the subbands). For comparison on Fig. 5 results of approximation “Hubbard-I” [7] is also plotted. In the point of energy gap vanishing \( (\frac{U}{w})_c = 1.672 \) what is very close to result of “Hubbard-III” approximation [22].

At increase of temperature in metallic state the overlapping of subbands decreases and temperature induced transition from metallic to insulating state can occur at some values of parameter \( \frac{U}{w} \) (Fig. 6). The obtained results allows us to draw the \((w/U, T)\) phase diagram of the model (Fig. 7). This phase diagram can explain the experimentally observed transitions from metallic to insulating state with increase of temperature and from insulating to metallic state with increase of bandwidth (under external pressure) in paramagnetic state.

4 Ground state energy

The ground state energy of the model

\[
\frac{E_0}{N} = \frac{1}{N} \langle \sum_{ij\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} \rangle + Ud,
\]

(22)

calculated using single particle Green function (17) and expressions (20)-(21) for the concentration of polar states has the form:

\[
\frac{E_0}{N} = -\frac{w}{2} + \frac{U}{4} (1 + 3d) - \frac{U^2}{2w} \frac{(1 - 4d)}{4(1 - 2d)^2 - 1}
\]

(23)

if \( (\frac{U}{w}) \leq (\frac{U}{w})_c \) and

\[
\frac{E_0}{N} = -\frac{1}{2} \sqrt{U^2 + w^2} + 2U(\frac{1}{4} - d)
\]

(24)

if \( (\frac{U}{w}) > (\frac{U}{w})_c \). In Fig. 8 the dependence of the ground state energy on parameter \( \frac{U}{w} \) given by Eqs.(23)-(24) is compared with the exact result, found
in one-dimensional case \[24\]. The upper and lower bounds on ground state energy in one-dimensional case found in paper \[25\] are also shown. Our result for the ground state energy in metallic state lies slightly lower than exact one and in insulator state fits the exact ground state energy very well.

In Fig. 9 our plot of the ground state energy is compared with the best upper and lower bounds on ground state energy in infinite-dimensional case \[26\]. In Fig. 10 we have the comparison with bounds on ground state energy for three-dimensional simple cubic lattice obtained in paper \[25\]. In Figs. 8-10 the ground state energy per electron is normalized by averaged band energy in absence of correlation \(\varepsilon_0\); in considered case and rectangular density of states \(\varepsilon_0 = -\frac{w}{2}\). Figs. 8-10 show that our result present a good approximation for the ground state energy of the system. In Fig. 11 we plot our result for the kinetic part of ground state energy. This plot describes the same behavior of kinetic energy of electrons with change of correlation strength in paramagnetic state as respective result of work \[23\]: in metallic state absolute value of kinetic energy decrease rapidly due to rapid decrease of doublon (hole) concentration. In insulating state absolute value of kinetic energy decrease slowly what in the approximation of effective Hamiltonian (obtained for the case \(\frac{t_{ij}}{U} \ll 1\)) is equivalent to the interaction of local magnetic moments.

5 Conclusions

In this paper we have studied electron correlations in narrow energy bands using recently proposed approximation \[11\]. We assume that state of the narrow-band system is paramagnetic insulator or paramagnetic metal. The single-particle Green function and energy spectrum dependent on model parameters and on polar states concentration (thus on temperature) have been found in paramagnetic state at half-filling \((n = 1)\). The obtained expression for energy gap allows to describe MIT at changes of bandwidth (under external pressure) or temperature. The comparison of calculated ground state energy with results of other approximations and the exact result found in one-dimensional case shows that the used method is a good approximation for the model under consideration. The obtained phase diagram of the model can explain the transitions from paramagnetic metal state to paramagnetic insulator state at increase of temperature and the paramagnetic insulator - paramagnetic metal transitions under external pressure observed in the
systems NiS$_{2-x}$Se$_x$, (V$_{1-x}$Cr$_x$)$_2$O$_3$ and Y$_{1-x}$Ca$_x$TiO$_3$.

It is worthwhile to note that approximation used in this paper can be generalized to describe effects of antiferromagnetic ordering. Such a generalization will be considered in subsequent paper.

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Figure captions

Fig.1 The dependence of doublon concentration \( d \) on \( U/w \) at zero temperature.

Fig.2 The comparison of \( d(U/w) \) dependences: solid line - our result, dashed line - iterative-perturbative theory [9,23], circles - QMC method [23].

Fig.3 The dependences of doublon concentration \( d \) on \( U/w \) at different temperatures: lower curve corresponds to \( kT/w = 0.16 \), middle curve corresponds to \( kT/w = 0.08 \), upper curve corresponds to \( kT/w = 0 \).

Fig.4 The dependences of doublon concentration \( d \) on temperature at different \( U/w \): values of \( U/w \) from down to up are 3, 2, 1.5, 1, 0.5, 0.

Fig.5 The dependences of energy gap width on \( U/w \): “Hubbard-I” approximation (upper curve), our result (middle curve), approximation [13] (lower curve).

Fig.6 The dependences of energy gap width on temperature at different \( U/w \): values of \( U/w \) from down to up are 0.5, 1.2, 1.5.

Fig.7 The obtained \( (kT,w/U) \)-phase diagram of the model.

Fig.8 The comparison of ground state energies in one-dimensional case: dashed curves correspond to upper and lower bounds given by Langer and Mattis [25], upper solid curve corresponds to exact ground state (Lieb and Wu [24]) lower solid curve corresponds to result of this paper.

Fig.9 The ground state energy found in this paper (upper curve), best upper (middle curve) and lower (lower curve) bounds on ground state energy in infinite-dimensional case.

Fig.10 The upper (upper curve) and lower (lower curve) bounds on ground state energy in three-dimensional case [25] and the ground state energy found in this paper (middle curve).

Fig.11 The kinetic part of ground state energy as a function of \( U/w \).