Metal-insulator transition in the Hubbard model: a simple description including the Kondo effect

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The electron spectrum structure in the half-filled Hubbard model is considered in terms of the one-particle Green’s functions within many-electron representation. A simple analytical generalization of the single-site Hubbard-III approximation is obtained, which takes into account the Fermi excitations (Kondo terms). The problem of the metal-insulator transition is investigated. The occurrence of a three-peak density-of-states structure including the “Kondo” peak at the Fermi level is discussed. A comparison with large-d calculations is performed.

I. INTRODUCTION

The problem of strong correlations in many-electron systems is one of the most important in the solid state theory. The simplest model to describe correlation effects is the Hubbard model [1] which includes the on-site Coulomb interaction. One of most interesting phenomena is the correlation-driven metal-insulator transition (MIT), which takes place in a number of transition metal compounds. A simple description of MIT was given by Hubbard [2] who started from the atomic-level picture and proposed a simple interpolation self-consistent scheme.

Since the Hubbard works of 60’s, a great progress has been achieved in understanding electronic structure of highly-correlated systems. Last time, the role of the Kondo effect has been discussed within the large-d approach (d is space dimensionality) which reduces the original periodic Hubbard model to an effective Anderson impurity model [3–5]. Such an approach (dynamical mean-field theory, DMFT) turned out to be rather successful. The corresponding density of states (DOS) has three-peak rather than two-peak structure: an additional “Kondo” quasiparticle resonance at the Fermi level occurs owing to scattering by the local moment. The spectrum structure in large-d approaches is confirmed by the quantum Monte-Carlo (QMC) calculations (see, e.g., [6]) and some spectroscopic experimental results. Unfortunately, there exist some difficulties in numerical calculations within QMC and large-d approaches, so that one needs often to introduce rather high temperatures to resolve these problems. The three-peak structure is not reproduced by most preceding analytical approaches, in particular, by the single-site Hubbard-III approximation [2], the reason being in that they do not take into account contributions of Fermi-like excitations in a proper way. Thus these approaches do not describe the Brinkman-Rice effective-mass enhancement which is important from the experimental point of view. Recently, an attempt has been made to improve the Hubbard-III approximation by calculating corrections owing to correlation effects [7]; however, the results remained qualitatively unchanged.

A detailed analysis of Hubbard-III-like approximations was performed in Refs. [8,9] within the large-z expansion, z being the nearest-neighbor number. In the zero order this approach reduces to the simplest Hubbard-I approximation [1]. General expressions for 1/z-corrections in the limit $U \to \infty$ were obtained in Ref. [8]. The problem of MIT within this approach was treated in Ref. [9]. Unfortunately, only a classical approximation (the large-S limit of the s-d model which generalizes the Hubbard model) was considered, and the terms with the one-particle occupation numbers, which just describe the Kondo effect in narrow bands [10], were neglected.

In the present paper we present a treatment that is based on the method of equations of motion for the many-electron Hubbard operators [11,12] and is a much more simple than the large-d approach. In Sec. II, the decoupling scheme with account of the Fermi excitations is developed. In Sec. III, we present the results of numerical calculations and carry out a comparison with previous works.

II. THE DECOUPLING SCHEME

We start from the Hubbard model with the electron concentration $n = 1$ (the half-filled case). The corresponding Hamiltonian reads

$$
\mathcal{H} = \sum_{k \sigma} t_{k \sigma} c_{k \sigma}^\dagger c_{k \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow},
$$

(1)
where \( n_{\sigma} = c_{\sigma}^\dagger c_{\sigma} \), \( c_{\sigma} \), and \( c_{\sigma}^\dagger \) are the one-electron operators in the Wannier and quasimomentum representation. We pass to the Hubbard I-X-operat0

\[
X_i^{\alpha \beta} = |i\alpha\rangle \langle i\beta|, \quad X_i^{\sigma \gamma} X_i^{\tau \varepsilon} = \delta_{\beta \gamma} X_i^{\sigma \varepsilon}, \quad \sum_\alpha X_i^{\alpha \alpha} = 1,
\]

so that

\[
c_{\sigma}^\dagger = \sum_{\alpha, \beta} \langle i\alpha| c_{\sigma}^\dagger | i\beta\rangle X_i^{\alpha \beta} = X_i^{\sigma 0} + \sigma X_i^{2-\sigma}.
\]

Then the interaction Hamiltonian takes a diagonal form and we obtain

\[
\mathcal{H} = \sum_{k\sigma} t_k (X_k^{\sigma 0} + \sigma X_k^{2-\sigma}) (X_k^{\sigma 0} + \sigma X_k^{2-\sigma}) + U \sum_i X_{i2}^2.
\]

Using (4) we have for the one-electron anti-commutator retarded Green's function

\[
G_{k\sigma}(E) = \langle \langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle \rangle_E = \langle \langle X_k^{\sigma 0} | c_{k\sigma}^\dagger \rangle \rangle_E + \sigma \langle \langle X_k^{2-\sigma} | c_{k\sigma}^\dagger \rangle \rangle_E.
\]

The energy \( E \) is supposed to be referred to the chemical potential which equals \( U/2 \) in our case. We write down the system of equation of motion

\[
E \langle \langle A| B \rangle \rangle_E = \langle \{A, B\} \rangle_E + \langle [A, \mathcal{H}] | B \rangle_E
\]

for the pair of the Green's functions in the right-hand side of (4). Using (2) we obtain in the non-magnetic case

\[
\begin{align*}
(E + U/2) \langle \langle X_k^{\sigma 0} | c_{k\sigma}^\dagger \rangle \rangle_E &= \frac{1}{2} (1 + t_k \langle \langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle \rangle_E) \\
&+ \sum_q t_q \langle \langle \delta(X_{k-q}^{00}) + \delta(X_{k-q}^{\sigma\sigma}) \rangle \rangle_E c_{q\sigma} | c_{k\sigma}^\dagger \rangle \rangle_E \\
&+ \sum_q t_q \langle \langle X_{k-q}^{\sigma\sigma} c_{q\sigma}^\dagger + \sigma c_{q\sigma}^\dagger X_{k+q}^{22} \rangle \rangle_E,
\end{align*}
\]

\[
\sigma(E - U/2) \langle \langle X_k^{2-\sigma} | c_{k\sigma}^\dagger \rangle \rangle_E = \frac{1}{2} (1 + t_k \langle \langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle \rangle_E) \\
+ \sum_q t_q \langle \langle \delta(X_{k-q}^{\sigma\sigma}) + \delta(X_{k+q}^{2-\sigma}) \rangle \rangle_E c_{q\sigma}^\dagger | c_{k\sigma} \rangle \rangle_E \\
- \sum_q t_q \langle \langle X_{k-q}^{\sigma\sigma} c_{q\sigma} + \sigma c_{q\sigma} X_{k+q}^{22} \rangle \rangle_E,
\]

where \( \delta A = A - \langle A \rangle \) is the fluctuation of the operator. Solving the system (3), (5) we derive

\[
G_{k\sigma}(E) = G_{k\sigma}^0(E) \left( 1 - \frac{U}{E} \frac{1}{\Gamma_{k\sigma}(E)} \right),
\]

\[
\Gamma_{k\sigma}(E) = \sum_q t_q \langle \langle \delta(X_{k-q}^{00} + X_{k-q}^{\sigma\sigma}) c_{q\sigma} + X_{k-q}^{\sigma\sigma} c_{q\sigma}^\dagger + \sigma c_{q\sigma}^\dagger X_{k+q}^{22} \rangle \rangle_E.
\]

Here

\[
G_{k\sigma}^0(E) = \frac{1}{F_0(E) - t_k}, \quad F_0(E) = E - \frac{U^2}{4E}
\]

is the Green’s function of the Hubbard-I approximation (which plays the role of a mean-field approximation for our problem), \( F_0(E) \) being the corresponding inverse locator. The Hubbard-I spectrum contains two correlation subbands defined by the poles of (6)

\[
E_{k1,2} = \frac{1}{2} (t_k \pm \varepsilon_k), \quad \varepsilon_k = \sqrt{U^2 + t_k^2}.
\]
The Green’s function $\Gamma_{k\sigma}(E)$ describes fluctuation corrections. The corresponding collective excitations are described by spin and charge operators.

$$S_q^\sigma = X_{q-\sigma}^+, \quad S_q^z = \frac{1}{2}(X_{q-\sigma}^z - X_{q-\sigma}^-),$$
$$\rho_q^+ = X_{q-20}^+, \quad \rho_q^- = \frac{1}{2}(X_{q-00}^2 - X_{q-00}^0).$$

Further we write down the system of equations for the fluctuation Green’s functions and perform the decouplings which correspond to the first order in the formal parameter $1/z$ (strictly speaking, this expansion is justified in the case of long-range electron hopping). For the half-filled band, we have to take into account particle and hole excitations in an equal way. However, decouplings can violate the particle-hole symmetry. To preserve this symmetry, we make an identical transformation by taking in (9) the Green’s functions with symmetrized operator products, e.g.,

$$\langle \langle X_{k-q}^{-\sigma}\sigma c_{q-\sigma}^+ | c_{k\sigma}^+ \rangle \rangle_E \to \frac{1}{2} \langle \langle X_{k-q}^{-\sigma}\sigma c_{q-\sigma} - c_{q-\sigma} X_{k-q}^{-\sigma}\sigma c_{k\sigma}^+ \rangle \rangle_E.$$

We also use in the equations of motion the Hamiltonian in the symmetrized form,

$$t_{k\sigma}c_{k\sigma}^+ c_{k\sigma} - t_{k受贿}c_{k\sigma}^+ c_{k\sigma}^+.$$

Then we obtain for the transverse spin fluctuation contribution

$$(E^2 - U^2/4 - Et_q)\langle \frac{1}{2} \langle \langle X_{k-q}^{-\sigma}\sigma c_{q-\sigma} - c_{q-\sigma} X_{k-q}^{-\sigma}\sigma c_{k\sigma}^+ \rangle \rangle_E = (E + U/2)(t_q - t_k)(f_q - \frac{1}{2})G_{k\sigma}(E) - U(t_k(X_{k-q}^{-\sigma}\sigma c_{k+q}^+ - c_{k+q}\sigma X_{k-q}^{-\sigma})),$$

$$+ (t_q - t_k)(\frac{1}{2}[X_{-q}\sigma, X_{q+q}^{\sigma}\sigma] - \sigma X_{q-00}^{\sigma}\sigma)G_{k\sigma}(E),$$

$$- (E + U/2)(f_q - \frac{1}{2}) + U(\frac{1}{2}[X_{-q}\sigma, X_{q}^{\sigma}\sigma])$$

$$- \sigma X_{-q}\sigma X_{q}^{0-\sigma} - X_{k-q}\sigma X_{k+q}^{-\sigma}\sigma.$$

Note that, as well as the standard Kondo terms, the “many-electron” terms come from the spin-flip processes, but not from longitudinal spin fluctuations. For the “transverse” charge contribution we have

$$\sigma(E^2 - U^2/4 - Et_q)\langle \frac{1}{2} \langle \langle c_{q-\sigma}^+ X_{k+q}^{02} | c_{k\sigma}^+ \rangle \rangle_E = (E + U/2)(t_q + t_k)(f_q - \frac{1}{2})G_{k\sigma}(E)$$

$$+ U(t_k(X_{k-q}^{02}X_{k+q}^\sigma + (t_q + t_k)(\sigma X_{q}^{\sigma}\sigma)X_{q}^{0-\sigma})$$

$$+ \frac{1}{2}[X_{-q}\sigma, X_{q}^{\sigma}\sigma]G_{k\sigma}(E)$$

$$+ (E + U/2)(f_q - \frac{1}{2}) - U(\frac{1}{2}[X_{-q}\sigma, X_{q}^{2\sigma}])$$

$$- \sigma X_{-q}\sigma X_{q}^{0-\sigma} - X_{k-q}\sigma X_{k+q}^{02}\sigma.$$

A symmetry of spin and charge degrees of freedom occurs for a symmetric conduction band.

Further we neglect $q$-dependence of spin and charge correlations functions and replace them by single-site averages, so that

$$\langle S_{q-\sigma}^\sigma S_{q-\sigma}^{-\sigma} \rangle = 2\langle S_{q-\sigma}^z S_{q-\sigma}^z \rangle = \langle X_{q-\sigma}^\sigma \rangle,$$

$$\langle \rho_{q-\sigma}^\sigma \rho_{q-\sigma}^{-\sigma} \rangle = 2\langle \rho_{q-\sigma}^z \rho_{q-\sigma}^z \rangle = \langle X_{q-\sigma}^{00} \rangle.$$

Such an approximation is made (although as a rule implicitly) in practically all works on the MIT problem. This corresponds to neglecting dynamics of low-energy Bose excitations and may be justified not only in high-temperature limit, but also within the $1/z$-expansion. For the local-spin subsystem, this approximation is in spirit of the mean-field theory. Main part of charge dynamics (the Hubbard splitting $U$) is also already taken into account in the zero-order (Hubbard-I) approximation. A consistent consideration of dynamics can be made in higher orders in $1/z$. This may lead to a change in details of the MIT picture. However, this problem is rather difficult.

Taking into account (11) we can use the sum rule in (12) to obtain
\[ G_k(E) = \frac{a(E)}{b(E) - a(E)t_k} = \frac{1}{F(E) - t_k}, \quad F(E) = \frac{b(E)}{a(E)}, \quad (12) \]

\[
\begin{align*}
 a(E) &= 1 + \frac{3U^2}{4E^2} \sum_q t_q \frac{1}{F_0(E) - t_q} + \frac{2U}{E} \sum_q t_q \frac{f_q}{F_0(E) - t_q}, \quad (13a) \\
 b(E) &= F_0(E) + \frac{2U}{E} \sum_q t_q^2 \frac{f_q}{F_0(E) - t_q}, \quad (13b)
\end{align*}
\]

We have substituted here the one-particle correlation functions in the Hubbard-I approximation,

\[
\langle c_{q\sigma}^\dagger X_{q0}^\sigma \rangle = \frac{1}{2\varepsilon_q}[(E_{q1} - U)f(E_{q1}) - (E_{q2} - U)f(E_{q2})],
\]

\[
\langle c_{q\sigma}^\dagger X_{q-\sigma}^\sigma \rangle = -\frac{\sigma}{2\varepsilon_q}[E_{q1}f(E_{q1}) - E_{q2}f(E_{q2})],
\]

\[
f_q \equiv \langle c_{q\sigma}^\dagger c_{q\sigma} \rangle = \frac{1}{\varepsilon_q}[(E_{q1} - U/2)f(E_{q1}) - (E_{q2} - U/2)f(E_{q2})].
\]

Due to the symmetry of the bare band, we have

\[
\sum_q f(E_{q,2})\Phi(t_q) = \sum_q [1 - f(E_{q1})]\Phi(-t_q).
\]

As a result of our way of decoupling, we have in the sums \( f(E_{q1}) \to f(E_{q1}) - 1/2 \), and the DOS of the interacting system remains symmetric.

To obtain the self-consistent (SC) approximation we have to replace in (10) the Hubbard-I Green’s functions by the exact ones,

\[
G_q^0(E) = \frac{1}{F_0(E) - t_q} \to G_q(E) = \frac{1}{F(E) - t_q},
\]

and the Fermi functions \( f_q \) by the exact occupation numbers \( n_q \), according to the spectral representation,

\[
n_q = -\frac{1}{\pi} \int dE f(E) \text{Im}G_q(E).
\]

Then we have the SC equation for the one-electron Green’s function in the form (12) with

\[
\begin{align*}
 a(E) &= 1 + \frac{3U^2}{4E^2} \sum_q t_q G_q(E) + \frac{2U}{E} \sum_q t_q G_q(E)n_q, \quad (14a) \\
 b(E) &= F_0(E) + \frac{2U}{E} \sum_q t_q^2 G_q(E)n_q. \quad (14b)
\end{align*}
\]

Unlike the simplest self-consistency scheme considered in Ref. [8] [see eq. (32) of that paper], the approximation (14), as well as the standard Hubbard-III approximation, does not result in a violation of analytical properties.

### III. RESULTS AND DISCUSSION

To investigate the MIT problem, we calculate the single-particle density of states

\[
N(E) = -\frac{1}{\pi} \text{Im} \sum_k G_k(E).
\]

The results for the approximations (13) and (14) are shown in Figs. 1–4, and the critical values for MIT are given in Table I. The numerical calculation were performed for the square and two cubic lattices with a symmetric bare DOS. We also treat the Bethe lattice, i.e. the model semielliptic bare conduction band with
metal-insulator transition at $U$. This fact is just due to many-electron corrections. Therefore the non-self-consistent (NSC) formulas (13) yield an approximation (see the discussion in Ref. [8]).

Then the quantity $\mu_2$ has equal expressions in terms of $W$ for the Gaussian and semielliptic bare DOS’s. It is important that the quantity $F(E)$, unlike $F_0(E)$, does not diverge at $E \to 0$, i.e. in the centre of the band. This fact is just due to many-electron corrections. Therefore the non-self-consistent (NSC) formulas (13) yield a metal-insulator transition at $U \neq 0$, unlike NSC local approximations. However, the corresponding critical value $U_{c}^{\text{NSC}}$ is rather small. The “false” singularities at the edges of the Hubbard-I bands occur at large $U$ in our NSC approximation (see the discussion in Ref. [8]).

The critical value for MIT $U_c$ in the standard Hubbard-III approximation [4] for an arbitrary bare DOS is given by

$$U_c^{\text{III}} = 2\sqrt{3\mu_2}. \quad (15)$$

The critical value in the SC approximation [14] is changed somewhat in comparison with the Hubbard-III result (see Table II). Unlike Ref. [4], where the critical value was decreased by fluctuations, $U_c/W = 0.67$ for the Bethe lattice, our approach yields an opposite tendency, in agreement with the results of the QMC calculations at finite temperatures, $U_c/W \approx 1$ (see Table II). Within the “linearized” DMFT [13], an analytical expression $U_c$ can be obtained, which exceeds the Hubbard-III value,

$$U_c^{\text{I}} = \sqrt{3}U_c^{\text{III}} = 6\sqrt{\mu_2}. \quad (16)$$

As follows from comparison with Table II, this approximation seems to overestimate somewhat $U_c$.

The account of the Fermi excitations results in a modification of the DOS form (cf. Ref. [9]). In a comparison with the Hubbard-III approximation, a pronounced pseudogap exists near MIT at $U < U_c$. The same feature can be seen from the results of Ref. [4]. At small $U$, a three-peak structure can be seen in Figs. 1 and 2, which becomes smeared with approaching MIT (the central peak becomes wide, and a pseudogap occurs). The three-peak structure is more pronounced in the NSC approximation. The details of our MIT scenario differ from the DMFT picture where the central quasiparticle peak is expected to shrink gradually at $U \to U_c - 0$. Probably, this discrepancy is connected with the overestimation of the role of the damping in our approach. The correct treatment of the damping is a difficult problem. To avoid this problem, most large-d calculations are performed at finite temperatures. It should be noted that various DMFT versions give somewhat different MIT pictures. In some calculations, a pseudogap develops in the metallic phase near MIT (see, e.g., Refs. [13,12]), as well as in our picture. The occurrence in some works of a very high and narrow peak with lowering temperature, even not too close to $U_c$, is probaly an unphysical drawback. In a number of large-d calculations (see Refs. [3,4,12]) the height of the peak does not change when approaching MIT.

In the case of square lattice, the situation is more complicated owing to the Van Hove singularity at the band centre. The underestimation of $U_c$ in the Hubbard-III approximation is confirmed by the calculations of Ref. [22] where $U_c \approx 1.5W$. More weak Van Hove singularities are present for cubic lattices. One can see from Table I that the difference between our calculations and Hubbard-III results becomes rather strong for these lattices .

To conclude, we have demonstrated that a simple decoupling scheme enables one to reproduce the non-trivial spectrum structure in the half-filled Hubbard model. Our approach yields a qualitative agreement with the results of large-d approaches and QMC calculations. At the same time, this can be easily applied for arbitrary two- and three-dimensional lattices. In principle, the many-electron Hubbard operator method enables one to consider in a regular way the problem of electron structure of systems with the Hubbard splitting. Various types of slave boson and fermion representations combined with diagram techniques can be used to this end.

Since our approach starts from Hubbard’s subbands and includes large incoherent contributions, this does not reproduce properly the Fermi-liquid (FL) description of quasiparticle states. An account of low-energy spin and
charge dynamics would be useful to describe the electron spectrum picture in more detail. A possibility of the transition from FL to non-FL behavior which can take place near MIT should be also taken into account.

The work is supported in part by the Grant of RFFI No. 00-15-9654 (Support of Scientific Schools).

**TABLE I.** Critical values of metal-insulator transition for different bare DOS forms in the Hubbard-III approximation, $U^\text{H}_c$, “linearized” DMFT, $U^\text{L}_c$, and NSC and SC approximations (13) and (14), $U^{\text{NSC}}_c$ and $U^{\text{SC}}_c$.

| DOS                  | $U^\text{H}_c/W$ | $U^\text{L}_c/W$ | $U^{\text{NSC}}_c/W$ | $U^{\text{SC}}_c/W$ |
|----------------------|------------------|------------------|----------------------|---------------------|
| rectangular          | 1                | 1.73             | 0.99                 | 1.22                |
| semielliptic         | $\sqrt{3}/2 = 0.866$ | 1.5             | 0.87                 | 1.06                |
| Gaussian             | $\sqrt{3}/2 = 0.866$ | 1.5             | 0.87                 | 1.06                |
| square               | 0.866            | 1.5              | 0.87                 | 1.06                |
| simple cubic         | 0.707            | 1.22             | 0.76                 | 0.99                |
| bcc                  | 0.612            | 1.06             | 0.67                 | 0.92                |

**TABLE II.** Critical values for the metal-insulator transition for the Bethe lattice, $U^\text{B}_c$, and in the large-$d$ case, $U^\text{G}_c$, from different works.

| $U^\text{B}_c/W$ | $U^\text{G}_c/W$ | Refs. | Method            |
|------------------|------------------|-------|-------------------|
| 1.20             |                  | [14]  | QMC               |
| 1.64             |                  | [16]  | PT$^a$, QMC       |
| 1.262            | 1.273            | [17]  | MFT, IPT$^b$      |
| 1.45             | 1.273            | [18]  | QMC               |
| 1.47             | 1.45             | [19]  | MFT, QMC          |
| 0.67             |                  | [6]   | PSCA$^c$          |
| 1.2              |                  | [7]   | QMC               |
| 1.47             |                  | [20]  | DMFT              |
| 0.67             |                  | [21]  | improved Hubbard III |

$^a$Perturbation Theory.
$^b$Iterated Perturbation Theory.
$^c$Projective SC Approximation.
$^d$Numerical Renormalization Group.
FIG. 1. Density of states for the semielliptic DOS (a) approximation [14] (b) SC approximation [14].
FIG. 2. Density of states for the Gaussian DOS (a) approximation (13) (b) SC approximation (14).
FIG. 3. Density of states for the simple cubic lattice (a) approximation [13] (b) SC approximation [14].
FIG. 4. Density of states for the square lattice (a) approximation [13] (b) SC approximation [13].

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