Eur. Phys. J. B **38**, 563–570 (2004)
DOI: 10.1140/epjb/e2004-00153-6

THE EUROPEAN PHYSICAL JOURNAL B

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

V.Yu. Irkhin[a] and A.V. Zarubin

Institute of Metal Physics, S.Kovalevskay str. 18, 620219 Ekaterinburg, Russia

Received 5 January 2004
Published online 8 June 2004 –

Abstract. 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 in the paramagnetic phase 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.

PACS. 71.10.Fd Lattice fermion models (Hubbard model, etc.) – 71.27.+a Strongly correlated electron systems; heavy fermions – 71.30.+h Metal-insulator transitions and other electronic transitions

1 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. Previously, 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., Ref. [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 references [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 reference [8]. The problem of MIT within this approach was treated in reference [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 Section 2, the decoupling scheme with account of the Fermi excitations is developed. In Section 3, we present the results of numerical calculations and carry out a comparison with previous works.

[a] e-mail: valentin.irkhin@imp.uran.ru

2 The decoupling scheme

We consider the Hubbard model with the electron concentration $n = 1$ (the half-filled case) in the paramagnetic state. The corresponding Hamiltonian reads

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} t_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$, $c^{\dagger}_{i\sigma}$ and $c^{\dagger}_{\mathbf{k}\sigma}$ are the one-electron operators in the Wannier and quasimomentum representation. We pass to the Hubbard X-operators

$$X_i^{\alpha\beta} = |i\alpha\rangle\langle i\beta|, \quad X_i^{\alpha\beta} X_i^{\gamma\varepsilon} = \delta_{\beta\gamma} X_i^{\alpha\varepsilon}, \quad \sum_{\alpha} X_i^{\alpha\alpha} = 1, \tag{2}$$

so that

$$c^{\dagger}_{i\sigma} = \sum_{\alpha,\beta} \langle i\alpha | c^{\dagger}_{i\sigma} | i\beta \rangle X_i^{\alpha\beta} = X_i^{\sigma 0} + \sigma X_i^{2-\sigma}. \tag{3}$$

Then the interaction Hamiltonian takes a diagonal form and we obtain

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} t_{\mathbf{k}} (X^{\sigma 0}_{-\mathbf{k}} + \sigma X^{2-\sigma}_{-\mathbf{k}})(X^{0\sigma}_{\mathbf{k}} + \sigma X^{-\sigma 2}_{\mathbf{k}}) + U \sum_{i} X_i^{22}. \tag{4}$$

Using (3) we have for the one-electron anticommutator retarded Green's function

$$G_{\mathbf{k}\sigma}(E) = \langle\langle c_{\mathbf{k}\sigma} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E = \langle\langle X^{0\sigma}_{\mathbf{k}} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E + \sigma \langle\langle X^{-\sigma 2}_{\mathbf{k}} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E. \tag{5}$$

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

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

for the pair of the Green's functions in the right-hand side of (5). Using (2) we obtain in the non-magnetic case

$$(E + U/2)\langle\langle X^{0\sigma}_{\mathbf{k}} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E = \frac{1}{2}(1 + t_{\mathbf{k}} \langle\langle c_{\mathbf{k}\sigma} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E) + \sum_{\mathbf{q}} t_{\mathbf{q}} \langle\langle (\delta(X^{00}_{\mathbf{k}-\mathbf{q}}) + \delta(X^{\sigma\sigma}_{\mathbf{k}-\mathbf{q}})) c_{\mathbf{q}\sigma} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E + \sum_{\mathbf{q}} t_{\mathbf{q}} \langle\langle X^{-\sigma\sigma}_{\mathbf{k}-\mathbf{q}} c_{\mathbf{q}-\sigma} + \sigma c^{\dagger}_{\mathbf{q}-\sigma} X^{02}_{\mathbf{k}+\mathbf{q}} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E, \tag{6}$$

$$\sigma(E - U/2)\langle\langle X^{-\sigma 2}_{\mathbf{k}} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E = \frac{1}{2}(1 + t_{\mathbf{k}} \langle\langle c_{\mathbf{k}\sigma} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E) + \sum_{\mathbf{q}} t_{\mathbf{q}} \langle\langle (\delta(X^{-\sigma-\sigma}_{\mathbf{k}-\mathbf{q}}) + \delta(X^{22}_{\mathbf{k}-\mathbf{q}})) c_{\mathbf{q}\sigma} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E - \sum_{\mathbf{q}} t_{\mathbf{q}} \langle\langle X^{-\sigma\sigma}_{\mathbf{k}-\mathbf{q}} c_{\mathbf{q}-\sigma} + \sigma c^{\dagger}_{\mathbf{q}-\sigma} X^{02}_{\mathbf{k}+\mathbf{q}} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E, \tag{7}$$

where $\delta A = A - \langle A \rangle$ is the fluctuation of the operator. Solving the system (6), (7) we derive

$$G_{\mathbf{k}\sigma}(E) = G^0_{\mathbf{k}}(E)(1 - \frac{U}{E} \Gamma_{\mathbf{k}\sigma}(E)), \tag{8}$$

$$\Gamma_{\mathbf{k}\sigma}(E) = \sum_{\mathbf{q}} t_{\mathbf{q}} \langle\langle \delta(X^{00}_{\mathbf{k}-\mathbf{q}} + X^{\sigma\sigma}_{\mathbf{k}-\mathbf{q}}) c_{\mathbf{q}\sigma} + X^{-\sigma\sigma}_{\mathbf{k}-\mathbf{q}} c_{\mathbf{q}-\sigma} + \sigma c^{\dagger}_{\mathbf{q}-\sigma} X^{02}_{\mathbf{k}+\mathbf{q}} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E. \tag{9}$$

Here

$$G^0_{\mathbf{k}}(E) = \frac{1}{F_0(E) - t_{\mathbf{k}}}, \quad F_0(E) = E - \frac{U^2}{4E} \tag{10}$$

is the Green's function of the Hubbard-I approximation (which plays the role of a mean-filed 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 (10)

$$E_{\mathbf{k}1,\,2} = \frac{1}{2}(t_{\mathbf{k}} \pm \varepsilon_{\mathbf{k}}), \quad \varepsilon_{\mathbf{k}} = \sqrt{U^2 + t^2_{\mathbf{k}}}.$$

The Green's function $\Gamma_{\mathbf{k}\sigma}(E)$ describes fluctuation corrections. The corresponding collective excitations are described by spin and charge operators.

$$S^{\sigma}_{\mathbf{q}} = X^{\sigma-\sigma}_{\mathbf{q}}, \quad S^{z}_{\mathbf{q}} = \frac{1}{2}(X^{++}_{\mathbf{q}} - X^{--}_{\mathbf{q}}),$$
$$\rho^{+}_{\mathbf{q}} = X^{20}_{\mathbf{q}}, \quad \rho^{z}_{\mathbf{q}} = \frac{1}{2}(X^{22}_{\mathbf{q}} - X^{00}_{\mathbf{q}}).$$

Now 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.,

$$\langle\langle X^{-\sigma\sigma}_{\mathbf{k}-\mathbf{q}} c_{\mathbf{q}-\sigma} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E \to \frac{1}{2} \langle\langle \{X^{-\sigma\sigma}_{\mathbf{k}-\mathbf{q}}, c_{\mathbf{q}-\sigma}\} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E = \frac{1}{2} \langle\langle X^{-\sigma\sigma}_{\mathbf{k}-\mathbf{q}} c_{\mathbf{q}-\sigma} + c_{\mathbf{q}-\sigma} X^{-\sigma\sigma}_{\mathbf{k}-\mathbf{q}} | c^{\dagger}_{\mathbf{k}\sigma} \rangle\rangle_E.$$

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

$$t_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \to \frac{1}{2} t_{\mathbf{k}} (c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - c_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}\sigma}).$$

Then we obtain for the transverse spin fluctuation contribution

$$(E^2 - U^2/4 - Et_{\mathbf{q}})\langle\langle \frac{1}{2}\{X^{-\sigma\sigma}_{\mathbf{k}-\mathbf{q}}, c_{\mathbf{q}-\sigma}\}|c^\dagger_{\mathbf{k}\sigma}\rangle\rangle_E =$$
$$(E+U/2)(t_{\mathbf{q}}-t_{\mathbf{k}})(f_{\mathbf{q}}-\frac{1}{2})G_{\mathbf{k}\sigma}(E)$$
$$-U(t_{\mathbf{k}}\langle X^{-\sigma\sigma}_{\mathbf{k}-\mathbf{q}}X^{\sigma-\sigma}_{-\mathbf{k}+\mathbf{q}}\rangle + (t_{\mathbf{q}}-t_{\mathbf{k}})\langle\frac{1}{2}[X^{-\sigma 0}_{-\mathbf{q}}, X^{0-\sigma}_{\mathbf{q}}]$$
$$-\sigma X^{2\sigma}_{-\mathbf{q}}X^{0-\sigma}_{\mathbf{q}}\rangle G_{\mathbf{k}\sigma}(E) - (E+U/2)(f_{\mathbf{q}}-\frac{1}{2})$$
$$+U\langle\frac{1}{2}[X^{-\sigma 0}_{-\mathbf{q}}, X^{0-\sigma}_{\mathbf{q}}] - \sigma X^{2\sigma}_{-\mathbf{q}}X^{0-\sigma}_{\mathbf{q}} - X^{-\sigma\sigma}_{\mathbf{k}-\mathbf{q}}X^{\sigma-\sigma}_{-\mathbf{k}+\mathbf{q}}\rangle.$$

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

$$\sigma(E^2 - U^2/4 - Et_{\mathbf{q}})\langle\langle \frac{1}{2}\{c^\dagger_{\mathbf{q}-\sigma}X^{02}_{\mathbf{k}+\mathbf{q}}\}|\, c^\dagger_{\mathbf{k}\sigma}\rangle\rangle_E =$$
$$(E+U/2)(t_{\mathbf{q}}+t_{\mathbf{k}})(f_{\mathbf{q}}-\frac{1}{2})G_{\mathbf{k}\sigma}(E)$$
$$+U(t_{\mathbf{k}}\langle X^{20}_{-\mathbf{k}-\mathbf{q}}X^{02}_{\mathbf{k}+\mathbf{q}}\rangle + (t_{\mathbf{q}}+t_{\mathbf{k}})\langle\sigma X^{2\sigma}_{-\mathbf{q}}X^{0-\sigma}_{\mathbf{q}}$$
$$+\frac{1}{2}[X^{2\sigma}_{-\mathbf{q}}, X^{\sigma 2}_{\mathbf{q}}]\rangle)G_{\mathbf{k}\sigma}(E) + (E+U/2)(f_{\mathbf{q}}-\frac{1}{2})$$
$$-U\langle\frac{1}{2}[X^{2\sigma}_{-\mathbf{q}}, X^{\sigma 2}_{\mathbf{q}}] - \sigma X^{2\sigma}_{-\mathbf{q}}X^{0-\sigma}_{\mathbf{q}} - X^{20}_{-\mathbf{k}-\mathbf{q}}X^{02}_{\mathbf{k}+\mathbf{q}}\rangle.$$

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

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

$$\langle S^\sigma_{-\mathbf{q}}S^{-\sigma}_{\mathbf{q}}\rangle = 2\langle S^z_{-\mathbf{q}}S^z_{\mathbf{q}}\rangle = \langle X^{\sigma\sigma}\rangle,$$
$$\langle \rho^\sigma_{-\mathbf{q}}\rho^{-\sigma}_{\mathbf{q}}\rangle = 2\langle \rho^z_{-\mathbf{q}}\rho^z_{\mathbf{q}}\rangle = \langle X^{22}\rangle = \langle X^{00}\rangle. \qquad (11)$$

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. The 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 is rather difficult and can be made in higher orders in $1/z$. This may lead to a change in details of the MIT picture. Roughly speaking, we work above the magnetic ordering temperature. The latter quantity is always small in comparison with the bandwidth and Hubbard parameter U, and is known to be low (of order of $10 \div 100$ K) in most transition-metal compounds of interest.

Taking into account (11) we can use the sum rule in (2) to obtain

$$G_{\mathbf{k}}(E) = \frac{a(E)}{b(E) - a(E)t_{\mathbf{k}}} = \frac{1}{F(E) - t_{\mathbf{k}}},$$
$$F(E) = \frac{b(E)}{a(E)}, \qquad (12)$$

$$a(E) = 1 + \frac{3}{4}\frac{U^2}{E^2}\sum_{\mathbf{q}} t_{\mathbf{q}}\frac{1}{F_0(E) - t_{\mathbf{q}}}$$
$$+\frac{2U}{E}\sum_{\mathbf{q}} t_{\mathbf{q}}\frac{f_{\mathbf{q}}}{F_0(E) - t_{\mathbf{q}}}, \qquad (13a)$$

$$b(E) = F_0(E) + \frac{2U}{E}\sum_{\mathbf{q}} t^2_{\mathbf{q}}\frac{f_{\mathbf{q}}}{F_0(E) - t_{\mathbf{q}}}. \qquad (13b)$$

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

$$\langle c^\dagger_{\mathbf{q}\sigma}X^{0\sigma}_{\mathbf{q}}\rangle = \frac{1}{2\varepsilon_{\mathbf{q}}}[(E_{\mathbf{q}1} - U)f(E_{\mathbf{q}1})$$
$$-(E_{\mathbf{q}2} - U)f(E_{\mathbf{q}2})],$$
$$\langle c^\dagger_{\mathbf{q}\sigma}X^{-\sigma 2}_{\mathbf{q}}\rangle = \frac{-\sigma}{2\varepsilon_{\mathbf{q}}}[E_{\mathbf{q}1}f(E_{\mathbf{q}1}) - E_{\mathbf{q}2}f(E_{\mathbf{q}2})],$$
$$f_{\mathbf{q}} \equiv \langle c^\dagger_{\mathbf{q}\sigma}c_{\mathbf{q}\sigma}\rangle = \frac{1}{\varepsilon_{\mathbf{q}}}[(E_{\mathbf{q}1} - U/2)f(E_{\mathbf{q}1})$$
$$-(E_{\mathbf{q}2} - U/2)f(E_{\mathbf{q}2})].$$

Due to the symmetry of the bare band, we have

$$\sum_{\mathbf{q}} f(E_{\mathbf{q},2})\Phi(t_{\mathbf{q}}) = \sum_{\mathbf{q}}[1 - f(E_{\mathbf{q}1})]\Phi(-t_{\mathbf{q}}).$$

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

To obtain the self-consistent (SC) approximation we replace in (10) the Hubbard-I inverse locators by the exact ones,

$$G^0_{\mathbf{q}}(E) = \frac{1}{F_0(E) - t_{\mathbf{q}}} \to G_{\mathbf{q}}(E) = \frac{1}{F(E) - t_{\mathbf{q}}},$$

and the Fermi functions $f_{\mathbf{q}}$ by the exact occupation numbers $n_{\mathbf{q}}$, according to the spectral representation,

$$n_{\mathbf{q}} = -\frac{1}{\pi}\int dE f(E)\Im G_{\mathbf{q}}(E).$$

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

$$a(E) = 1 + \frac{3}{4}\frac{U^2}{E^2}\sum_{\mathbf{q}} t_{\mathbf{q}}G_{\mathbf{q}}(E) + \frac{2U}{E}\sum_{\mathbf{q}} t_{\mathbf{q}}G_{\mathbf{q}}(E)n_{\mathbf{q}}, \qquad (14a)$$

$$b(E) = F_0(E) + \frac{2U}{E}\sum_{\mathbf{q}} t^2_{\mathbf{q}}G_{\mathbf{q}}(E)n_{\mathbf{q}}. \qquad (14b)$$

Table 1. Critical values of metal-insulator transition for different bare DOS forms in the Hubbard-III approximation, $U_c^{\rm H}$, "linearized" DMFT, $U_c^{\rm L}$, and NSC and SC approximations (13) and (14), $U_c^{\rm NSC}$ and $U_c^{\rm SC}$.

DOS	$U_c^{\rm H}/W$	$U_c^{\rm L}/W$	$U_c^{\rm NSC}/W$	$U_c^{\rm SC}/W$
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

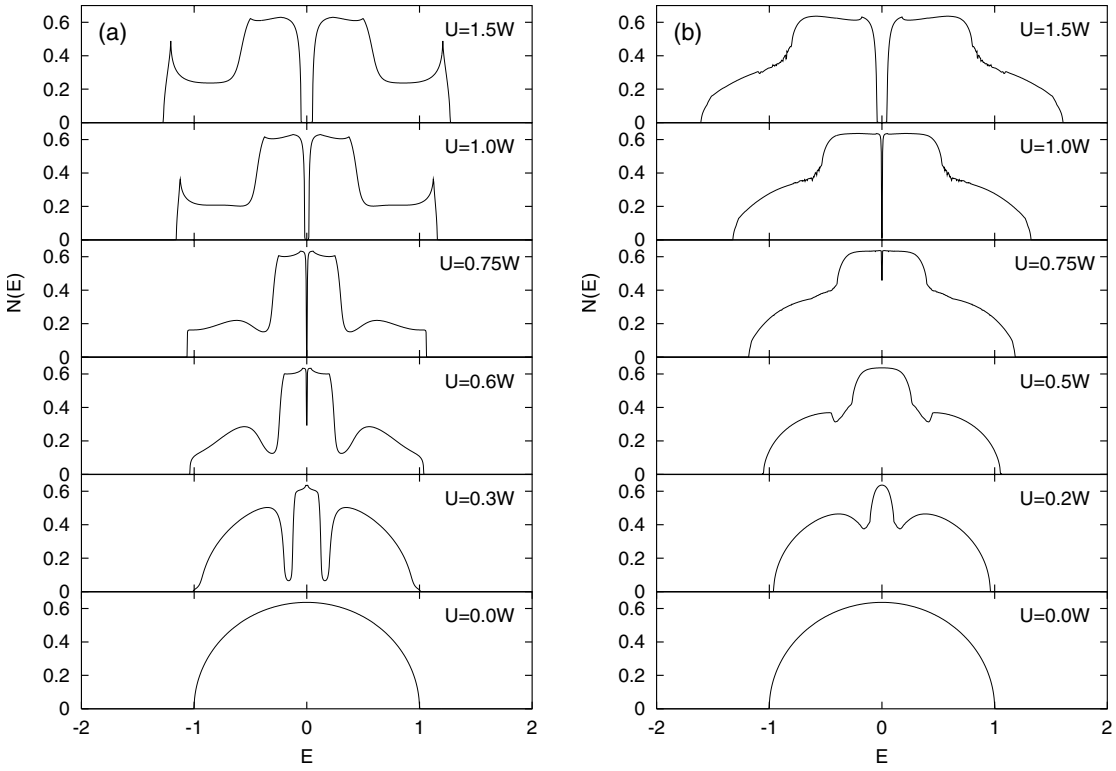

Fig. 1. Density of states for the semielliptic DOS (a) approximation (13), (b) SC approximation (14).

The approximation (14), as well as the standard Hubbard-III approximation, does not result in a violation of analytical properties of the Green's functions. Note that such a drawback is present for the simplest self-consistency scheme considered in reference [8] [see Eq. (32) of that paper], which does not use the locator representation.

3 Results and discussion

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

$$N(E) = -\frac{1}{\pi}\Im \sum_{\mathbf{k}} G_{\mathbf{k}}(E).$$

The results for the approximations (13) and (14) are shown in Figures 1–4, and the critical values for MIT are given in Table 1. The numerical calculations 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

$$N(E) = \frac{4}{\pi W}\sqrt{1 - \Big(\frac{2E}{W}\Big)^2},$$

(W is the bare bandwidth), the rectangular DOS, and the Gaussian DOS

$$N(E) = \frac{4}{\sqrt{2\pi}W} \exp\Big(-2\Big(\frac{2E}{W}\Big)^2\Big)$$

which corresponds to the hypercubic lattice in the large-d limit. The Gaussian DOS does not have band edges, so that the parameter W is determined from the second DOS

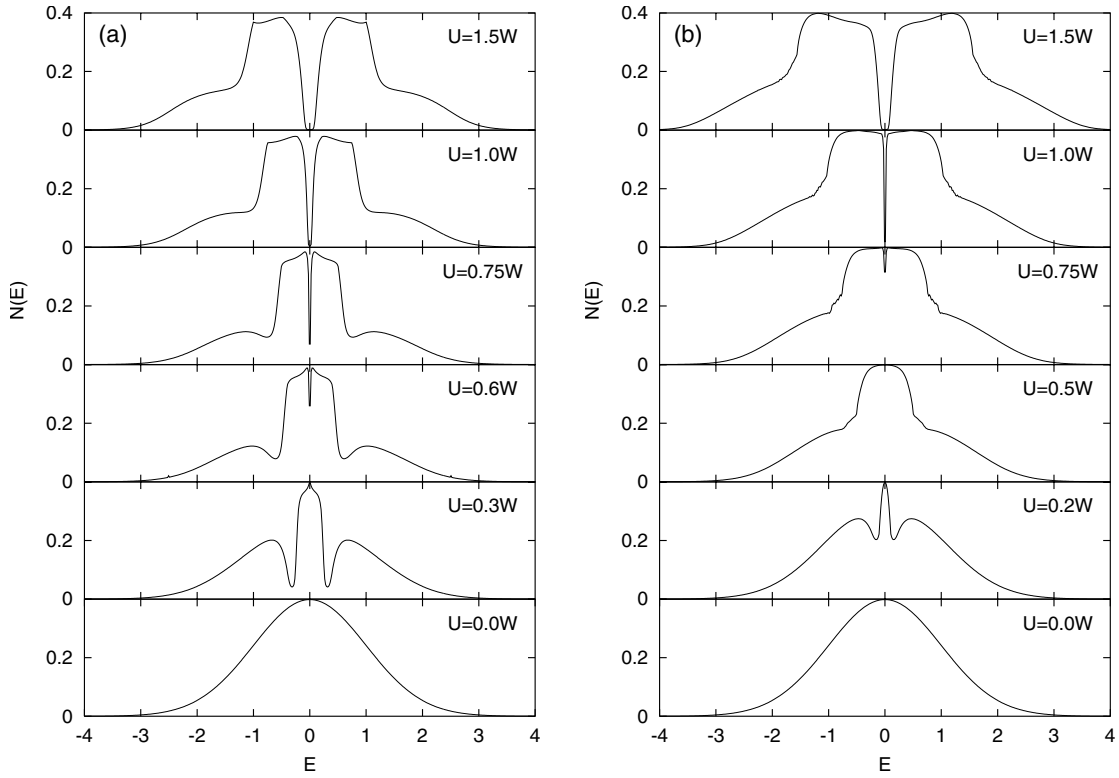

Fig. 2. Density of states for the Gaussian DOS (a) approximation (13), (b) SC approximation (14).

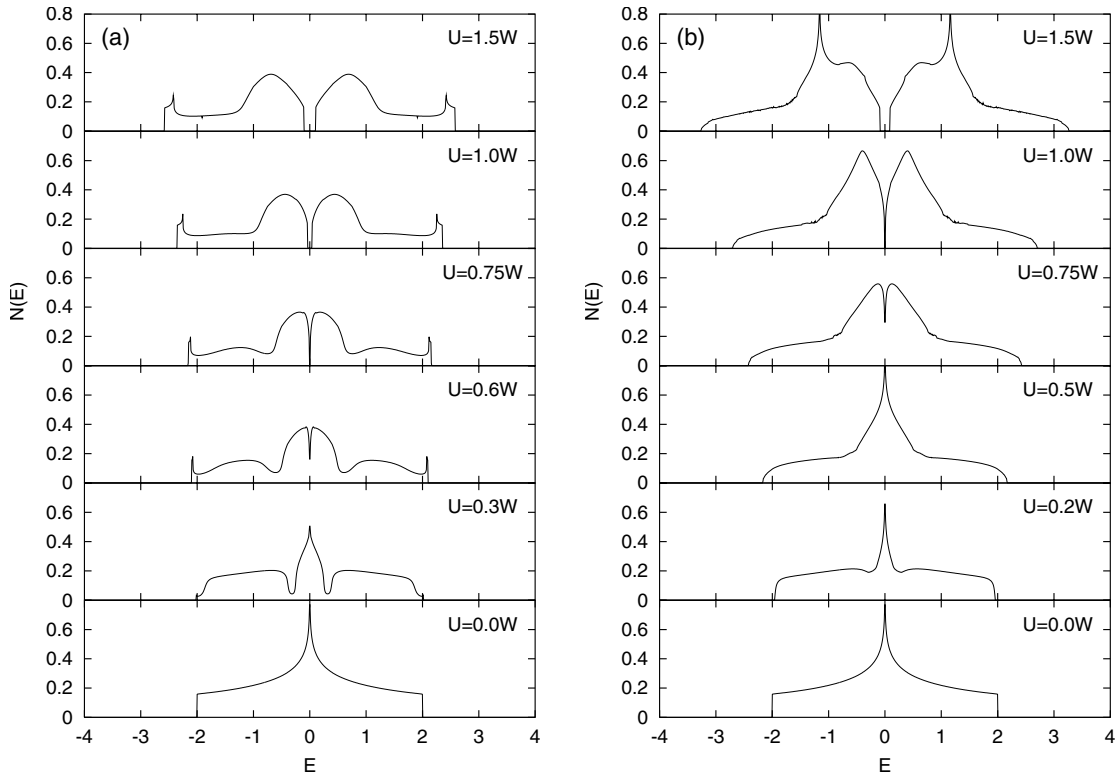

Fig. 3. Density of states for the square lattice (a) approximation (13), (b) SC approximation (14).

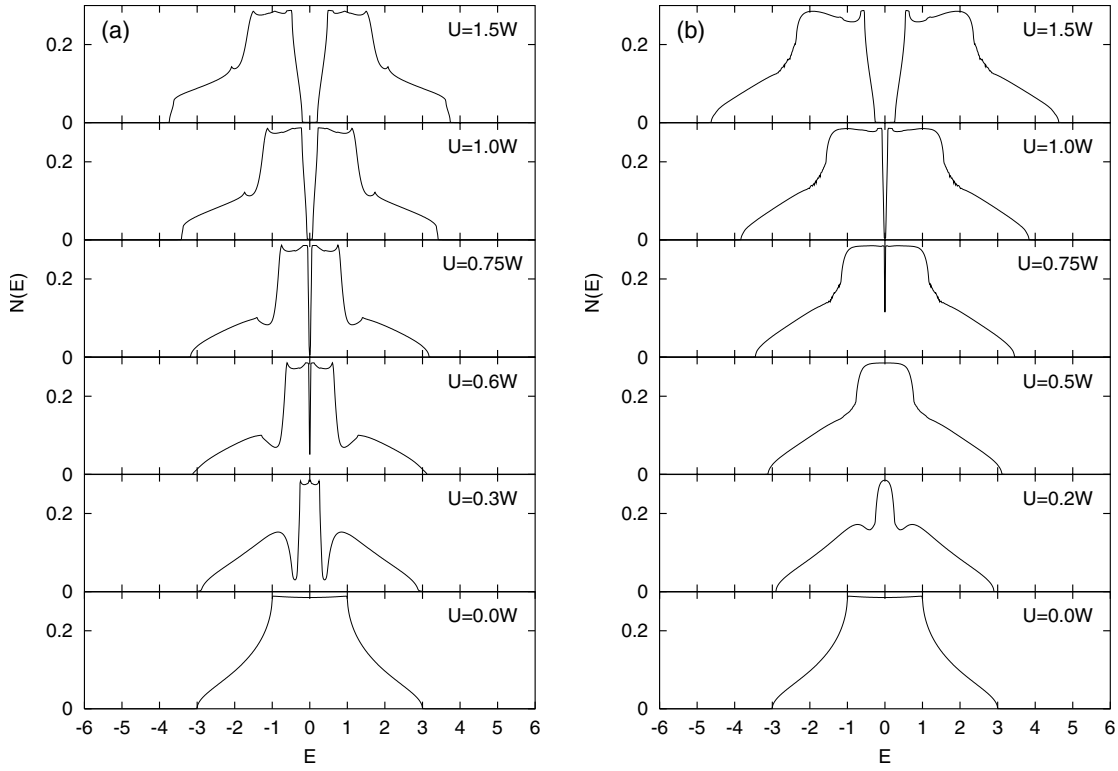

Fig. 4. Density of states for the simple cubic lattice (a) approximation (13), (b) SC approximation (14).

Table 2. Critical values for the metal-insulator transition for the Bethe lattice, $U^{\rm B}_{\rm c1,\,2}$, and for the hypercubic lattice in the large-d case, $U^{\rm G}_{\rm c1,\,2}$, from different works.

$U^{\rm B}_{\rm c1}/W$	$U^{\rm B}_{\rm c2}/W$	$U^{\rm G}_{\rm c1}/W$	$U^{\rm G}_{\rm c2}/W$	Refs.	Method
		1.202		[14]	QMC
		1.24		[15]	QMC
1.308	1.591	1.273	1.662	[16]	MFT, IPT
		1.273		[21]	QMC
1.3	1.64			[5]	MFT, QMC
1.25				[6]	QMC
1.25	1.47	1.15	1.45	[22,19]	DMFT, NRG, IPT
1.195	1.47			[17]	NRG
0.67				[7]	improved Hubbard III

Note: PT is Perturbation Theory, IPT is Iterated Perturbation Theory, NRG is Numerical Renormalization Group.

moment,

$$W = 4\sqrt{\mu_2}, \quad \mu_2 = \int E^2 N(E) dE.$$

Then the quantity μ_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 $U_{\rm c}^{\rm NSC}$ is rather small. The "false" singularities at the edges of the Hubbard-I bands occur for large U in our NSC approximation (see the discussion in Ref. [8]).

The critical value for MIT in the standard Hubbard-III approximation [2] for an arbitrary bare DOS is given by [9]

$$U_{\rm c}^{\rm H} = 2\sqrt{3\mu_2}. \tag{15}$$

The critical value in the SC approximation (14) is changed somewhat in comparison with the Hubbard-III result (see Tab. 1). Unlike reference [7], where the critical value was decreased by fluctuations, $U_{\rm c}/W = 0.67$ for the Bethe lattice, our approach yields an opposite tendency, in agreement with the results of the QMC calculations at finite temperatures, $U_{\rm c}/W \simeq 1$ (see Tab. 2). Within the "linearized" DMFT [13], an analytical expression $U_{\rm c}$ can be obtained, which exceeds the Hubbard-III value,

$$U_{\rm c}^{\rm L} = \sqrt{3} U_{\rm c}^{\rm H} = 6\sqrt{\mu_2}. \tag{16}$$

As follows from comparison with Table 2, 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 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 reference [7]. At small U, a three-peak structure can be seen in Figures 1–4, 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. Note that a pseudogap develops in the metallic phase near MIT in our picture, as well as in a number of other approaches (see, e.g., Refs. [14,15]). 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. A consistent treatment of the damping is a difficult problem, so that early DMFT calculations were performed at low temperatures; approximate solvers such as iterated perturbation theory (IPT) do not also deal correctly with this aspect [16]. On the other hand, NRG calculations demonstrate that DMFT does yield damping at $T \to 0$ [17].

In the case of square lattice the situation is more complicated than for the Bethe lattice 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 reference [18] where $U_c \simeq 1.5W$. More weak Van Hove singularities are present for cubic lattices. One can see from Table 1 that the difference between our calculations and Hubbard-III results becomes rather strong for these lattices.

In the metallic phase, the electron self-energy $\Sigma(E) = E - F(E)$ demonstrates in our theory the standard Fermi-liquid behavior: $\Re\Sigma(E \to 0) \propto E$, $\Im\Sigma(E \to 0) \propto E^2$ (Fig. 5); note that a consistent account of spin dynamics may be important for details of this behavior. The corresponding U-dependence of the quasiparticle weight (the Green's function residue),

$$Z = \left(1 - \left.\frac{\partial \Re\Sigma(E)}{\partial E}\right|_{E=0}\right)^{-1}, \qquad (17)$$

is shown in Figure 6. This quantity vanishes at $U \to U_c$, i.e., at closing the energy gap.

As confirm modern calculations, especially in the framework of the DMFT approach, two phase transitions with increasing U take place at very low temperatures [16,19]. The first transition corresponds to the first critical value, U_{c1}, at which the gap closes and the other one at a higher coupling, U_{c2}, at which the metallic solution disappears (i.e., the quasiparticle weight vanishes). Rather accurate values of both U_{c1} and U_{c2} for hypercubic and Bethe lattices were determined by recent methods, in particular by NRG method [13,16,17,19] (see Tab. 2). Since our consideration does not describe properly low-temperature behavior, we do not treat this problem in detail. Thus the metal-insulator transition in our theory

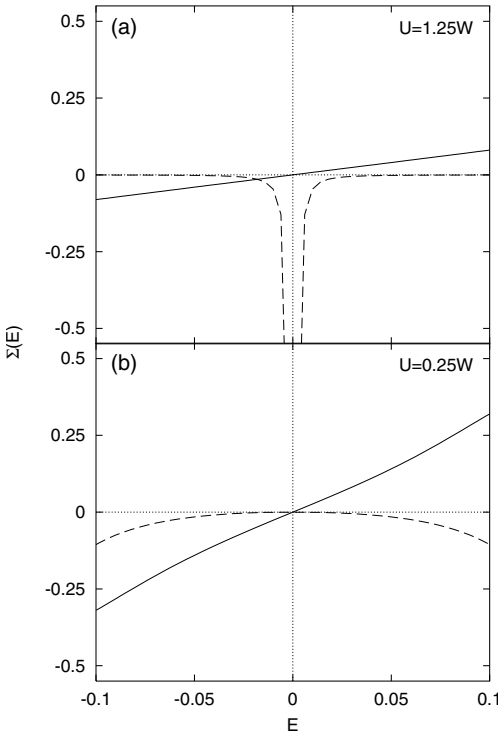

Fig. 5. Energy dependence of the electron self-energy $\Sigma(E)$ near the Fermi level (real part: solid line, imaginary part: dashed line) in SC approximation for the semielliptic bare DOS (a) $U/W = 1.25 > U_c/W$ (insulator phase), (b) $U/W = 0.25 < U_c/W$ (metallic phase).

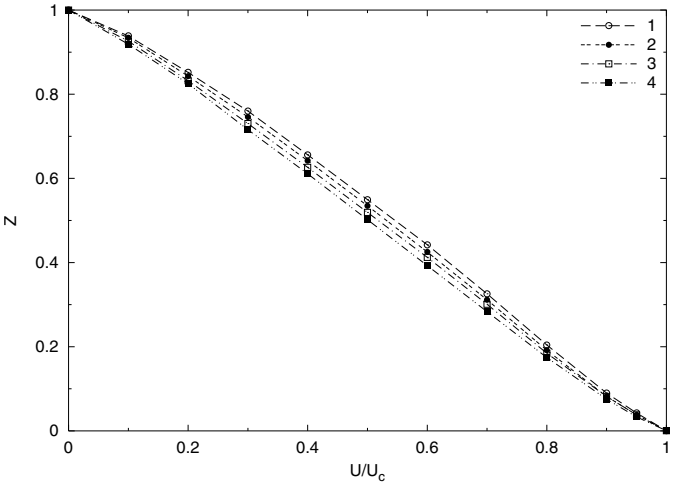

Fig. 6. The dependence of the quasiparticle weight Z vs. U for the semielliptic DOS (line 1), Gaussian DOS (line 2), square lattice (line 3), and simple cubic lattice (line 4) in SC approximation (14).

(as well as in classical MIT considerations in the Hubbard model) should be compared to that associated with U_{c1}.

It should be stressed once more that the picture considered corresponds to MIT in a paramagnetic phase. On the other hand, in the ground antiferromagnetic state the half-filled Hubbard model on a square, simple cubic and bcc lattices is an insulator for arbitrarily small U (see, e.g., Ref. [20]). Such an instability occurs because of the

nesting condition for the electron spectrum ($t_{\mathbf{k}+\mathbf{Q}} = -t_{\mathbf{k}}$ with $\mathbf{Q} = (\pi, \pi, \pi)$). However, the corresponding energy gap is exponentially small, so that such effects can be neglected at not too low temperatures.

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 a transition from FL to non-FL behavior which can take place near MIT (the existence of the second phase transition) should be also taken into account.

The work is supported in part by the Grant No. 747.2003.2 (Support of Scientific Schools) from the Russian Basic Research Foundation and by Program of General Physics Division, Grant N15.

References

1. J. Hubbard, Proc. Roy. Soc. A **276**, 238 (1963)
2. J. Hubbard, Proc. Roy. Soc. A **281**, 401 (1964)
3. A. Georges, G. Kotliar, Phys. Rev. B **45**, 6479 (1992); X.Y. Zhang, C.M. Zhang, Phys. Rev. B **49**, 7929 (1994); F.J. Ohkawa, J. Phys. Soc. Jpn **61**, 1615 (1992)
4. A. Georges, G. Kotliar, W. Krauth, M.J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996)
5. M.J. Rozenberg, X.Y. Zhang, G. Kotliar, Phys. Rev. Lett. **69**, 1236 (1992); M.J. Rozenberg, G. Kotliar, X.Y. Zhang, Phys. Rev. B **49**, 10181 (1994)
6. J. Schlipf, M. Jarrell, P.G.J. van Dongen, N. Blümer, S. Kehrein, Th. Pruschke, D. Vollhardt, Phys. Rev. Lett. **82**, 4890 (1999)
7. H.-G. Luo, S.-J. Wang, Phys. Rev. B **61**, 5158 (2000)
8. A.O. Anokhin, V.Yu. Irkhin, Phys. Status Solidi (b) **165**, 129 (1991)
9. A.O. Anokhin, V.Yu. Irkhin, M.I. Katsnelson, J. Phys.: Condens. Matter **3**, 1475 (1991)
10. V.Yu. Irkhin, A.V. Zarubin, Eur. Phys. J. B **16**, 463 (2000)
11. J. Hubbard, Proc. Roy. Soc. A **285**, 542 (1965)
12. V.Yu. Irkhin, Yu.P. Irkhin, Phys. Status Solidi (b) **183**, 9 (1994); `arXiv:cond-mat/9812072`
13. R. Bulla, M. Potthoff, Eur. Phys. J. B **13**, 257 (2000); Y. Ōno, R. Bulla, A.C. Hewson, Eur. Phys. J. B, **19**, 375 (2001); Y. Ōno, R. Bulla, A.C. Hewson, M. Potthoff, Eur. Phys. J. B **22**, 283 (2001); M. Potthoff, `arXiv:cond-mat/0306278`
14. M. Jarrell, Th. Pruschke, Z. Phys. B **90**, 187 (1993); M. Jarrell, Phys. Rev. Lett. **69**, 168 (1992)
15. Th. Pruschke, D.L. Cox, M. Jarrell, Phys. Rev. B **47**, 3553 (1993)
16. A. Georges, W. Krauth, Phys. Rev. B **48**, 7167 (1993)
17. R. Bulla, T.A. Costi, D. Vollhardt, Phys. Rev. B **64**, 045103 (2001)
18. F. Mancini, Europhys. Lett. **50**, 229 (2000)
19. R. Bulla, Adv. Solid State Phys. **40**, 169 (2000)
20. M.I. Katsnelson, V.Yu. Irkhin, J. Phys. C **17**, 4291 (1984)
21. M. Caffarel, W. Krauth, Phys. Rev. Lett. **72**, 1545 (1994)
22. R. Bulla, Phys. Rev. Lett. **83**, 136 (1999)