Mott transitions in correlated electron systems with orbital degrees of freedom

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Mott metal-insulator transitions in an M-fold orbitally degenerate Hubbard model are studied by means of a generalization of the linearized dynamical mean-field theory. The method allows for an efficient and reliable determination of the critical interaction $U_{\rm c}$ for any integer filling n and different M at zero temperature. For half-filling a linear dependence of $U_{\rm c}$ on M is found. Inclusion of the (full) Hund's rule exchange J results in a strong reduction of $U_{\rm c}$. The transition turns out to change qualitatively from continuous for $J = 0$ to discontinuous for any finite J. This result is confirmed using the exact-diagonalization method for $M = 2$.

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I. INTRODUCTION

The Mott metal-insulator transition (MIT) has been the subject of numerous experimental and theoretical investigations over the past decades[1–3]. As a transition from a paramagnetic metal to a paramagnetic insulator that is driven by the competition between the conduction electrons' kinetic energy and their mutual Coulomb repulsion, the Mott MIT represents a prime example for a quantum-phase transition. Realizations of the Mott transition can be found in different 3d transition-metal oxides[1,2] as well as in alkali-doped Fullerides[4,5], for example. Its description is a challenging task for many-body theory.

The minimal model to describe the Mott transition is the Hubbard model[6] which in its simplest form contains the local Coulomb interaction between the electrons in a conduction band formed by a *single* orbital only. The investigation of such a single-band model might be justified in some cases, in particular as an effective model for low-energy properties. A consistent description of the experimental observations for the above-mentioned systems, however, certainly requires the use of more realistic models which include orbital degrees of freedom, possible crystal field splittings, etc.

Theoretical advances in the past decade – mainly due to the development of the dynamical mean-field theory (DMFT)[7,8] – have led to an increased understanding of multi-orbital Hubbard models. Recent investigations have either concentrated on fundamental questions such as the nature of the Mott MIT as a function of orbital degeneracy[9–16] or, within the so-called LDA+DMFT approach[17], on a realistic description of the transition.

Nevertheless, there are still no reliable DMFT results for the zero-temperature ($T = 0$) Mott transition in general multi-band models: Numerical methods to solve the DMFT equations are either restricted to fairly large temperatures (quantum Monte-Carlo approach, QMC) or have not yet been extended to the multi-band case (numerical renormalization-group method, NRG). Additionally, due to the sign problem within the QMC approach only a simplified exchange part of the Coulomb interaction can be taken into account[13,18]. The exact-diagonalization method (ED) is restricted to rather small system sizes, and data are available for $M \leq 2$ orbitals only[16]. The M dependence of the critical interaction strength $U_{\rm c}$ for different integer fillings n is particularly interesting. Detailed results for $U_{\rm c}$ as a function of M and n are available from the Gutzwiller approximation and from a slave-boson approach[9,11]. Numerical DMFT-QMC calculations have been performed for $M \leq 3$[12,13]. Remarkably, in the limit of large orbital degeneracy $M \to \infty$ an analytical treatment of the DMFT becomes possible for the MIT[15]. A scaling $U_{\rm c} = U_{\rm c,2} \propto M$ for the actual transition is found while $U_{\rm c,1} \propto \sqrt{M}$ is obtained for the critical interaction where the insulating solution breaks down[15]. This is consistent with the linear dependence for large M found in Refs. 9, 11 and with the square-root dependence reported in Ref. 5. However, there is still a need for a DMFT method which works at $T = 0$ and which allows for an efficient and reliable determination of $U_{\rm c}$ for arbitrary n and M and for a model including the full exchange interaction.

Here we present and apply a proper multi-band generalization of the so-called linearized DMFT (L-DMFT)[19] which is a simple but rather successful technique that originally was developed for the critical regime of the Mott MIT in the single-band model. Within the L-DMFT the lattice problem is mapped onto an Anderson impurity model with a single bath site only by considering a simplified self-consistency condition just at the critical point. The approach can be considered to be the simplest non-trivial variant of the more systematic projective self-consistent method (PSCM) by Moeller et al[20]. It allows for extremely fast numerical calculations or even analytical results to estimate the critical parameters. Extensions have been considered for the (Mott-Hubbard or charge-transfer) MITs in a d-p model[21], for a quantum-critical point in the periodic Anderson model[22], and for

the $M = 2$ degenerate Hubbard model at half-filling and $J = 0$[16]. Furthermore, a general two-site DMFT[23] has been developed which reduces to the L-DMFT at the MIT but is not restricted to the critical point. An application to multi-band systems is likewise possible but has not yet been considered.

As concerns effective single-band models, the linearized DMFT has been tested extensively by comparing with numerical results from the full DMFT. For the standard Hubbard model[19,24] but also for different thin-film and semi-infinite surface geometries[25] as well as for the *d-p* model[26] a remarkable agreement has been found: Detailed trends of U_c as a function of electronic model parameters and as a function of parameters characterizing the lattice geometry are predicted reliably. For quantitative estimates errors of the order of a few percent have to be tolerated.

As it is demonstrated here, a straightforward extension of the method to multi-band systems is possible. We expect the L-DMFT to be a fast but reliable tool in this case as well since the effective impurity model includes the complete atomic part and the self-consistently determined bath with the complete degeneracy (although restricted to a single site only). Furthermore, the reliability of the L-DMFT for the multi-band case is checked by comparing with different fully numerical DMFT techniques whenever results are available. All DMFT calculations discussed in this paper were performed on a Bethe lattice with $t^2 = 1$, corresponding to bandwidth of 4.

II. MODEL AND LINEARIZED DMFT

We consider a multi-band Hubbard-type model $H = H_0 + H_1$ including an intra-orbital hopping

$$H_0 = \sum_{ij\alpha\sigma} t_{ij} c^\dagger_{i\alpha\sigma} c_{j\alpha\sigma} \tag{1}$$

and the direct and the exchange part of the on-site Coulomb interaction:

$$H_1 = \frac{1}{2} \sum_{i\alpha\alpha'\sigma\sigma'} U_{\alpha\alpha'}\, c^\dagger_{i\alpha\sigma} c^\dagger_{i\alpha'\sigma'} c_{i\alpha'\sigma'} c_{i\alpha\sigma} + \frac{1}{2} \sum_{i\alpha\alpha'\sigma\sigma'} J_{\alpha\alpha'}\, c^\dagger_{i\alpha\sigma} c^\dagger_{i\alpha'\sigma'} c_{i\alpha\sigma'} c_{i\alpha'\sigma}\,, \tag{2}$$

using standard notations. i is a site index, and $\sigma = \uparrow, \downarrow$ refers to the spin direction. The different orbitals labeled by $\alpha = 1, ..., M$ are considered to be equivalent, M is the orbital degeneracy. Exploiting atomic symmetries, we have $U_{\alpha\alpha'} = (U + 2J)\delta_{\alpha\alpha'} + U(1 - \delta_{\alpha\alpha'})$ and $J_{\alpha\alpha'} = J(1-\delta_{\alpha\alpha'})$ as usual (see e.g. Ref. 27). Opposed to calculations using the QMC method (see, e.g. Refs. 13, 18), H_1 includes the full exchange part and thus preserves rotational invariance.

The DMFT assumes the self-energy to be local. Furthermore, the self-energy as well as the Green function are diagonal with respect to the orbital index α for the model considered here. In case of equivalent orbitals and in the absence of any spontaneous symmetry breaking, we thus have $\Sigma_{ij\alpha\beta}(\omega) = \delta_{ij}\delta_{\alpha\beta}\Sigma(\omega)$ and likewise for the local Green function: $G_{ii\alpha\beta}(\omega) = \delta_{\alpha\beta}G(\omega)$. Within the framework of the DMFT, the model H is mapped onto an impurity model $H' = H'_0 + H'_1$ where H'_1 is the local part of the interaction (2) at a distinguished site i_0 and

$$H'_0 = \sum_{\alpha\sigma} t_0\, c^\dagger_{i_0\alpha\sigma} c_{i_0\alpha\sigma} + \sum_{\alpha\sigma,k=2}^{n_s} \epsilon_k\, a^\dagger_{k\alpha\sigma} a_{k\alpha\sigma} + \sum_{\alpha\sigma,k=2}^{n_s} V_k\, (c^\dagger_{i_0\alpha\sigma} a_{k\alpha\sigma} + \text{h.c.}) \tag{3}$$

with $t_0 = t_{ii}$. The self-energy $\Sigma(\omega)$ of H' is identified with the self-energy of the lattice model H and yields, via the lattice Dyson equation, the on-site Green function $G(\omega)$. The latter determines the one-particle parameters of H' or, equivalently, the hybridization function $\Delta(\omega) = \sum_k V_k^2/(\omega + \mu - \epsilon_k)$ via the DMFT self-consistency condition $\Delta(\omega) = \omega + \mu - t_0 - \Sigma(\omega) - 1/G(\omega)$.

Within the full DMFT an infinite number of bath degrees of freedom $n_s \to \infty$ are necessary to fulfill the self-consistency equation. This implies the need for further approximations to treat H'. Contrary, a simple two-site model is considered here. For $n_s = 2$ the model (3) can be solved exactly; however, a simplified self-consistency condition must be tolerated.

Our approach rests on the assumption that similar as for the single-band model, the MIT is characterized by a vanishing weight of a low-energy quasi-particle resonance. Close to the MIT it is then plausible to neglect any internal structure of the quasi-particle peak and to assume that there is no influence of high-energy features on the low-energy part of the excitation spectrum. The quasi-particle peak is then approximated by a single pole at the Fermi energy ($\epsilon_c \equiv \epsilon_{k=2} = \mu$) which reproduces itself in the DMFT self-consistency cycle. One can proceed as for the single-band model[19] and is finally left with the following simple algebraic self-consistency equation which determines the critical parameters ($V \equiv V_{k=2}$):

$$V^2 = z M_2^{(0)}\,. \tag{4}$$

Here $M_2^{(0)}$ is the second moment of the non-interacting density of states $M_2^{(0)} = \int dx\, x^2 \rho^{(0)}(x)$. Formally, Eq. (4) is the same as in the single-band model[19]. However, the quasi-particle weight z has to determined from the degenerate model (3). We calculate $z = 1/(1 - \Sigma'(0))$ from the spectral representation of $G(\omega)$ by summing the residua $\propto V^2$ in the limit $V \to 0$. The residua are obtained by standard (Brillouin-Wigner) degenerate perturbation theory up to the order V^2. This yields an expression $z = z(V, \epsilon_c, t_0, U, J) = V^2\, F(\epsilon_c - t_0, U, J)/M_2^{(0)} + \mathcal{O}(V^4)$. Using $\epsilon_c = \mu$ in the limit $V \to 0$ and setting $t_0 = t_{ii} = 0$ to fix the energy zero, we obtain from Eq.

(4) $F(\mu, U, J) = 1$ as a condition for the MIT. This condition is different for different orbital degeneracy M and integer filling $n = 1, ..., 2M - 1$.

III. RESULTS AND DISCUSSION

For an integer filling n and for any U larger than a critical interaction $U_c = U_c(n, M)$ there are two critical values for the chemical potential $\mu_\pm(U)$ which can be obtained by solving $F(\mu, U) = 1$ for μ (the case $J = 0$ is considered first). For $U > U_c(n, M)$ and $\mu_-(U) < \mu < \mu_+(U)$ the system is a Mott insulator with integer filling n. On the other hand, for $\mu < \mu_-(U)$ or $\mu > \mu_+(U)$, a non-integer filling is realized, and the system becomes metallic. The chemical potential is a continuous function of the filling n' in the vicinity of n for any $U < U_c(n, M)$ but $\mu(n')$ is discontinuous at $n' = n$ with a jump from $\mu_-(U)$ to $\mu_+(U)$ for $U > U_c(n, M)$. U_c is determined by minimization of the function $U(\mu)$ which is obtained by solving $F(\mu, U) = 1$ for U.

For half-filling $n = M$ and arbitrary M we succeeded with a completely analytical calculation for $F(\mu, U)$:

$$F(\mu, U)/M_2^{(0)} = \frac{1}{2}\left(\frac{M+1}{MU-\mu} + \frac{M}{\mu-(M-1)U}\right)^2 + \frac{1}{2}\left(\frac{M}{MU-\mu} + \frac{M+1}{\mu-(M-1)U}\right)^2 . \quad (5)$$

For $U < U_c$ and half-filling $n = M$ in the symmetric model, the chemical potential is fixed to $\mu = (M - \frac{1}{2})U$ due to particle-hole symmetry. Then we find $F = M_2^{(0)}(4M + 2)^2/U^2$ which results in the critical interaction

$$U_c(n = M, M) = (4M + 2)\sqrt{M_2^{(0)}} . \quad (6)$$

By solving $F(\mu, U) = 1$ with Eq. (5) for $U > U_c$ we obtain the jump in the chemical potential

$$\Delta\mu \equiv \mu_+ - \mu_- = U\sqrt{B - \sqrt{B^2 - 1 + \frac{U_c^2}{U^2}}} \quad (7)$$

where $B \equiv 1 + 1/(2(2M + 1)^2(U/U_c)^2)$. The result for $\Delta\mu(U)$ is shown in Fig. 1 for $M = 1, ..., 5$. Here and hereafter we set $M_2^{(0)} = 1$. For fixed M and $U \to \infty$, the jump in the chemical potential increases linearly with U. For $U \to U_c$, $\Delta\mu(U)$ shows a square-root behaviour.

Qualitatively and even quantitatively, this agrees well with results from numerical methods to solve the full DMFT equations. In particular, we compare with results from ED calculations which we have performed with $n_s = 6$ for $M = 2$ (circles) and with data available for $T = 0$ from the projective self-consistent method (crosses)[14]. The non-degenerate case $M = 1$ has already been discussed in Ref. 24. For $M = 2$ and $n_s = 6$ the error due to finite-size effects in the ED is almost negligible. One can state that the agreement of the L-DMFT results with the ED and PSCM data is equally good for both $M = 1$ and $M = 2$.

The generalized L-DMFT predicts $U_c(n = M, M)$ to depend linearly on M, see Eq. (6). This agrees with previous results from the Gutzwiller method[9], slave boson calculations[11], the non-crossing approximation for low temperature[28], and the projective technique for large M[15]. This finding can easily be understood by looking at the weight factors in the Lehmann representation of the spectral density of the two-site Anderson model. Expanding into the different configurations, one finds that the ground state is composed of the order of M singlet states in the limit $V \to 0$ and that there are of the order of M excited states coupling to the ground state. Hence, there are of the order of M^2 processes to be considered in the V-perturbation theory which are contributing to the spectral weight near $\omega = 0$. This implies $z \propto M^2V^2/U^2$ and eventually results in $U_c \propto M$.

In Fig. 2 the dependence of U_c on both n and M is shown for all integer fillings and $M \leq 5$. We find U_c to be reduced away from half-filling, consistent with previous results[5,9,12–14]. The fit shows an almost perfect quadratic dependence of U_c on the filling.

Let us now discuss the influence of the Hund's rule coupling J on the Mott transition at $T = 0$. Contrary to the QMC method, the full exchange part of the on-site Coulomb interaction can easily be included in the L-DMFT calculation. A quantitative influence, i.e. a reduction of U_c due to J has already been observed in Refs. 5, 13. This behavior is also evident from our L-DMFT results, as shown below.

The situation is, however, more complicated: It turns out that a finite J leads to a *qualitative* change of the nature of the $T = 0$ Mott transition. This is illustrated in Fig. 3 which shows the U-dependence of the quasiparticle weight z for various values of J and $n = M = 2$. Note that z is plotted not only close to the transition but also for U far below U_c which means that the self-

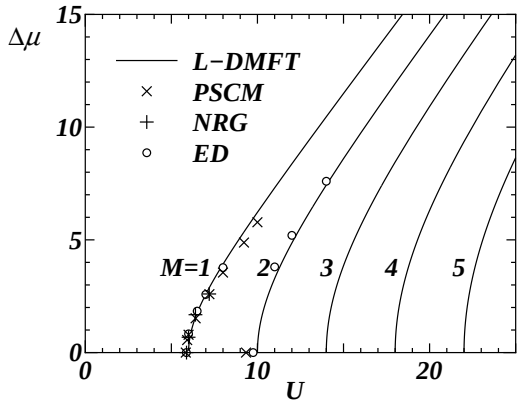

FIG. 1. $\Delta\mu(U)$ for half-filling $n = M$ and different M as obtained from Eq. (7). Results from the full DMFT using ED, NRG, and PSCM[14,20] are shown for comparison.

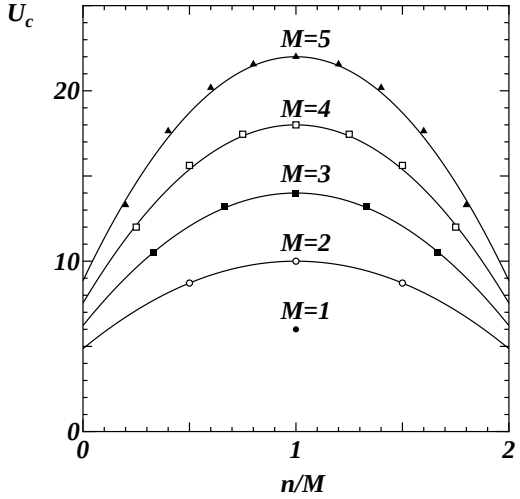

FIG. 2. Critical interaction U_c for different fillings $n = 1, 2, ..., 2M-1$ and different M as a function of n/M. Symbols: L-DMFT results. Lines: simple fit function $U_c(n,M) = U_c(n=M,M) - c(1-(n/M))^2$ and $c = -0.217 + 2.671M$.

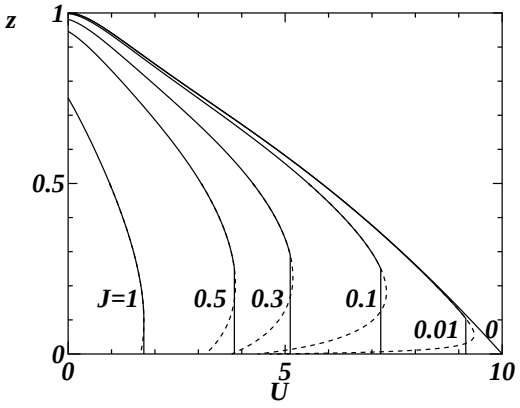

FIG. 3. U-dependence of the quasi-particle weight z for $n = M = 2$ and different J. Dashed lines correspond to metastable solutions; vertical lines indicate the actual Mott transition at $U = U_c$.

consistency relation (4) is used for any U. This is reasonable as long as there is a clear separation between the low-energy (quasi-particle) and the high-energy scale (Hubbard bands). Although the approximation becomes questionable for higher z and particularly in the limit $z \to 1$, the trend of $z(U)$ looks rather plausible in whole range.

In the critical regime where z goes to zero continuously, we find $z(U)$ to decrease with *decreasing* U which seems to be unphysical. In fact, this behavior belongs to a metastable state (dashed line) while for the true ground state (solid line) $z(U)$ is always decreasing with increasing U. The two metallic states with finite $z > 0$ but different slope dz/dU are coexisting in a finite range of interaction strengths, namely for U larger than $U_{c,2}$ (given by $z = 0$) and for U smaller than another critical value $U_{c,3} > U_{c,2}$ where they merge together[29].

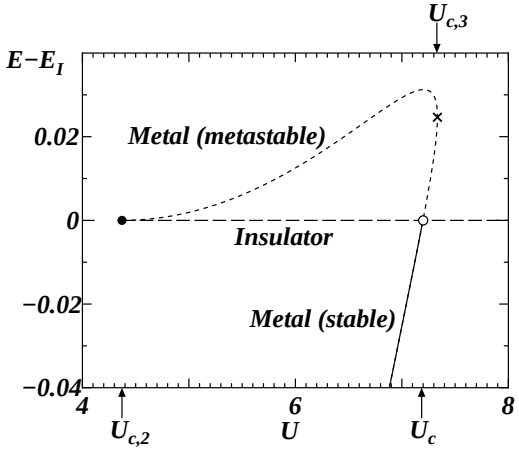

FIG. 4. Energy of the two metallic solutions relative to the energy of the insulator for $J = 0.1$. At $U_{c,2}$ (closed circle) the metastable metallic state continuously merges with the insulating state. At $U_{c,3}$ (cross) the two metallic states merge. The discontinuous phase transition takes place at U_c (open circle).

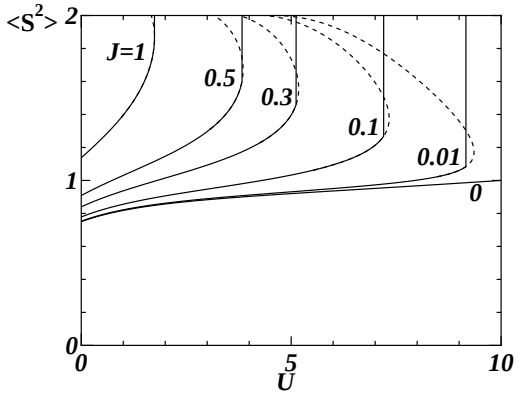

FIG. 5. Local moment at the impurity site $\langle \mathbf{S}^2 \rangle$ as a function of U for different J. Dashed lines: metastable solutions; vertical lines: actual Mott transition for $U = U_c$.

The actual critical interaction strength U_c where the transition to the insulator takes place must be determined by comparing the respective energies with the energy of the insulator. This is shown in Fig. 4 for $J = 0.1$. For any $J > 0$ it is found that $U_{c,2} < U_c < U_{c,3}$. At U_c the energies of the metallic and insulating states are crossing as functions of U. Consequently, the transition at $T = 0$ is discontinuous with a jump in physical quantities like the double occupancy $\langle n_\uparrow n_\downarrow \rangle = dE/dU$. Equivalently, one can look at the local magnetic moment at the impurity site $\langle \mathbf{S}^2 \rangle$ (see Fig. 5). The local moment increases with U, typical for a strongly correlated normal metal. At U_c it jumps to $\langle \mathbf{S}^2 \rangle = 2$ for any finite J. Similarly, the quasi-particle weigth z decreases with increasing U and drops to zero at U_c from a *finite* value $z > 0$. In Fig. 3 this is indicated by solid vertical lines.

The phase diagram in the (U,J)-plane is shown in Fig. 6. The critical interaction for the actual transition is

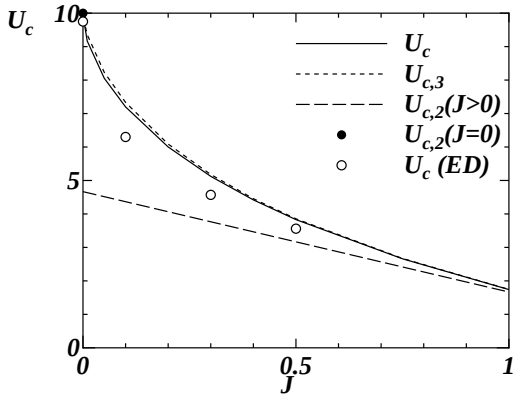

FIG. 6. (U,J) phase diagram for $n = M = 2$. U_c: critical interaction for the MIT. $U_{c,3}$: maximum U up to which a metallic solution is found. $U_{c,2}$: critical U where $z \to 0$ ($U_{c,2} = 14/3 - 3J$ for $J > 0$ and $M_2^{(0)} = 1$).

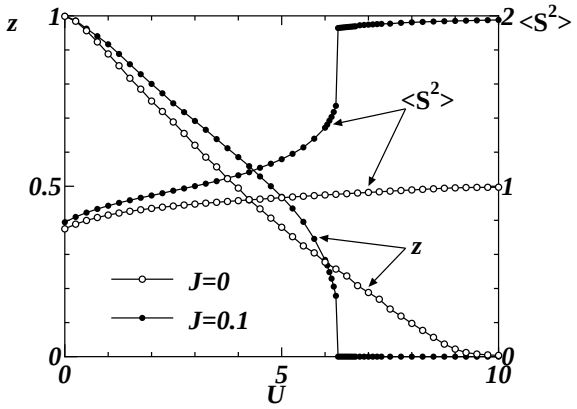

FIG. 7. DMFT-ED results ($n_s = 6$) for the U-dependence of the quasi-particle weight (left scale) and the local moment (right scale). $J = 0$ and $J = 0.1$ for $n = M = 2$.

plotted together with $U_{c,2}$ and $U_{c,3}$. U_c is found to be very close to $U_{c,3}$ for all J-values. Note that already a moderate value of $J \approx 0.3$ leads to a drastic reduction of U_c from $U_c = 10$ to $U_c \approx 5$.

Interestingly, similar results have been obtained beforehand by a rather different method: Applying a generalized Gutzwiller approximation to a degenerate two-band model, Bünemann et al.[10] found the Mott transition to be discontinuous for any finite $J > 0$ and to be continuous for $J = 0$ only. While the Gutzwiller method (for $J = 0$) significantly overestimates the critical interaction strength as compared to the L-DMFT, the reduction of U_c by a finite J is stronger. Common to both methods, however, is the qualitative change of the Mott transition for a finite J.

We have additionally checked the nature of the Mott transition by a fully numerical evaluation of the DMFT equations using the ED method with $n_s = 6$ sites for $n = M = 2$. The results for $J = 0$ and $J = 0.1$ are shown in Fig. 7. The critical interaction U_c is found to be somewhat smaller as compared to the L-DMFT result as shown in Fig. 6. More important, however, the ED calculations show the same qualitative trend: The slope of $z(U)$ approaches $-\infty$ at a critical value $U = U_{c,3}$. This clearly indicates a second metastable metallic solution and a discontinuous transition and thus corroborates our results discussed above. Fig. 7 also shows the U dependence of the local magnetic moment where the effect is even more pronounced. Note that in the insulator $\langle \mathbf{S}^2 \rangle$ is close but not equal to the prediction of the linearized DMFT $\langle \mathbf{S}^2 \rangle = 2$ (cf. Fig. 5). This is due to residual local fluctuations which are neglected by the L-DMFT for the insulating phase.

The limit $J \to 0$ which appears to be somewhat exceptional can be analyzed easily. From Fig. 3 it is obvious that the critical interaction $U_{c,2}$ at which $z \to 0$ in the metastable phase shows a discontinuous jump from a value $U_{c,2} \approx 5 < U_{c,3}$ for $J > 0$ to $U_{c,2} = 10 = U_{c,3}$ for $J = 0$. To find the physical reason for this discontinuity of $U_{c,2}$, one can again look at the Lehmann representation of the spectral density for $V \to 0$. The main difference between the case $J = 0$ and the case $J > 0$ consists in the fact that for $J > 0$ only those configurations with a triplet on the impurity site contribute to the (singlet) ground state in the limit $V \to 0$ (see Fig. 5). As compared with $J = 0$ this is about a factor of 2 configurations less. Thus, the discontinuous jump of $U_{c,2}$ is caused by a strong suppression of orbital fluctuations due to a finite J (a similar argument in a slightly different context has been put forward in Ref. 16). On the other hand, it should be stressed that the actual critical interaction U_c remains continuous in the limit $J \to 0$ as $U_c \to U_{c,3}$. Note that to uncover this subtle distinction it has been necessary to extend the theory beyond the $z \to 0$ limit.

IV. CONCLUSION

To summarize, we have presented an extension of the linearized dynamical mean-field theory (L-DMFT) to multi-orbital Hubbard models including the *full* exchange term. This allows a reliable calculation of the critical interaction strength U_c for the zero-temperature Mott transition analytically for all M at half-filling and numerically for all integer fillings $n \neq M$ and $M \leq 5$. We find a linear dependence of U_c on the number of orbitals. Remarkably, a qualitative change of the nature of the $T = 0$ Mott transition is observed for any finite J: the transition becomes discontinuous with a finite jump of the quasi-particle weight at U_c close to $U_{c,3}$.

For finite temperatures one might speculate that a finite J increases the tendency for a first-order Mott-transition. This could be of experimental relevance for the Mott-transition in transition-metal oxides.

The L-DMFT for correlated electron systems with orbital degrees of freedom is a handy and trustable approach with a large potential for future applications. One might consider, for instance, the multi-band Hubbard

model investigated in the context of the LDA+DMFT approach for the transition-metal oxide V_2O_3[18]. The L-DMFT can be easily extended to answer questions about the importance of the e_g^σ-bands (neglected in Ref. 18) on the Mott transition, or the influence of the *full* exchange term. We have already observed a significant quantitative change of U_c when excluding the spin-dependent part from the exchange term in (2). This should have consequences for a realistic description of the MIT in transition-metal oxides which are worth to be studied.

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