Simple treatment of the metal-insulator transition: Effects of degeneracy, temperature, and applied magnetic field

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A simple slave-boson representation combined with the Hartree-Fock approximation for Hund's rule coupling is introduced for a doubly degenerate narrow band, which bears a direct relation to that introduced previously in the nondegenerate case. Namely, one keeps the fermion representation of the spin operator to recover properly the energy of fermionic quasiparticles in the presence of an applied magnetic field. A simple two-parameter mean-field analysis of the metamagnetism is provided, with the emphasis on the role of Hund's rule coupling. We also analyze the appearance of the spin-split effective masses in the applied field and for the non-half-filled band situation. The Mott-Hubbard boundary is determined at nonzero temperature ($T>0$); it shifts towards lower interactions with increasing T and the field signaling the precursory localization effects, explicitly exhibited in the behavior of the magnetic susceptibility calculated in the Appendix. We also formulate a more general two-parameter rotationally invariant approach for an arbitrary degeneracy d of equivalent orbitals and show that the Mott-Hubbard transition at zero temperature and at any integer filling $n \geqslant 1$ is always discontinuous. A brief overview of the experimental situation is also given. [S0163-1829(98)04616-5]

I. INTRODUCTION

In recent years one observes a renewed interest in the metal-insulator transition (MIT) of the Mott-Hubbard type, with a particular emphasis on the effect of orbital degeneracy and associated with it Hund's rule coupling, both appearing as additional factors.[1] This interest is induced by the new works on perovskites,[2] $NiS_{2-x}Se_x$,[3] as well as on the canonical system $V_{2-y}O_3$.[4] In most of these compounds one observes an anomalous metallicity even in the paramagnetic state.[3,4] Among them is the metamagnetism and a relatively strong applied magnetic field dependence of thermodynamic properties,[5] in addition to the field induced metal-insulator transition.[6] These phenomena of localization occur in compounds of various crystal structure and even in the same magnetic phase, as in the case of $NiS_{2-x}Se_x$. Therefore, it seems that the underlying microscopic mechanism is rather general, neither strongly dependent on a particular crystallographic structure, nor on the form of the density of states near the Fermi energy and the type of magnetism. Additionally, electronic properties of the system $NiS_{2-x}Se_x$ are well described by considering a half-filled e_g band[7] composed of $3d$ states (due to Ni^{2+} ions), which hybridize with completely filled p states due to S^{2-} or Se^{2-} (the last states are believed to play only a passive role near the MIT).

The purpose of this paper is to carry out a simplified analysis for a system composed of orbitally degenerate but otherwise equivalent band states that nonetheless addresses some of the principal phenomena in an applied magnetic field and at nonzero temperature. Thus, one can examine the system behavior as a function of experimentally controllable parameters.

The analysis of Mott-Hubbard localization in the nondegenerate band case was based on the Hubbard model and provides a continuous transition at $T=0$ (Ref. 8) and a discontinuous transition at $T>0$.[9] These results were subsequently confirmed in the limit of infinite dimensions.[10] This means that this quantum phase transition possesses an upper critical dimension and the Gutzwiller approach represents a correct mean-field theory. Also, close to the localization, depending on the band filling, one observes metamagnetism[6] or metamagnetic behavior,[7,11] spin-split effective masses,[11,12] and a transition from an antiferromagnetic semimetal to an antiferromagnetic insulator.[4] The related Gutzwiller approximation scheme for a doubly degenerate Hubbard model provides a discontinuous transition already at $T=0$,[1] a change induced by Hund's rule coupling. Obviously, Hund's rule should make the localization easier (i.e., diminish the critical value U_c of the intraatomic interaction), since it favors energetically the high-spin atomic state against any normal Fermi-liquid state. Hence, we can separate the effects associated with the Coulomb interaction from those due to Hund's rule coupling.

The structure of this paper is as follows. In the next section we introduce a slave-boson approach combined with the Hartree-Fock approximation for the Hund's-rule term, which reproduces in a simple manner the similar results of the full slave-boson analysis by Hasegawa[1] in the paramagnetic state for zero field and temperature. Additionally, this representation provides a correct expression of the energy a fermionic quasiparticles in the applied magnetic field. Within this scheme we determine the magnetic susceptibility, metamagnetic properties, spin-dependent effective masses, as well as determine the Mott-Hubbard boundary at nonzero temperature, and its shift towards lower temperatures in the applied field. The similarities and differences with the nondegenerate-band case are stressed. In the second part we propose a simple rotationally invariant formulation of the problem for an arbitrary orbital degeneracy of electron states and compare it with the Gutzwiller approach. Within this approach, a difference between the Hund's rule and intersite magnetic coupling appears naturally, although the last point is not discussed in detail in the present paper. The correlated

metal-paramagnetic insulator transition takes place at any integer filling n and is discontinuous for $n \geqslant 1$.

II. PARAMAGNETIC AND METAMAGNETIC STATES OF THE DOUBLY DEGENERATE HUBBARD MODEL

A. Slave-boson method combined with the Hartree-Fock approximation for the exchange term

Doubly degenerate Hubbard model in the situation with equivalent orbitals is described by the Hamiltonian:

$$\mathcal{H}=\sum_{ijl\sigma}{}' t_{ij}a^{\dagger}_{il\sigma}a_{jl\sigma}+U\sum_{il} n_{il\uparrow}n_{il\downarrow}+(U'-\tfrac{1}{2}J)\sum_{i} n_{i1}n_{i2} -2J\sum_{i} \mathbf{S}_{i1}\cdot\mathbf{S}_{i2}-2h\sum_{il} S^{z}_{il}, \tag{1}$$

where $a_{il\sigma}$ is the annihilation operator of electron from lattice site i on orbital $l(=1,2)$ and with spin $\sigma(=\uparrow,\downarrow)$, $n_{il\sigma}$ is the particle number and $\mathbf{S}_{il}=(S^{+}_{il},S^{-}_{il},S^{z}_{il})$ is the spin operator, t_{ij} is the hopping integral, assumed for simplicity the same for the two orbitals (we choose also $t_{ii}=0$). Parameters U, U', and J are, respectively, the intraband Coulomb, the interband Coulomb, and Hund's-rule-exchange integrals. For the e_g band we have $U'=U-2J$. Finally, in the last term $h=\frac{1}{2}g\mu_B H_a$, where H_a is the applied magnetic field. Because of the vanishing orbital moment in the first order, the magnetic field affects the spin degrees only (we neglect also the Landau quantization effects for low fields).

We make the mean-field approximation for the exchange term. Likewise, we decouple in the same manner the interorbital term, since $U'-\frac{1}{2}J=U-\frac{5}{2}J$. Therefore, we have

$$n_{i1}n_{i2}=n_{i1}\langle n_{i2}\rangle+\langle n_{i1}\rangle n_{i2}-\langle n_{i1}\rangle\langle n_{i2}\rangle,$$

$$\mathbf{S}_{i1}\cdot\mathbf{S}_{i2}=S^{z}_{i1}\langle S^{z}_{i2}\rangle+\langle S^{z}_{i1}\rangle S^{z}_{i2}-\langle S^{z}_{i1}\rangle\langle S^{z}_{i2}\rangle, \tag{2}$$

where $\langle A\rangle=\mathrm{Tr}(Ae^{-\beta\mathcal{H}_{H-F}})$ is the average value of operator A with Hamiltonian $\mathcal{H}_{H-F}$:

$$\mathcal{H}_{H-F}=\sum_{ijl\sigma}{}' t_{ij}a^{\dagger}_{il\sigma}a_{jl\sigma}+U\sum_{il} n_{il\uparrow}n_{il\downarrow}+K\tfrac{1}{2}n\sum_{il} n_{il} -Jm\tfrac{1}{4}\sum_{il\sigma}\sigma n_{il\sigma}-h\sum_{il\sigma}\sigma n_{il\sigma}-\tfrac{1}{4}KNn^2+\tfrac{1}{8}JNm^2 -\mu N_e. \tag{3}$$

In this equation we have added the chemical potential part $(-\mu N_e)$, with N_e being the number of electrons in the system. The n and m are defined by equations

$$\langle n_{il}\rangle\equiv\tfrac{1}{2}n, \tag{4}$$

$$2\langle S^{z}_{il}\rangle\equiv\tfrac{1}{2}m, \tag{5}$$

and N is the number of sites, $K=U'-\frac{1}{2}J$. The mean values of n_{il} and S^{z}_{il} are independent of site and orbital indexes because of translational symmetry and the equivalence of the orbitals for half- or nearly-half-filled band configurations (in this part we consider mainly the limit of n equal to or close to two).

We employ the slave boson representation of Kotliar and Ruckenstein[13] in the form

$$|0,il\rangle\equiv e^{\dagger}_{il}|v\rangle, \tag{6a}$$

$$a^{\dagger}_{il\sigma}|0,il\rangle\equiv|\sigma,il\rangle\equiv f^{\dagger}_{il\sigma}p^{\dagger}_{il\sigma}|v\rangle, \tag{6b}$$

$$\sigma a^{\dagger}_{il\sigma}a^{\dagger}_{il\bar{\sigma}}|0,il\rangle\equiv|2,il\rangle\equiv\sigma f^{\dagger}_{il\sigma}f^{\dagger}_{il\bar{\sigma}}d^{\dagger}_{il}|v\rangle, \tag{6c}$$

where we introduced new boson-fermion vacuum $|v\rangle$ instead of the Fock-space vacuum $\{|0,il\rangle\}$. So, we have added only the orbital index to the original formulation. The operators $e^{\dagger}_{il}$, $p^{\dagger}_{il\sigma}$, and $d^{\dagger}_{il}$ are boson operators and $f^{\dagger}_{il\sigma}$ is fermion operator. This representation must be supplemented by the constraints

$$Q_{il\sigma}\equiv f^{\dagger}_{il\sigma}f_{il\sigma}-p^{\dagger}_{il\sigma}p_{il\sigma}-d^{\dagger}_{il}d_{il}=0 \tag{7}$$

and

$$P_{il}\equiv e^{\dagger}_{il}e_{il}+\sum_{\sigma} p^{\dagger}_{il\sigma}p_{il\sigma}+d^{\dagger}_{il}d_{il}-1=0\,. \tag{8}$$

The relation between original $(a_{il\sigma})$ and new $(f_{il\sigma})$ fermion operators is

$$a_{il\sigma}=(e^{\dagger}_{il}p_{il\sigma}+d_{il}p^{\dagger}_{il\,\bar{\sigma}})f_{il\sigma}=z_{il\sigma}f_{il\sigma}. \tag{9}$$

The constraints given by Eqs. (7) and (8) can be enforced by Lagrange multipliers $\lambda^{(1)}_{il}$ and $\lambda^{(2)}_{il\sigma}$. We obtain the following Hamiltonian:

$$\mathcal{H}_{\mathrm{tot}}\equiv\mathcal{H}_{H-F}+\mathcal{H}_{\mathrm{con}} =\sum_{ijl\sigma}{}' t_{ij}z^{\dagger}_{il\sigma}z_{jl\sigma}f^{\dagger}_{il\sigma}f_{jl\sigma}+U\sum_{il} d^{\dagger}_{il}d_{il} +\sum_{il\sigma}[(\tfrac{1}{2}Kn-\mu)-\sigma(h+\tfrac{1}{4}Jm)]f^{\dagger}_{il\sigma}f_{il\sigma}+\mathcal{H}_{\mathrm{con}}+C, \tag{10}$$

where

$$C\equiv-\tfrac{1}{4}KNn^2+\tfrac{1}{8}JNm^2, \tag{11}$$

and

$$\mathcal{H}_{\mathrm{con}}\equiv\sum_{il}\lambda^{(1)}_{il}P_{il}+\sum_{il\sigma}\lambda^{(2)}_{il\sigma}Q_{il\sigma}. \tag{12}$$

Note that, using the fermion representation for the spin operator $S^{z}_{il}=\frac{1}{2}(f^{\dagger}_{il\uparrow}f_{il\uparrow}-f^{\dagger}_{il\downarrow}f_{il\downarrow})$, we obtain correctly the Zeeman term and, also, the Hund's rule coupling in the form of a molecular field. Equivalently, one could utilize the Bose representation $S^{z}_{il}=\frac{1}{2}(p^{\dagger}_{il\uparrow}p_{il\uparrow}-p^{\dagger}_{il\downarrow}p_{il\downarrow})$, but then only the z-component is well defined and the result in the saddle-point approximation does not provide the quasiparticle energies with the proper Zeeman term (see the discussions of this point in Ref. 6(b), where the full spin rotation invariant form of the SB representation is invoked).

The factor $z_{il\sigma}$ is not unique, but when we make the choice,[13]

$$z_{il\sigma}\rightarrow(1-d_{il}^{\dagger}d_{il}-p_{il\sigma}^{\dagger}p_{il\sigma})^{-1/2}z_{il\sigma}(1-e_{il}^{\dagger}e_{il}-p_{il\bar{\sigma}}^{\dagger}p_{il\bar{\sigma}})^{-1/2}, \tag{13}$$

we obtain the correct result in the saddle-point solution.

The partition function is given by

$$Z=\int D[e,e^{\dagger}]D[p,p^{\dagger}]D[d,d^{\dagger}]D[f,f^{\dagger}]\prod_{il\sigma}d\lambda_{il}^{(1)}d\lambda_{il\sigma}^{(2)} \times\exp\left[-\int_0^{\beta}\mathcal{L}(\tau)d\tau\right], \tag{14}$$

where $\beta=1/k_BT$ is the inverse temperature,

$$\begin{aligned}\mathcal{L}(\tau)=&\sum_{ijl\sigma}f_{il\sigma}^{\dagger}[[\partial_{\tau}-\tilde{\mu}-\sigma(h+\tfrac{1}{4}Jm)+\lambda_{il\sigma}^{(2)}]\delta_{ij}\\&+t_{ij}z_{il\sigma}^{\dagger}z_{jl\sigma}]f_{jl\sigma}+\sum_{il}e_{il}^{\dagger}(\partial_{\tau}+\lambda_{il}^{(1)})e_{il}\\&+\sum_{il\sigma}p_{il\sigma}^{\dagger}(\partial_{\tau}+\lambda_{il}^{(1)}-\lambda_{il\sigma}^{(2)})p_{il\sigma}\\&+\sum_{il}d_{il}^{\dagger}\left(\partial_{\tau}+\lambda_{il}^{(1)}-\sum_{\sigma}\lambda_{il\sigma}^{(2)}+U\right)d_{il}-\sum_{il}\lambda_{il}^{(1)}+C,\end{aligned} \tag{15}$$

is the system Lagrangian, and

$$\tilde{\mu}=\mu-\tfrac{1}{2}Kn. \tag{16}$$

is the effective chemical potential.

Next, we make the saddle-point approximation, i.e., assume that Bose fields and Lagrange multipliers do not depend on time τ, number of site i, and orbital index l, so $e_{il}(\tau)\rightarrow e$, $p_{il\sigma}(\tau)\rightarrow p_{\sigma}$, $d_{il}(\tau)\rightarrow d$, $\lambda_{il\sigma}^{(2)}\rightarrow\lambda_{\sigma}^{(2)}$, and $\lambda_{il}^{(1)}\rightarrow\lambda$. To obtain the saddle-point solution we must minimize free energy with respect to boson fields and Lagrange multipliers. From partition function (14) we obtain the following expression for the free energy:

$$\begin{aligned}F=&-k_BT\sum_{\mathbf{k}l\sigma}\ln\left[1+\exp\left(\frac{\tilde{\mu}-E_{\mathbf{k}\sigma}}{k_BT}\right)\right]+\tfrac{1}{8}NJm^2+2NUd^2\\&-2N\sum_{\sigma}\lambda_{\sigma}^{(2)}(p_{\sigma}^2+d^2)+2N\lambda^{(1)}\left(e^2+\sum_{\sigma}p_{\sigma}^2+d^2-1\right)\\&-\tfrac{1}{4}NKn^2+\mu Nn.\end{aligned} \tag{17}$$

The Fermi quasiparticle energy $E_{\mathbf{k}\sigma}$ is given by

$$E_{\mathbf{k}\sigma}=q_{\sigma}\epsilon_{\mathbf{k}}-\sigma(h+\tfrac{1}{4}Jm)+\lambda_{\sigma}^{(2)}, \tag{18}$$

where $\epsilon_{\mathbf{k}}$ is bare band energy, $q_{\sigma}\equiv z_{\sigma}^2$, and

$$z_{\sigma}^2=\frac{(ep_{\sigma}+dp_{\bar{\sigma}})^2}{(1-d^2-p_{\sigma}^2)(1-e^2-p_{\bar{\sigma}}^2)}. \tag{19}$$

Thus, one encounters here two molecular fields: one coming from the Hund's rule and the other $(\lambda_{\uparrow}^{(2)}-\lambda_{\downarrow}^{(2)})$ coming from the electronic correlations.

Differentiation of the free energy with respect to Lagrange multipliers provides the mean-field version of the constraints:

$$\frac{\partial F}{\partial\lambda_{\sigma}^{(2)}}=0\Rightarrow p_{\sigma}^2+d^2=\frac{1}{N}\sum_{\mathbf{k}}n_{\mathbf{k}\sigma}=\tfrac{1}{2}n_{\sigma}, \tag{20}$$

$$\frac{\partial F}{\partial\lambda^{(1)}}=0\Rightarrow 1-e^2-\sum_{\sigma}p_{\sigma}^2-d^2=0, \tag{21}$$

where

$$n_{\mathbf{k}\sigma}=\frac{1}{1+\exp[\beta(E_{\mathbf{k}\sigma}-\tilde{\mu})]} \tag{22}$$

is the Fermi-Dirac function. From Eqs. (4) and (14) we obtain that $\langle n_{il\sigma}\rangle=\frac{1}{2}n_{\sigma}=(n+\sigma m)/4$. Instead of computing the derivatives with respect to the remaining fields we set e and p_{σ} expressed via d, n, and m into free energy (17). Next, we introduce new variables β_3 and β_0, such that $\lambda_{\sigma}^{(2)}=\beta_0+\sigma\beta_3$. We obtain the following free energy:

$$\begin{aligned}\frac{F}{N}=&-2k_BT\frac{1}{N}\sum_{\mathbf{k}\sigma}\ln\left[1+\exp\left(\frac{\bar{\mu}-E_{\mathbf{k}\sigma}}{k_BT}\right)\right]+\tfrac{1}{8}Jm^2+2Ud^2\\&-\beta_3m+\tfrac{1}{4}Kn^2+\bar{\mu}n.\end{aligned} \tag{23}$$

Quasiparticle energy is given by

$$E_{\mathbf{k}\sigma}=q_{\sigma}\epsilon_{\mathbf{k}}-\sigma(h+\tfrac{1}{4}Jm-\beta_3), \tag{24}$$

and the effective chemical potential by

$$\bar{\mu}=\tilde{\mu}-\beta_0=\mu-\tfrac{1}{2}Kn-\beta_0. \tag{25}$$

From Eq. (19) we obtain q_{σ} in a form

$$q_{\sigma}=4\frac{\left(\sqrt{1-\frac{1}{2}n+d^2}\sqrt{n+\sigma m-4d^2}+d\sqrt{n-\sigma m-4d^2}\right)^2}{(4-n-\sigma m)(n+\sigma m)}. \tag{26}$$

This factor is the mass enhancement and in the general case $(n\neq 2)$ leads to the spin-dependent effective masses.

One should justify the approximations made. First, for e_g band $J\simeq 0.2U$, and therefore $U'=U-2.5J\simeq 0.5U$. Hence one can say that making the Hartree-Fock approximation for the interorbital-interaction part is qualitatively correct even for $U\sim W$. Below we make this argument more quantitative by comparing the ground-state energy obtained within different approximation schemes. Mixing the slave-boson scheme with the Hartree-Fock approximation for the Hund's rule exchange has this advantage: that we can single out what feature is specifically due to Hund's rule coupling, as discussed next.

B. Case $n=2$, $T=0$, and $h=0$: Effect of exchange interaction on the metal-insulator transition

We consider first the simplest situation: a paramagnetic state in the half-filled band case and at zero temperature and in zero applied magnetic field.[1]

At temperature $T=0$ the distribution function (22) takes the form

$$n_{\mathbf{k}}=\Theta(\overline{\mu}-E_{\mathbf{k}})=\begin{cases}0 & \text{when } E_{\mathbf{k}}>\overline{\mu},\\ 1 & \text{when } E_{\mathbf{k}}\leqslant\overline{\mu},\end{cases} \tag{27}$$

where $E_k=\Phi_0\epsilon_{\mathbf{k}}$ and $\Phi_0\equiv q_\sigma=q_{\bar\sigma}=8d^2(1-2d^2)$. We obtain following expression for the ground-state energy:

$$\begin{aligned}E_0&=-2\sum_\sigma\int_{-W/2}^{W/2}d\epsilon\rho(\epsilon)(\overline{\mu}-\Phi_0\epsilon)\Theta(\overline{\mu}-\Phi_0\epsilon)\\&\quad+2Ud^2+2\overline{\mu}\\&=2\Phi_0\overline{\epsilon}+2Ud^2+K,\end{aligned} \tag{28}$$

where:

$$\overline{\epsilon}\equiv 2\int_{-W/2}^{W/2}d\epsilon\rho(\epsilon)\epsilon n(\epsilon) \tag{29}$$

is the mean bare-band energy, $n(\epsilon)=\Theta(\overline{\mu}-\Phi_0\epsilon)$, and $\rho(\epsilon)$ is density of states. Minimizing the functional (28) with respect d^2 we obtain the solution

$$d^2=\frac{1}{4}\left(1-\frac{U}{8|\overline{\epsilon}|}\right), \tag{30}$$

which coincides with the results in the nondegenerate-band case,[8,9] i.e., the metallic state would become unstable for $U=U_0\equiv 8|\overline{\epsilon}|$ if the system evolves continuously with growing U. However, we shall see that in the degenerate system this instability point U_0 is replaced by a critical point $U_c<U_0$, at which a discontinuous transition takes place.

The ground-state energy of the metallic state can be expressed explicitly as

$$E_0^M=-2|\overline{\epsilon}|-\frac{1}{32}\frac{U^2}{|\overline{\epsilon}|}+\frac{3}{2}U-\frac{5}{2}J. \tag{31}$$

In the Mott-insulating spin-disordered state, i.e., for $d^2=0$, we have

$$E_0^I=K-\tfrac{1}{2}J=U-3J. \tag{32}$$

Equating the energies (32) and (28) we determine the critical value of $J=J_c$ and $U=U_c$, for which the transition from a correlated metal to a paramagnetic Mott insulator takes place:

$$J_c=4|\overline{\epsilon}|\left(1-\frac{U_c}{8|\overline{\epsilon}|}\right)^2. \tag{33}$$

For $J<J_c$ the metallic state is stable. Also, for $J>0$ the transition is of first order, whereas for $J=0$ it is continuous and corresponds to that for the nondegenerate case. For example, for $J/U=0.1$ we obtain the critical value $U=U_c=5.1|\overline{\epsilon}|$. The diminution of U_c below U_0 is obviously caused by the Hund's rule favoring the high-spin state on each atom.

C. Case $n=2$, $T=0$, and $h\geqslant 0$: Metamagnetic transition

We discuss next the homogeneous magnetized state starting from the paramagnetic state at $T=0$. From Eq. (26) we obtain the band narrowing factor in this case in the form

$$\Phi\equiv q_\sigma=\frac{16d^2}{4-m^2}[1-2d^2+\tfrac{1}{2}\sqrt{4(1-2d^2)^2-m^2}]. \tag{34}$$

Thus, the effective mass will not depend on spin for the half-filled band case.

The average occupancy of each orbital state with spin σ is

$$\begin{aligned}n_\sigma&=\frac{2}{N}\sum_{\mathbf{k}}n_{\mathbf{k},\sigma}=2\int_{-W/2}^{W/2}d\epsilon\rho(\epsilon)n_\sigma(\epsilon)\\&=2\int_{-W/2}^{[\overline{\mu}+\sigma(h-\beta_3+Jmm/4)]q_\sigma}d\epsilon\rho(\epsilon),\end{aligned} \tag{35}$$

where $n_\sigma(\epsilon)=\Theta(\overline{\mu}+\sigma(h-\beta_3+Jm/4)-q_\sigma\epsilon)$. We choose the featureless (rectangular) density bare of states:

$$\rho(\epsilon)=\begin{cases}\dfrac{1}{W} & \text{for } \epsilon\in[-W/2,W/2],\\ 0 & \text{otherwise.}\end{cases} \tag{36}$$

The overall features should be independent of the detailed shape of $\rho(\epsilon)$, as we determine global quantities (m, E_G, d^2) involving integrals over the filled part of the relevant bands. Putting above density of states (DOS) into Eq. (35) we obtain

$$\begin{aligned}n_\sigma&=\frac{2}{W}\int_{-W/2}^{[\overline{\mu}+\sigma(h-\beta_3+Jmm/4)]/\Phi}d\epsilon\\&=\frac{1}{W\Phi}\left[\left(h-\beta_3+\frac{1}{4}Jm\right)\sigma+\overline{\mu}+\frac{W\Phi}{2}\right].\end{aligned} \tag{37}$$

Summation over σ of the above equation leads to the condition $\overline{\mu}=0$, but multiplying it by σ and then summing over σ leads to the expression for the molecular field of the form

$$\beta_3=-\tfrac{1}{4}\Phi Wm+h+\tfrac{1}{4}Jm. \tag{38}$$

Because Φ is nonlinear in magnetic moment m, the molecular field β_3 depends also on m in the same manner. Inserting β_3 into Eq. (23) for $T=0$, we obtain

$$E_M\equiv\frac{F}{NW}=-(4-m^2)\Phi/8+2ud^2-hm-\tfrac{1}{8}jm^2+k, \tag{39}$$

where the reduced parameters are

$$u=U/W,\quad j=J/W,\quad k=K/W,\quad h\to h/W. \tag{40}$$

We determine the saddle-point solution minimizing E_M with respect d^2 and m. Differentiation with respect to m leads to

$$d^4(m^2-16a)+a(16d^2+m^2-4)=0, \tag{41}$$

where $a=(h+jm/4)^2$. The differentiation with respect d^2 yields

$$\tfrac{1}{2}(u+4d^2-1)\sqrt{4(1-2d^2)^2-m^2}-(1-2d^2)^2+\tfrac{1}{4}m^2 +2d^2(1-2d^2)=0. \tag{42}$$

For $h=0$ and $u\leqslant 2$ from Eq. (30) we obtain $d^2=(1-u/2)/4$. The change of direction of magnetic field h does not change d^2; thus $(\partial d^2/\partial h)_{h=0}=0$. Next, differentiating with respect to h, Eq. (41), and taking into account the above relations, we obtain the following expression for the magnetic susceptibility:

$$\chi(0)\equiv\left.\frac{\partial m}{\partial h}\right|_{h=0}\frac{1}{4}\chi_0=\frac{\chi_0}{\dfrac{2-u}{2+u}-j}, \tag{43}$$

where $\chi_0=2\mu_B^2/W$ is the Pauli susceptibility (cf. the Appendix). The magnetic susceptibility was derived for the metallic state, so from taking into account the condition (33) we obtain the metallic state for $j<(1-u/2)^2\leqslant(1-u/2)/(1+u/2)\leqslant 1$. From, the last inequality we obtain the condition for the magnetization in small fields:

$$m\approx\left.\frac{\partial m}{\partial h}\right|_{h=0}h=\frac{4h}{\dfrac{2-u}{2+u}-j}>\frac{4h}{1-j}. \tag{44}$$

This condition reduces solutions of Eq. (41) to

$$d^2=\frac{-8a+m\sqrt{a(16a+4-m^2)}}{m^2-16a}. \tag{45}$$

Substituting d^2 into Eq. (42) we obtain the following equation for magnetization:

$$-64a^3+12a^2m^2-3am^4/4+m^6/64+64a^2u-m^4u/4 -16au^2+32a^2u^2+m^2u^2+12am^2u^2+m^4u^2/8 -16au^3-m^2u^3-4au^4+m^2u^4/4=0. \tag{46}$$

The pair of solutions (m,d^2) determines the ground-state energy (39). The ground-state energy of a Mott-Hubbard insulator in the spin disordered state is

$$E_I=-2h-j/2+k. \tag{47}$$

From the preceding subsection we know that the metal-insulator transition take place for $j=(1-u/2)^2$. From the expression (43) for the magnetic susceptibility we see that except for the case $j=0$ and $u=2$, *there is no singularity in* χ *at the transition.* This means that the transition for $j>0$ is of the first order. For $j=0$ we have second-order transition, as in the nondegenerate band case, where χ is singular (cf. the Appendix).

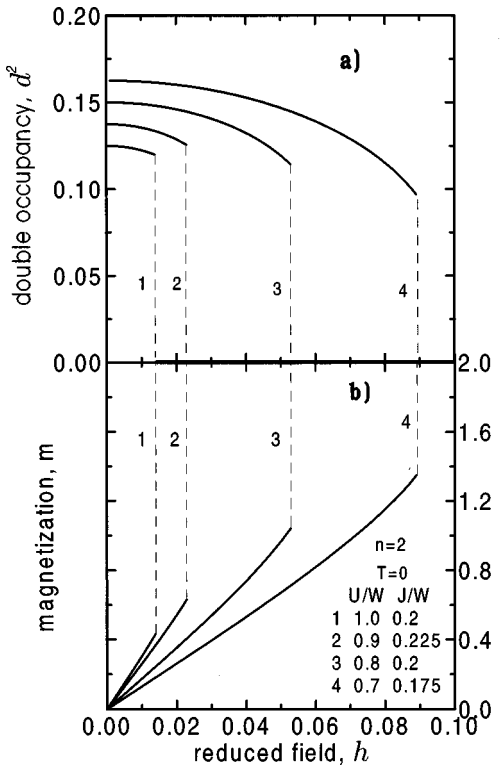

FIG. 1. Field dependences of double occupancy d^2 per orbital (a) and magnetization m per atom (b), both for $T=0$ and $n=2$.

Field dependences of d^2 and m are displayed on Figs. 1(a),(b), respectively. Close to the transition point the system exhibits a metamagnetic behavior, i.e., the $m(h)$ dependence is curved upwards. With the increasing field h the doubly occupancy diminishes because of the growing spin polarization and at the transition point d^2 jumps to zero, while the magnetic moment jumps to its saturation value. The magnitude of magnetization jump Δm and the critical field h_c depend on the values of j and u, as shown in Fig. 2. One observes here an example of a magnetic-field-induced localization, with a formation of a ferromagnetic (field-induced) insulator. The transition from the metal to the insulator can be either the first or second kind, depending on values u and j. Regimes of u and j, where the particular kind of a transition takes place, are displayed in Fig. 3. We mark the area of the insulating phase in zero field bounded by the curve determined from Eq. (33). The insulator polarizes at $T=0$ to a saturated state in an infinitesimal field; the jump of the magnetization is then equal to $\Delta m=2$. Upon increasing j the critical field h_c decreases; likewise the magnetization jump. From Fig. 2 and Fig. 3 one could seen that for $u>0.5$ a second-order transition does not occur. Obviously, our analysis is valid quantitatively only for j substantially smaller than u. Also, the critical field for metamagnetic transition becomes experimentally accessible only close to MIT ($u\to 2$) and reduces gradually to zero with growing j. This prediction could be tested experimentally (see below).

D. Case $n<2$ and $T=0$: Spin-split masses, and MIT for $n=1$

Consider now briefly the situation $n<2$ when the metallic state is stable. We examine the effect of magnetic field on the

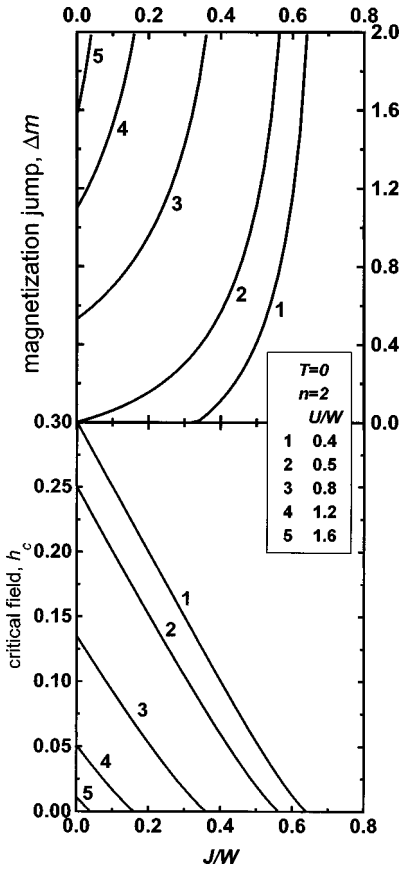

FIG. 2. Jump of the magnetization Δm per atom and the critical magnetic field h_c both as a function of exchange interaction J/W and calculated at the metal-insulator transition for $T=0$ and $n=2$.

transition to the saturated state, as a function of the parameters u and j. The ground-state energy for a polarized state is provided by the expression

$$E_M(n)\equiv\frac{F}{NW}=-\tfrac{1}{16}\sum_{\sigma} q_{\sigma}(4-n-\sigma m)(n+\sigma m)+2ud^2$$

$$-\tfrac{1}{8}jm^2-hm+\tfrac{1}{4}kn^2. \qquad (48)$$

The energy of the saturated state is obtained by taking into account Eq. (26) and making the substitution $d^2\rightarrow 0$ and $m\rightarrow n$ in Eq. (48). We have then

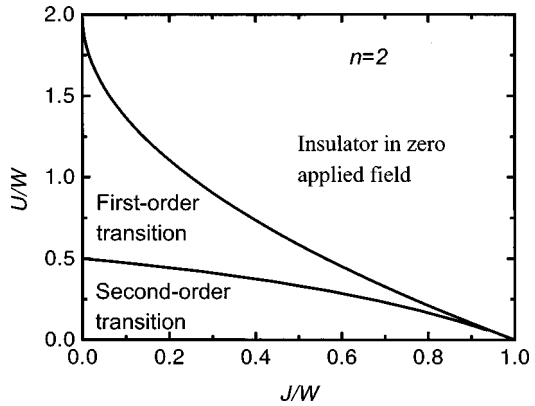

FIG. 3. Regimes of U/W and J/W for the half-filled band configuration comprising both first- and second-order transition regimes in an applied magnetic field.

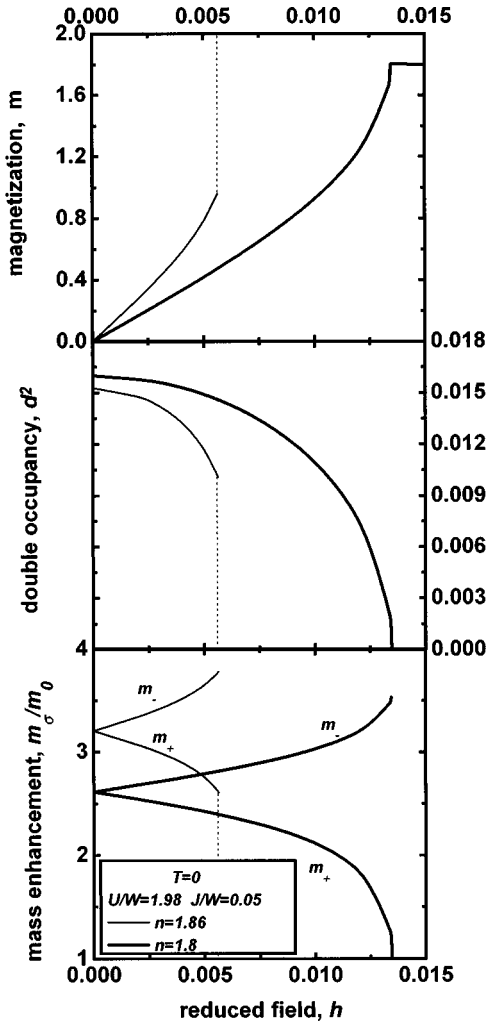

FIG. 4. Field dependences of magnetization m per atom, double occupancy d^2 per orbital, and the spin-dependent mass enhancement m_σ/m_0, all for $n<2$ (from the top to the bottom, respectively).

$$E_I(n)\equiv-\tfrac{1}{2}n(2-n)-\tfrac{1}{8}jn^2-hn+\tfrac{1}{4}kn^2. \qquad (49)$$

In Fig. 4 we display magnetization m, doubly occupancy d^2, and the mass enhancement q_σ^{-1} as a function of applied magnetic field for $u=1.98$ and $j=0.05$, for the band fillings $n=1.86$ and $n=1.8$. The important feature is that the mass enhancement is spin dependent (see the lowest panel). Also, there is a possibility of first- and second-order transitions to a saturated state. Regimes of u and j, where these two types of transition are possible for filling $n=1.8$ are shown in Fig. 5(a). By comparing this figure with Fig. 3 we see that regime of stability of an insulator for $n=2$ corresponds here to the area Ib with excluded doubly occupancy (EDO), when the system is in a magnetically saturated state in a vanishing field. In the case of one-band model, i.e., $j=0$, EDO state for $n\neq 1$ is reached for $u\rightarrow+\infty$ in $h=0$. For $j\neq 0$, the doubly degenerate case, this state is achieved for finite u.

One should note that the effect of spin-split masses arising in the magnetically polarized state is not associated with the emergence of the spin-dependent density of states in the bare band. This can be seen from the fact that the quasipar-

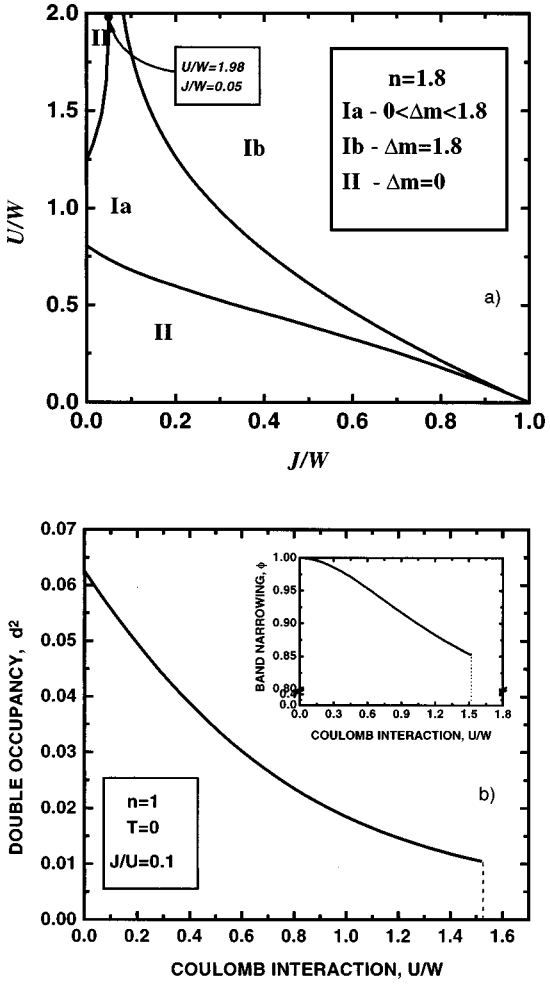

FIG. 5. (a) Regimes of U/W and J/W of first- and second-order transitions in applied magnetic field for $T=0$. (b) The metal-insulator transition for $n=1$, (for $J/U=0.1$), as exemplified by d^2 vs U/W dependence. The band narrowing is exhibited in the inset.

ticle energies $E_{\mathbf{k}\sigma}$ [cf. Eq. (24)] lead to the following density of states:

$$\rho_\sigma(E)=\frac{1}{q_\sigma}\rho_\sigma^{(0)}\left(\varepsilon-\frac{\sigma\left(h+\frac{1}{4}Jm-\beta_3\right)}{q_\sigma}\right), \tag{50}$$

where $\rho_\sigma^{(0)}(\varepsilon)$ is the density of bare states per spin. Thus, the enhancement due to the correlations is distinct from the shift of the density of states caused by the presence of the effective field. The many-body nature of the enhancement factor can be also seen by writing the quasiparticle energy in the form

$$\begin{aligned}E_{\mathbf{k}\sigma}&=\varepsilon_{\mathbf{k}}-\sigma h+(q_\sigma-1)\varepsilon_{\mathbf{k}}-\sigma(\tfrac{1}{4}Jm-\beta_3)\\&\equiv\varepsilon_{\mathbf{k}}-\sigma h-\Sigma_\sigma(\omega=\varepsilon_{\mathbf{k}}),\end{aligned} \tag{51}$$

where the self-energy is

$$\Sigma_\sigma(\omega)=-(1-q_\sigma)\omega-\sigma(\tfrac{1}{4}Jm-\beta_3). \tag{52}$$

Taking into account the well-known definition of the mass enhancement in the Fermi liquid,

$$\frac{m_0}{m^*}=\lim_{\omega\to\mu}\left(1+\frac{\partial}{\partial\omega}\mathrm{Re}\Sigma_\sigma(\omega)\right), \tag{53}$$

we have that $m_0/m^*=q_\sigma$, i.e., is indeed spin dependent. This spin dependence, which will lead to the strong field dependence of the linear specific heat close to the metamagnetic transition (see Spałek *et al.*[11]) is characteristic of the almost localized fermions and should be determined experimentally. Note that it is the same for all $\mathbf{k}$ states.

One should observe that a discontinuous transition is possible also for $n=1$. In Fig. 5(b) we display the double occupancy d^2 as a function of U/W and show the transition at $U_c/W=1.52$ for $J/U=0.1$; the associated with it band-narrowing-factor change is included in the inset. One sees a clear difference with the approach in Ref. 1, where the same transition is continuous. The difference disappears at nonzero temperature, where it is always discontinuous (cf. Ref. 9 and the discussion below). In our case the first-order transition is driven by the difference in the interorbital Coulomb term $\sim Kn^2$, which is absent in the insulating phase. Thus the first-order nature of MIT here is common to both $n=1$ and $n=2$ cases. Also, the critical value of U_c for $n=1$ is higher than that for $n=2$, for the same reason. The field and temperature dependences of the physical quantities for $n=1$ are similar to the those for $n=2$, so we will not repeat them here.

III. MOTT-HUBBARD BOUNDARY AT NONZERO TEMPERATURE

A. Phase diagram: $h\geqslant 0$

In the preceding section we considered the system properties at zero temperature. We concentrate now on a more realistic case of nonzero temperature in the half-filled band case. The low-temperature (Sommerfeld) expansion[9] of the free energy (23) for the metallic phase leads to the following expression for the constant DOS:

$$\frac{F_M}{NW}=-(4-m^2)\Phi/8+2ud^2-hm-\frac{1}{8}jm^2+k-\frac{2\pi^2}{3\Phi}\tau^2, \tag{54}$$

where $\tau=k_BT/W$. No higher-order term in τ appears for this DOS.

Hamiltonian describing the insulating phase can be rewritten in the form

$$\begin{aligned}\mathcal{H}_I&=K\sum_i n_{i1}n_{i2}-2J\sum_i \mathbf{S}_{i1}\cdot\mathbf{S}_{i2}-2h\sum_{il}S_{il}^z\\&=\sum_i\left[Kn_{i1}n_{i2}-J(\mathbf{S}_i^2-\mathbf{S}_{i1}^2-\mathbf{S}_{i2}^2)-2hS_i^z\right],\end{aligned} \tag{55}$$

where $\mathbf{S}_i=\mathbf{S}_{i1}+\mathbf{S}_{i2}$ is the total spin per site. The eigenstates of H_I are singlet and triplet configurations. The partition function is then given by

$$\begin{aligned}Z&=\mathrm{Tr}(e^{-\beta\mathcal{H}_I})\\&=e^{-\beta KN}[e^{-3\beta J/2}+e^{\beta J/2}+e^{\beta J/2}(e^{2\beta h}+e^{-2\beta h})]^N\\&=e^{-\beta KN}[e^{-3\beta J/2}+e^{\beta J/2}(1+2\cosh(2\beta h))]^N.\end{aligned} \tag{56}$$

This expression leads to the free energy for the Mott insulating state in the following form:

$$\frac{F_I}{NW} = -\frac{1}{NW\beta}\ln[Z]$$
$$= k - \frac{1}{W\beta}\ln[e^{-3\beta J/2} + e^{\beta J/2}(1+2\cosh(2\beta h))]$$
$$= k - \tau\ln[e^{-3j/2\tau} + e^{j/2\tau}(1+2\cosh(2h/\tau))]. \quad (57)$$

The result in the limit $\tau \to 0$ reduces to the expression (47). The magnetization in this state is

$$m \equiv 2\mathrm{Tr}(S_i^z e^{-\beta\mathcal{H}_I})$$
$$= 2\frac{e^{-\beta KN}e^{\beta J/2}(e^{2\beta h} - e^{-2\beta h})}{e^{-\beta KN}[e^{-3\beta J/2} + e^{\beta J/2}(1+2\cosh(2\beta h))]}$$
$$= \frac{4\sinh(2\beta h)}{e^{-2J\beta} + 1 + 2\cosh(2\beta h)} = \tanh(h/\tau)\frac{2}{\dfrac{e^{-2j/\tau}-1}{4\cosh^2(h/\tau)} + 1}, \quad (58)$$

For $j = 0$ we obtain $m = 2\tanh(h/\tau)$, the expression for the magnetization of noninteracting spins. Such a situation arises because the saddle-point approximation in its essence is a single-site approximation (the intersite interaction arises from the quantum Gaussian fluctuations around it).

The field dependences of the magnetization and of the double occupancy are shown in Fig. 6. We see that upon increasing j while keeping fixed u the critical metamagnetic field is reduced. It indicates, as before for $T = 0$, a significant role of exchange interaction and, associated with it, Hund's rule. Also, the magnetization curve is slightly curved upwards in small fields. The upper part of the $m(h)$ curve reflects magnetization of the localized-moment system. Thus we have a transition from an itinerant (albeit metamagnetic) to localized-type behavior as a function of h.

Substituting the expressions for m and d^2 taken from the Appendix into the free energy (54) we can determine the system behavior in the vicinity of $h = 0$. The phase diagram for cases $h = 0$ and 0.01, for different values of J/U is exhibited in Fig. 7. Upon increasing of J/U the paramagnetic insulating (PI) phase expands at the expense of the paramagnetic metallic (PM) phase. In the applied field the boundaries shift towards lower temperatures. We see also a typical reentrant metallic behavior at high temperatures. Namely, with rising temperature the system evolves from a metal through an insulator back to the metallic state. In the inset we display the temperature dependence of the free energies for PM and PI states.

The shape of the phase boundary is essentially the same as in the nondegenerate-band case.[9] However, it is shifted remarkably towards lower values of U/W already for rather small values of J/W. The boundary is of first order apart from the point specified. The upper part of the curve is only qualitative, particularly if a realistic DOS is used, as higher-order contribution in τ will become important. In fact, the solution of the Hubbard model in the infinite-dimension limit[10] provides only a crossover behavior, not a weakly discontinuous retrograde behavior.

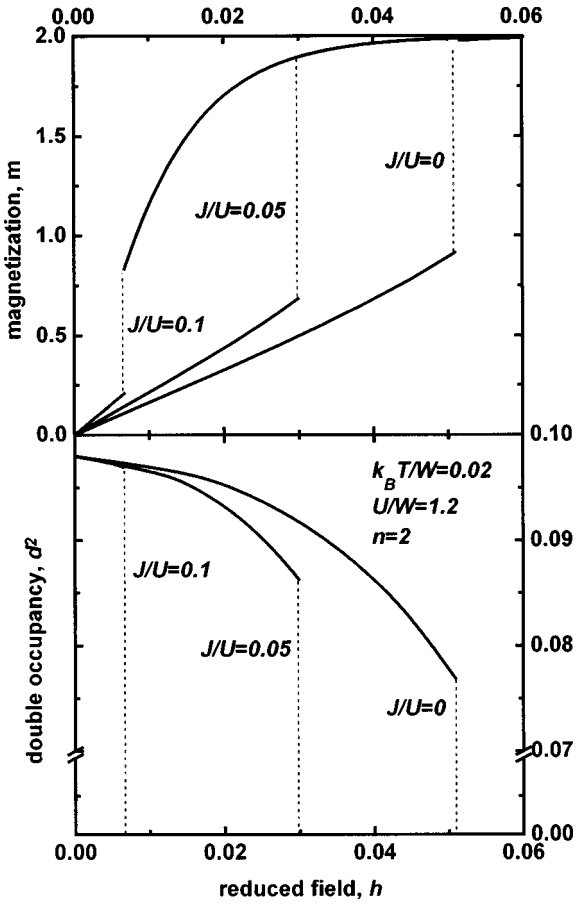

FIG. 6. Field dependences of the magnetization and double occupancy for different values of J/U.

One may ask if the low-T analysis is realistic, since in the mean-field slave-boson analysis the low-energy spin fluctuations (quantum Gaussian fluctuations around the saddle point here) have been neglected. Those spin fluctuations lead to the contribution $\sim T^4\ln(T/\theta)$ in the free energy.[14] This con-

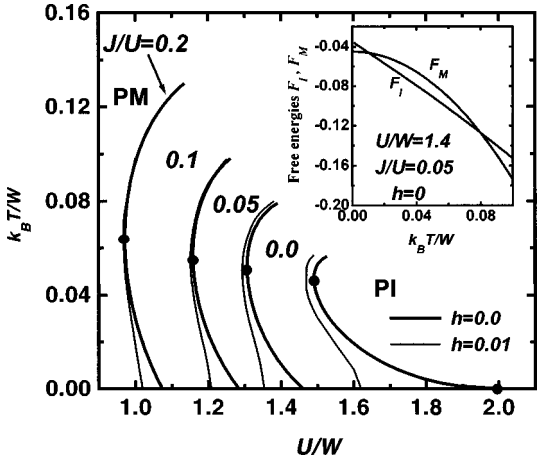

FIG. 7. The PM–PI phase boundaries as a function of U/W for $n = 2$ (thick lines), and their shift in the applied magnetic field (fine lines). The inset displays the free energies for PM and PI states as a function of temperature.

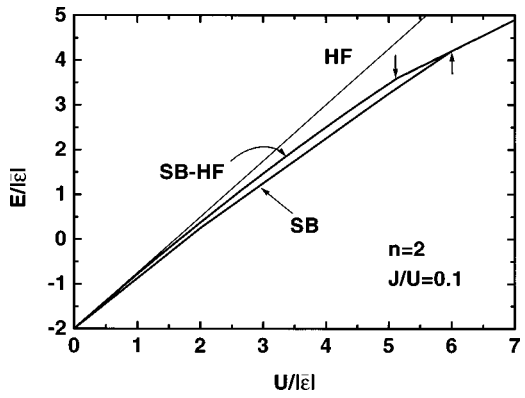

FIG. 8. Comparison ground-state energies for $T=h=0$, $n=2$, and $J/U=0.1$ obtained from these methods: Hartree-Fock, slave boson, and slave boson combined with Hartree-Fock. The arrows indicate the position of MIT in the two last approximation schemes.

tribution is of higher order than the T^2 contribution coming from the quasiparticle excitations across the Fermi surface. Therefore, the analysis is realistic, but only to the leading order in low-T expansion, as we have done it.

B. Physical discussion

The evolution of the almost localized fermions discussed above for the half-filled band case can be explained nicely from a physical point of view. Namely, for $U\rightarrow U_c$ the renormalized band ($\Phi\overline{\epsilon}$) and the correlation (Ud^2) energies *almost compensate each other.* In such a situation, much smaller entropy ($\sim TS$) or applied field ($\sim\mu_B H_a$) energies tip the balance towards either the M or I phase. Explicitly, at low temperatures, the spin-disordered magnetic insulator has much larger entropy contribution ($-k_B T\ln 2$, per orbital) than that of the almost localized Fermi liquid [$-\gamma_0 T^2/(2\Phi)$, with $\gamma_0=(2/3)\pi^2 k_B^2\rho$]. This circumstance tips the balance from the PM state (with $E_G<0$, but small entropy contribution) towards the PI state (with $E_G=0$, but much larger entropy contribution). At much higher temperatures the balance is tipped back towards the PM phase, since eventually the entropy of the metallic state grows and approaches the asymptotic value $2k_B\ln 2$ per orbital. Thus the reentrant metallic behavior is driven by the entropy. It is observed in both $(V_{1-x}Cr_x)_2O_3$ (Ref. 15) and $NiS_{2-x}Se_x$ (Ref. 3) systems. It can be applied also to explain the low-temperature reentrant liquid behavior in liquid ^{3}He.[16] In our view the reentrant behavior appearing either as a crossover or as a discontinuous transition (^{3}He) is uniquely present in the Mott-Hubbard systems defined as systems, for which the band and the Coulomb parts of their energy almost compensate each other. The intra-atomic exchange contribution tips the balance further towards the localized state.

Obviously, the first-order nature of the transition will lead to the coexistence of the two phases, with localized and itinerant electrons, respectively. However, this mixed phase can be discussed only when the magnetism is included, and we will not elaborate on it here.

As mentioned at the beginning, the present formulation represents for $H_a=T=0$ a simplified version of the full slave-boson and Gutzwiller treatments[1] discussed recently. In Fig. 8 we have compared the Hartree-Fock (HF), ours (SB-HF), and full slave-boson (SB) results for the ground-state energies for $h=0$ and $n=2$. The arrows denote the position of the Mott-Hubbard boundary in the two latter schemes. The energy difference diminishes rapidly with growing h. The difference for physical quantities is only quantitative, not qualitative, though the SB approach[1] has slightly lower energy, since it contains many more variational parameters. In the next section we extend the main features of our solution to arbitrary J/W and higher degeneracy d of equivalent orbitals and an arbitrary filling.

IV. METAL-INSULATOR TRANSITION FOR ARBITRARY ORBITAL DEGENERACY AND FILLING: A SPIN ROTATION INVARIANT MODEL

A. Global (site) representation of the intraatomic interaction

We now generalize the principal features of our argument to the case of orbital degeneracy. First, we represent the intraatomic part in terms of global (site) representation. For that purpose we start from the following expression of that part:

$$\mathcal{H}_I=U\sum_{il} n_{il\uparrow}n_{il\downarrow}+\frac{1}{2}K\sum_{ill\sigma\sigma'}{}' n_{il\sigma}n_{il'\sigma'}-J\sum_{ill'}{}' \mathbf{S}_{il}\cdot\mathbf{S}_{il'}, \tag{59}$$

where now l and l' assume the values $1,2,\ldots,d$, and the primed summation is taken for $l\neq l'$. We introduce the global spin and particle number operators through the relations

$$\mathbf{S}_i\equiv(S_i^+,S_i^-,S_i^z)\equiv\sum_{l=1}^{d}\mathbf{S}_{il}, \tag{60}$$

and

$$n_i\equiv\sum_{\sigma} n_{i\sigma}\equiv\sum_{l\sigma} n_{il\sigma}. \tag{61}$$

We have the following relations between global and previously introduced operators:

$$\sum_{ll'} n_{il}n_{il'}=n_i^2-n_i-2\sum_{l} n_{il\uparrow}n_{il\downarrow}, \tag{62}$$

and

$$\sum_{ll'}{}' \mathbf{S}_{il}\cdot\mathbf{S}_{il'}=\mathbf{S}_i^2+\frac{3}{2}\sum_{l} n_{il\uparrow}n_{il\downarrow}-\frac{3}{4}n_i. \tag{63}$$

Hence, up to a constant $\mathcal{H}_I$ takes the form

$$\mathcal{H}_I=\frac{1}{2}K\sum_{i} n_i^2-J\sum_{i}\mathbf{S}_i^2+I\sum_{il} n_{il\uparrow}n_{il\downarrow}, \tag{64}$$

where $I=U-K-\frac{3}{2}J$.

For a particular example of the e_g band we have

$$\mathcal{H}_I=\tfrac{1}{2}(U-\tfrac{5}{2}J)\sum_{i} n_i^2-J\sum_{i}\mathbf{S}_i^2+J\sum_{il} n_{il\uparrow}n_{il\downarrow}. \tag{65}$$

The first term represents charge fluctuations, the second the atomic Hund's rule. Moreover, unlike in a nondegenerate band the intraorbital intraatomic (Hubbard) parameter (J) is much smaller than U. Additionally, the first two terms are proportional to d^2 while the third is $\sim d$. Hence, the last term can become the smallest, particularly for highly degenerate systems. In general, the Hamiltonian (64) expresses the so-called minimum polarity model of Van Vleck (charge fluctuations suppressed by growing U), as well as the separation of the dynamic processes into inequivalent charge and spin degrees of freedom in the effective one-band model introduced by Hubbard.[17] For highly degenerate systems we can approximate

$$I\sum_{il} n_{il\uparrow}n_{il\downarrow} \simeq I\sum_{il} \frac{n_{i\uparrow}}{d}\cdot\frac{n_{i\downarrow}}{d} = \frac{I}{d}\sum_{i} n_{i\uparrow}n_{i\downarrow}. \tag{66}$$

Noting that

$$n_{i\uparrow}n_{i\downarrow} = \frac{n_i^2}{4} - (\boldsymbol{\mu}_i\cdot\mathbf{S}_i)^2, \tag{67}$$

where $\boldsymbol{\mu}_i$ is unit vector along an arbitrarily oriented spin quantization axis for the spin $\mathbf{S}_i$, one has finally

$$\mathcal{H}_I \simeq \frac{\widetilde{U}}{4}\sum_i n_i^2 - J\sum_i \mathbf{S}_i^2 - \frac{I}{d}\sum_i (\boldsymbol{\mu}_i\cdot\mathbf{S}_i)^2, \tag{68}$$

where $\widetilde{U}\equiv 2K + I/d$. For a particular case of a nondegenerate band ($d=1$), $K=J=0$, we recover the earlier results[18] with $\widetilde{U}=U$, and $I=U$. For $d\to\infty$ the last term is absent and the correlated paramagnetic state at $T=0$ is described by two variational parameters:

$$\lambda \equiv \langle n_i^2\rangle, \tag{69}$$

and

$$m \equiv \langle \mathbf{S}_i^2\rangle. \tag{70}$$

Note that in this section m represent the local-moment magnitude. The third parameter describing the long-range order is obtained by making the Hartree-Fock approximation,

$$\frac{I}{d}\sum_i (\boldsymbol{\mu}_i\cdot\mathbf{S}_i)^2 \simeq \frac{I}{d}\sum_i (\boldsymbol{\mu}_i\cdot\langle\mathbf{S}_i\rangle)\boldsymbol{\mu}_i\cdot\mathbf{S}_i. \tag{71}$$

The collinear magnetic ordering is expressed then through $\langle S_i^z\rangle = \boldsymbol{\mu}_i\cdot\langle\mathbf{S}_i\rangle$. Since in this section we consider only a paramagnetic state at $T=H_a=0$, we neglect in our analysis the last term. Note however, that the present parameters λ, m, and $\langle\boldsymbol{\mu}_i\cdot\mathbf{S}_i\rangle$ for arbitrary d correspond directly to the parameters d^2, $p_\uparrow^2$, and $p_\downarrow^2$ in the preceding section (e^2 is removed via the completeness condition $e^2+p_\uparrow^2+p_\downarrow^2+d^2=1$).

B. Magnitude of local-moment and charge fluctuations: First-order transition to the insulating state at $T=0$

In direct analogy to the doubly degenerate case discussed in Sec. II, we express the ground-state energy in the form

$$\frac{E_G}{N} = \Phi(\lambda,m)\overline{\epsilon} + \frac{\widetilde{U}}{4}\lambda - Jm, \tag{72}$$

where now the band narrowing factor Φ depends on λ and $\overline{\epsilon}$ represent the average band energy for a degenerate system. Without a loss of generality one can assume that $\Phi(\lambda,m) = \Lambda(m)G(m)$. In accordance with our simple derivation of the mean-field (Gutzwiller) approach in the half-filled band case[19] we make an expansion:

$$\Lambda(\lambda) = l_0 + l_1\lambda + l_2\lambda^2, \tag{73}$$

and

$$G(m) = g_0 + g_1 m + g_2 m^2. \tag{74}$$

Note that $0\leqslant\Phi\equiv\Lambda G\leqslant 1$. The expansion has the meaning of a Landau expansion, and the coefficients can be determined by calculating E_G explicitly in limiting situations. For example, in the Hartree-Fock approximation we have $\Lambda = G = 1$ and thus elementary analysis provides us with

$$\lambda\equiv\lambda_0 = n + n^2\left(1 - \frac{1}{2d}\right), \tag{75}$$

and

$$m\equiv m_0 = \frac{3}{4}n\left(1 - \frac{n}{2d}\right), \tag{76}$$

where n is the band filling ($n=d$ corresponds to the half-filling). Analogously, for $\widetilde{U}\to\infty$ and $J\to\infty$, the quantities λ_0 and m_0 will approach their atomic values λ_∞, m_∞:

$$m\equiv m_\infty = \begin{cases} \frac{3}{4} & \text{for } n\leqslant 1 \\ \frac{n}{2}\left(\frac{n}{2}+1\right) & \text{for } n\geqslant 1, \end{cases} \tag{77}$$

and

$$\lambda\equiv\lambda_\infty = \begin{cases} n & \text{for } n\leqslant 1 \\ n^2 & \text{for } n\geqslant 1. \end{cases} \tag{78}$$

Additionally, applying the equilibrium conditions

$$\frac{\partial E_G}{\partial\lambda_0} = \frac{\partial E_G}{\partial m_0} = 0, \tag{79}$$

we obtain the expression

$$\lambda = \lambda_0\left[1 - \frac{\widetilde{U}}{8l_2\lambda_0|\overline{\epsilon}|G(m)}\right], \tag{80}$$

$$m = m_0\left[1 + \frac{J}{2g_2 m_0|\overline{\epsilon}|\Lambda(\lambda)}\right]. \tag{81}$$

As in nondegenerate case, the charge fluctuations are suppressed with increasing $\widetilde{U}$. On the contrary, the magnetic moment grows with increasing J. Additionally, using the conditions $\Lambda(\lambda_0)=G(m_0)=1$ we obtain

$$\Lambda(\lambda) = 1 + l_2(\lambda-\lambda_0)^2, \tag{82}$$

$$G(m)=1+g_2(m-m_0)^2. \tag{83}$$

The coefficients l_2 and g_2 are determined from the condition that for any integer band filling $n\geqslant 1$ we have that $\Lambda(\lambda_\infty)=0$, and $G(m_\infty)=n_\sigma/n=1/2$ (this result is valid for the paramagnetic configuration only and reflects the Pauli exclusion). So, finally we have

$$\Lambda(\lambda)=1-\left(\frac{\lambda-\lambda_0}{\lambda_\infty-\lambda_0}\right)^2, \tag{84}$$

and

$$G(m)=1-\frac{1}{2}\left(\frac{m-m_0}{m_\infty-m_0}\right)^2. \tag{85}$$

Substituting these expressions into the expression (72) for E_G, we obtain the explicit form in the terms of variational variables λ and m. Making use of the conditions $\partial E_G/\partial m=\partial E_G/\partial\lambda=0$ we arrive at the algebraic equations, which may be transformed into the following equations for the functions G and Λ taken at the extremal points:

$$G^3-G^2\left[1-2\frac{\tilde{U}}{U_0}+\left(\frac{J}{J_c}\right)^2\frac{1}{g_2}\right]+G\frac{\tilde{U}}{U_0}\left(\frac{\tilde{U}}{U_0}-2\right)-\left(\frac{\tilde{U}}{U_0}\right)^2=0, \tag{86}$$

and

$$\Lambda^3-\Lambda^2\left[1+2\frac{J}{J_c}+\left(\frac{\tilde{U}}{U_0}\right)^2\frac{1}{l_2}\right]+\Lambda\frac{J}{J_c}\left(\frac{J}{J_c}+2\right)-\left(\frac{J}{J_c}\right)^2=0, \tag{87}$$

with $U_0=8|\overline{\epsilon}|$, and $J_c=2|\overline{\epsilon}|$. These two equations can be transformed into each other by changes $\Lambda\leftrightarrow G$, $g_2\leftrightarrow l_2$, and $J/J_c\leftrightarrow-\tilde{U}/U_0$. Hence, it is sufficient to solve numerically one of them and adapt it subsequently for the second equation. One should notice that the nondegenerate-band-case result $\lambda=\lambda_\infty$ (i.e., $d^2=0$) is recovered for $U/U_0=1$.

Before going into the numerical analysis let us summarize the above subsection. We have developed a relatively simple scheme of calculating the magnitudes of local moment $\langle\mathbf{S}_i^2\rangle$ and of the charge fluctuations $\langle n_i^2\rangle$, which is equivalent to the Gutzwiller-Brinkman-Rice scheme[8] for $d=1$. These magnitudes are calculated from a relative balance between the renormalized band energy from one side, and the correlation energies $[(\tilde{U}/4)\lambda^2-Jm^2]$ from the other. The method involves an interpolation between low- and high-correlation regimes (note that the mean-field slave-boson theory requires such an interpolation to the $U\rightarrow 0$ limit[13,12]).

C. Numerical analysis for arbitrary degeneracy and filling

We define the reduced variables

$$\lambda_R=\frac{\lambda-\lambda_0}{\lambda_\infty-\lambda_0}, \tag{88}$$

and

$$m_R=\frac{m-m_0}{m_\infty-m_0}. \tag{89}$$

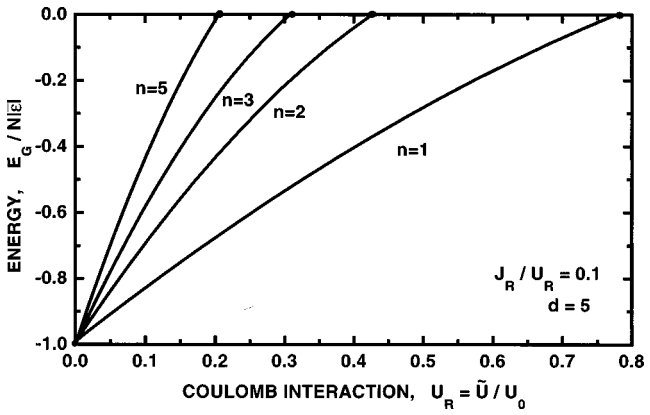

FIG. 9. The ground-state energy per site (in units of $|\overline{\epsilon}|$) as a function of the Coulomb interaction $U_R=\tilde{U}/U_0\equiv\tilde{U}/8|\overline{\epsilon}|$. A transition to the Mott-Hubbard insulating state takes place for each (integer) band filling n for the value of U_R at which $E_G=0$.

In this manner, the values $\lambda_R=m_R=0$ corresponds to the Hartree-Fock approximation, whereas the limit with $\lambda_R=m_R=1$ corresponds to the exact atomic limit, which for an integer $n\geqslant 1$ corresponds to the Mott-Hubbard insulator. In Fig. 9 we have plotted E_G as a function of $U_R\equiv\tilde{U}/U_0=\tilde{U}/8|\overline{\epsilon}|$, for $J_R/U_R=0.1$, which corresponds to $J/\tilde{U}=0.4$. The bare band energy for the featureless density of states is $\overline{\epsilon}=-(W/2)n(1-n/2d)$. One sees that $E_G=0$ for a critical value of U_R. At this point the values λ_∞ and m_∞ are reached for $n>1$ in a discontinuous way, as illustrated in Figs. 10(a),(b). The localization threshold diminishes with n. This is because the band energy varies roughly $\sim n$, while the interaction energy is $\sim n^2$. The transition to the localized-moment state is determined by the interplay between the exchange and the Coulomb interaction. This is illustrated in Figs. 11(a),(b), where the band-narrowing factors Λ and G have been specified. In most situations the part $G(m)$ changes from its Hartree-Fock value only a little. This provides an *a posteriori* justification of the Hartree-Fock approximation for the exchange term. The dominant role of the term $\sim n_i^2$ over the Hund's rule term gives some support to the interpretation of the local-moment formation in the terms of a nondegenerate Hubbard model. This becomes clear if one notices that in that case

$$\lambda=\langle n_i^2\rangle=n+2\langle n_{i\uparrow}n_{i\downarrow}\rangle=n+2d^2, \tag{90}$$

and hence $\lambda=\lambda_\infty=n$ correspond to the limit $d^2=0$ ($\Lambda=0$). In the situation depicted in Fig. 11(a) $\Lambda\approx 0.6$ at the transition. However, unlike the nondegenerate system, the spin-charge fluctuation coupling is leading to the discontinuous character of this transition for $n\geqslant 1$.

The discontinuous nature of the metal-insulator transition induces only a weak enhancement of the effective mass close to the transition [the curves in Fig. 10(b) are physically meaningful only below the discontinuity points]. The results in this respect are valid universally for arbitrary $d>1$ and $n\geqslant 1$.

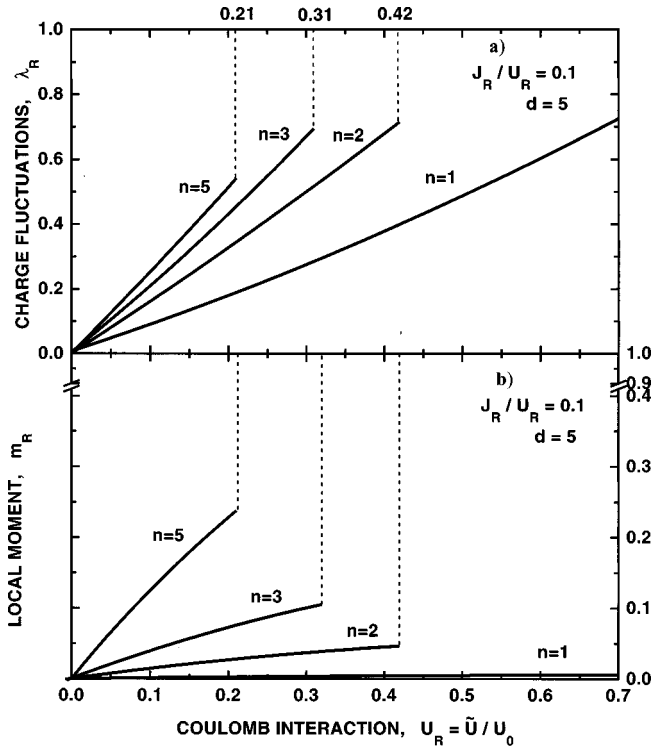

FIG. 10. (a) The relative magnitude of the charge fluctuations $\lambda_R=(\lambda-\lambda_0)/(\lambda_\infty-\lambda_0)$ versus U_R. Note a discontinuous nature of the transition to the atomic configuration $\lambda=\lambda_\infty$ at a critical value of U_R specified for each $n>1$. (b) The relative magnitude of the local moment $m_R=(m-m_0)/(m_\infty-m_0)$, as a function of U_R. The discontinuous jump in m reflects the same behavior as of λ_R.

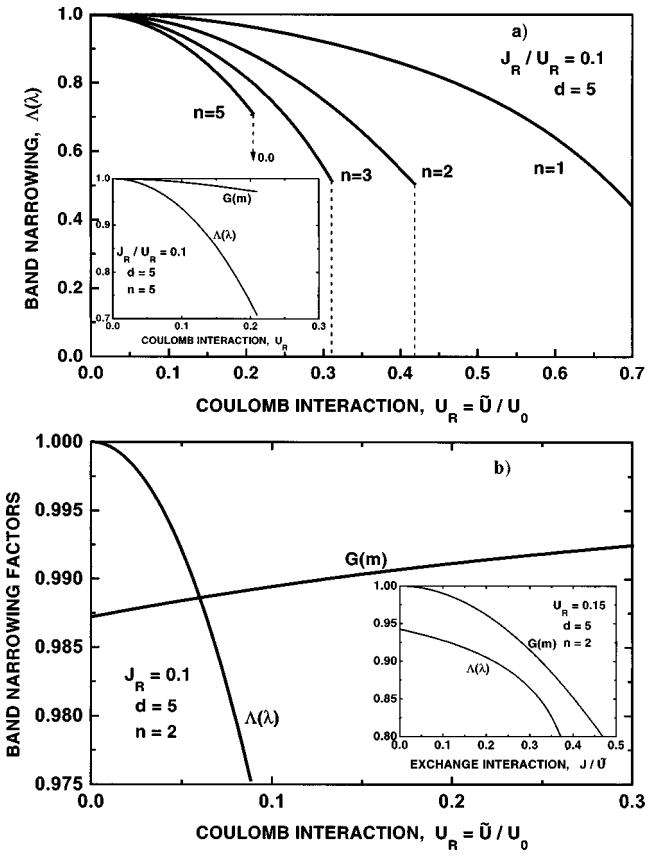

FIG. 11. (a) The band-narrowing parts $\Lambda(\lambda)$ and $G(m)$ as the magnitude of the Coulomb interaction. The inset compares the two narrowing factors, both diminishing with increasing U_R. (b) The charge- and spin-fluctuation parts of the band narrowing as a function of the Coulomb interaction, for the value of U_R below the Mott transition. The inset displays the different trend as a function of the $J/\tilde{U}$ ratio.

V. CONCLUSIONS

In this paper we have put an emphasis on the similarities and differences of the Mott localization in a degenerate-band system with the extensive analysis of MIT existing for the nondegenerate-band case. For that purpose we have made in the first part the Hartree-Fock approximation for the exchange interaction. This approximation is applicable in the limit when J is substantially smaller than U, as is usually the case for $3d$ bands. This scheme provides us with the physically plausible conclusion that the metal-insulator transition is mainly driven by the intraatomic Coulomb interaction; the intraatomic exchange is responsible for the first-order nature of the transition already at $T=0$. Also, with this approach one can see that the correlated systems, whether orbitally degenerate or not, can in the mean-field approximation be described as systems of fermionic quasiparticles with spin-split masses (in the magnetically polarized state) and a nonlinear molecular field coming from the correlations, in addition to the usual exchange field.

The fundamental question is whether the present approach (as well as those listed in Ref. 1) provide a proper mean-field theory of a correlated state near the metal-insulator transition. It seems so and the proper order parameter in the orbitally nondegenerate paramagnetic system is either Φ or d^2, which are nonzero in the metallic phase and vanish in the insulating state. What is more important, since for $n=2$ the band-narrowing factor Φ in the PM state can be directly related[20] to the physical quantity $Z(=\Phi)$ representing the discontinuity of the Fermi-Dirac distribution at the Fermi energy, the order parameter is a measurable quantity for this quantum phase transition at $T=0$. In the magnetically ordered state the system is additionally characterized by a staggered moment $\langle S_i^z\rangle$. In the second part of this paper we have shown that even in the paramagnetic state the orbitally degenerate system is additionally characterized by the parameter $\langle \mathbf{S}_i^2\rangle$ describing the local moment magnitude. Thus, in our view, the set of the parameters: $d^2 \Leftrightarrow \langle n_i^2\rangle$, $\langle \mathbf{S}_i^2\rangle$, and $\mu_i \cdot \langle \mathbf{S}_i\rangle$ compose a *minimal set* describing the metal-insulator transition in the degenerate system and associated with it the magnetic transition [in a nondegenerate system $\langle \mathbf{S}_i^2\rangle = \frac{3}{4}(1-2d^2)$]. Obviously, the full slave-boson and Gutzwiller approaches[1] provide essentially the same qualitative picture, although they contain more parameters, which are eliminated by implementing the constraints appearing as consistency conditions. In this respect, our simplified approach provides didactical guidance for more complicated analysis. For example, the effect of quantum Gaussian fluctuations in auxiliary Bose fields[14] neglected so far will introduce intersite exchange interactions, which will not introduce any additional order parameter, though the detailed thermodynamic properties will contain the contribution coming from the interaction between the quasiparticles with the characteristics (q_σ, β_3, β_0), which appeared on the mean-field level.

The slave-boson approach has been recently extended[22] to describe the antiferromagnetic phase in the half-filled doubly degenerate Hubbard model. However, the temperature dependence of MIT in the paramagnetic phase is still important, since in $NiS_{2-x}Se_x$ (Ref. 3) one observes a transition to the semiconducting phase upon heating the system, when the system crosses the Néel point (cf. Fig. 7 for $H_a=0$, where the M→I transition is observed upon heating the system). The detailed analysis requires the discussion of antiferromagnetic insulating and metallic states at $T>0$ before any direct comparison with the experiment is made. Also, in the case of a quarter-filled band the system undergoes a transition from a ferromagnetic metal [as observed in CoS_2 (Ref. 23)] to a ferromagnetic insulator with an orbital ordering.[24] Therefore, the role of both magnetic ordering near MIT, as well as of degeneracy (albeit weak[25]) must be determined in detail.

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APPENDIX: MAGNETIC SUSCEPTIBILITY AND DOUBLE OCCUPANCY OF THE METALLIC STATE CLOSE TO THE MOTT-HUBBARD LOCALIZATION

We start from the expression (54) for the free-energy functional for a constant DOS and in the half-band case:

$$f=\frac{F_M}{NW}=-(4-m^2)\Phi/8+2ud^2-hm-\frac{1}{8}jm^2-\frac{2\pi^2}{3\Phi}\tau^2+k, \tag{A1}$$

where Φ is defined by Eq. (34).

Minimizing above expression with respect to m we obtain

$$0=\frac{\partial f}{\partial m}=\frac{d^2m}{\sqrt{4(1-2d^2)^2-m^2}}-h-\frac{1}{4}jm+\frac{2\pi^2}{3\Phi^2}\Phi_m\tau^2, \tag{A2}$$

where $\Phi_m=\partial\Phi/\partial m$. Differentiating the above equation with respect to h and taking $h=0$, for which $m=0$, we have

$$\frac{d^2}{1-2d^2}m_0'-2-\frac{1}{2}jm_0'-\frac{8\pi^2\tau^2}{3}\Phi_m\Phi_h\Phi^{-3}|_0+\frac{4\pi^2\tau^2}{3}\Phi_{mh}\Phi^{-2}|_0=0, \tag{A3}$$

where $m_0'=(dm/dh)_{h=0.}$ The derivative Φ for $m=h=0$ is

$$\left.\frac{\partial\Phi}{\partial m}\right|_0=\left\{\frac{32d^2}{(4-m^2)^2}[1-2d^2+\tfrac{1}{2}\sqrt{4(1-2d^2)^2-m^2}]m-\frac{8d^2}{(4-m^2)\sqrt{4(1-2d^2)^2-m^2}}m\right\}_{h=0}. \tag{A4}$$

We see that $\Phi_{m=0}=0$. Also, $(d^2)_0'=0$; this is because both Φ and d^2 depend only on even powers of either m or h. In that situation

$$\left.\frac{\partial^2\Phi}{\partial m\,\partial h}\right|_0=2d^2(1-2d^2+\sqrt{1-4d^2+4d^4})m_0'-\frac{d^2}{\sqrt{1-4d^2+4d^4}}m_0'=\frac{4d^2(1-2d^2)^2-d^2}{1-2d^2}m_0'=\frac{d^2(4d^2-3)(4d^2-1)}{1-2d^2}m_0'. \tag{A5}$$

So, we obtain the magnetic susceptibility $\chi\equiv dm/dh$ in the form

$$m_0'=2\left(\frac{d^2}{1-2d^2}-\frac{1}{2}j+\frac{\pi^2(4d^2-3)(4d^2-1)}{48d^2(1-2d^2)^3}\tau^2\right)^{-1}. \tag{A6}$$

We use also the low-temperature expansion of d^2 derived earlier:

$$d^2=\frac{1}{4}\left(1-\frac{u}{2}\right)-\frac{\tau^2\pi^2u}{6\left(1-\frac{1}{4}u^2\right)^2}. \tag{A7}$$

Expanding m_0' to the first order in τ^2 we arrive at the expression for χ in physical units:

$$\chi=\chi_0\left(\frac{1}{\frac{2-u}{2+u}-j}+\frac{16}{3}\pi^2u^2\times\frac{u^2+4u-4}{(4-u^2)^2(-2+u+2j+ju)^2}\tau^2\right) \tag{A8}$$

where χ_0 is the susceptibility for noninteracting particles.

We see that for $u>-2+2\sqrt{2}\approx0.83$ the susceptibility is always rising with temperature. Note that for DOS smoothly varying around the Fermi energy this increase is solely due to the correlations and corresponds to the approaching the localization boundary depicted in Fig. 7. In the nondegenerate case and for $T=0$, the corresponding Brinkman-Rice formula reads:

$$\chi=\chi_0\frac{2+u}{2-u}. \tag{A9}$$

Now we derive d^2 in small magnetic field and temperature. Because of time reversal symmetry d^2 depends only on even power of h. We determine nonvanishing term $\sim h^2$ at $T=0$. Substituting into Eq. (42) first the expression for m in the first order of h given by (44) and subsequently differen-

tiating twice, thus obtained formula we see that doubly-occupancy probability diminishes with growing T and/or h according to:

$$d^2=\frac{1}{4}\left(1-\frac{u}{2}\right)-\frac{\pi^2 u}{6\left(1-\frac{u^2}{4}\right)^2}\tau^2-\frac{4}{(-2+u+2j+ju)^2}h^2. \tag{A10}$$

The decrease of η with T and h signals a precursory localization effects discussed in Sec. II E.

We now generalize the results to the case with arbitrary DOS. We start from the expression (23) for the free energy with the condition

$$1=\sum_\sigma \int_{-W/2}^{W/2}\rho(\epsilon)n_\sigma(\epsilon)d\epsilon, \tag{A11}$$

for the chemical potential; $n_\sigma(\epsilon)$ is given by Eq. (22). Defining $H\equiv h+\frac{1}{4}Jm-\beta_3$, we obtain the following expression of m to the first order:

$$m=2\int_{-W/2}^{W/2}\rho(\epsilon)\sum_\sigma \sigma\left(\frac{1}{1+e^{(\phi\epsilon-\mu/k_BT)}}+\frac{1}{(1+e^{(\phi\epsilon-\mu/k_BT)})^2}e^{(\phi\epsilon-\mu/k_BT)}\frac{\sigma}{k_BT}H\right)d\epsilon \tag{A12}$$

or, explicitly

$$m=2(h+\tfrac{1}{4}Jm-\beta_3)K, \tag{A13}$$

with

$$K\equiv\int_{-W/2}^{W/2}\frac{2}{(1+e^{(\phi\epsilon-\mu/k_BT)})^2}\frac{e^{(\phi\epsilon-\mu/k_BT)}}{k_BT}\rho(\epsilon)d\epsilon. \tag{A14}$$

Differentiating the above equation with respect to h and taking $h=0$ we have

$$m_0'=2(1+\tfrac{1}{4}Jm_0'-\beta_{3,h=0}')K(h=0). \tag{A15}$$

Differentiating the free energy with respect to m we obtain the relation

$$\tfrac{1}{4}Jm-\beta_3+2\sum_\sigma\int_{-W/2}^{W/2}\rho(\epsilon)(\Phi_m\epsilon-\sigma\tfrac{1}{4}J)n_\sigma(\epsilon)=0, \tag{A16}$$

and hence,

$$\beta_3=2\Phi_m\sum_\sigma\int_{-W/2}^{W/2}\epsilon\rho(\epsilon)n_\sigma(\epsilon), \tag{A17}$$

which, when differentiated with respect to h, leads to

$$\beta_{3,h=0}'=4\Phi_{mh}|_0\int_{-W/2}^{W/2}\epsilon\rho(\epsilon)n_0(\epsilon), \tag{A18}$$

where $\Phi_{mh}|_0$ is given by Eq. (A5). From Eq. (A15) we have

$$\left.\frac{dm}{dh}\right|_{h=0}=2\frac{K}{-\frac{1}{2}KJ+4K\overline{\epsilon}(T)\frac{d^2(4d^2-3)(4d^2-1)}{1-2d^2}+1}, \tag{A19}$$

where all quantities on the right-hand side are taken for $h=0$, and $\overline{\epsilon}(T)$ is average band energy per site and orbital.

Next, we expand $\overline{\epsilon}(T)$, d^2, and K in the powers of T. From Ref. 20 we have that

$$d^2=\frac{1}{4}(1-I)-\frac{2\pi^2}{3}\frac{I\rho}{U_0}\left(\frac{k_BT}{\Phi_0}\right)^2, \tag{A20}$$

$$\Phi=\Phi_0-\frac{16\pi^2}{3}\frac{I^2\rho}{U_0}\left(\frac{k_BT}{\Phi_0}\right)^2, \tag{A21}$$

and

$$\overline{\epsilon}(T)=-\frac{U_0}{8}+\frac{1}{3}\pi^2\rho\left(\frac{k_BT}{\Phi_0}\right)^2. \tag{A22}$$

where $I\equiv U/U_0$, and $U_0\equiv 8|\overline{\epsilon}|$. Defining $\mu^*=\mu/\Phi$, and $T^*=T/\Phi$, we can write

$$\begin{aligned}K&=\int_{-W/2}^{W/2}\frac{2}{(1+e^{(\epsilon-\mu*/k_BT^*)})^2}\frac{e^{(\epsilon-\mu^*/k_BT^*)}}{k_BT}\rho(\epsilon)d\epsilon\\&=-\frac{2}{\Phi}\int_{-W/2}^{W/2}f'\left(\frac{\epsilon-\mu^*}{k_BT^*}\right)\rho(\epsilon)d\epsilon\\&=-\frac{2}{\Phi}\int_{(-W/2-\mu^*/k_BT^*)}^{(W/2-\mu^*/k_BT^*)}f'(x)\rho(xk_BT^*+\mu^*)dx\\&=-\frac{2}{\Phi}\sum_n(k_BT^*)^{2n}\frac{\rho^{(2n)}(\mu^*)}{(2n)!}\int_{-\infty}^{+\infty}x^{2n}f'(x)dx\end{aligned} \tag{A23}$$

where $f'(x)$ is the derivative of the Fermi-Dirac function. Noting that

$$\int_{-\infty}^{+\infty}\frac{df(x)}{dx}dx=-1,\quad \int_{-\infty}^{+\infty}x^2\frac{df(x)}{dx}dx=-\frac{1}{3}\pi^2, \tag{A24}$$

we arrive at the expression

$$K=\frac{2}{\Phi}[\rho(\mu^*)+\tfrac{1}{6}\pi^2\rho''(\mu^*)(k_BT^*)^2]. \tag{A25}$$

From Ref. 20 we also have

$$\mu^*(T)=\epsilon_F-\frac{\pi^2}{6}(k_BT^*)^2\frac{\rho'}{\rho}, \tag{A26}$$

and thus

$$K=\frac{2\rho}{\Phi}\left[1-\frac{\pi^2}{6}\left(\frac{k_BT}{\Phi}\right)^2\left(\left(\frac{\rho^{(1)}}{\rho}\right)^2-\frac{\rho^{(2)}}{\rho}\right)\right]$$
$$=2\rho\left(\frac{1}{\Phi_0}+\frac{16\pi^2}{3\Phi_0^2}\frac{I^2}{U_0}\rho(k_BT^*)^2\right)-2\rho\frac{\pi^2}{6\Phi_0}(k_BT^*)^2r, \tag{A27}$$

with $r=(\rho^{(1)}/\rho)^2-(\rho^{(2)}/\rho)$. We substitute Eqs. (A20), (A22), and (A27) into Eq. (A19). As a result, the susceptibility $\chi=(1/4\rho)\,\chi_0(dm/dh)_{h=0}$ is of the form

$$\chi=\frac{\chi_0}{S}\left[1-a\frac{\pi^2(k_BT)^2}{6\Phi_0^2S}\right], \tag{A28}$$

where

$$S=\Phi_0\left(1-U\rho\frac{1+I/2}{(1+I)^2}\right)-J\rho, \tag{A29}$$

and

$$a=8I^2(I^2+2I+3)(1+I)^{-2}\rho^2-\frac{32I^2\rho}{Uc}+r\Phi_0. \tag{A30}$$

Neglecting higher-order contribution in I, the result reduces to the usual Stoner form $\chi(T=0)=\chi_0[1-\rho(U+J)]^{-1}$. Formula (A28) generalizes the result of Brinkman and Rice[8] obtained for a nondegenerate case at $T=0$, and its generalization[20] to $T>0$. The Hund's rule coupling enhances the susceptibility and can be the source of a ferromagnetic instability.

With the help of the expression for Φ one can determine the first nontrivial contribution to the specific heat in the applied field. Namely, one has $C_v=(\gamma_0/\Phi_0)T+bH_a^2T$, where b is a constant divergent at the localization point. This increase is connected with the narrowing of the band with the growing field.

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