Interplay of Mott transition and ferromagnetism in the orbitally degenerate Hubbard model

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A slave-boson representation for the degenerate Hubbard model is introduced. The location of the metal-to-insulator transition that occurs at commensurate densities is shown to depend weakly on the band degeneracy M. The relative weights of the Hubbard subbands depend strongly on M, as well as the magnetic properties. It is also shown that a sizable Hund's rule coupling is required in order to have a ferromagnetic instability appearing. The metal-to-insulator transition driven by an increase in temperature is a strong function of it. [S0163-1829(97)02144-9]

There has been dramatic progress in our understanding of the Mott transition in the last few years. Careful experimental studies of systems in the vicinity of the Mott transition have been carried out.[1] Two new theoretical tools, slave-boson mean-field theories (see, for instance, Frésard and Wölfle[2] and references therein), and the limit of infinite dimensions have been adapted to its study. For a review see Georges *et al.*[3] Most of the modern work has focused on the *single-band Hubbard model*. Now that both the metallic and the Mott insulating states of the (doped) titanate and vanadiates have been studied experimentally[1,4] (corresponding to $3d1$ and $3d2$ configurations in the Mott insulating state), there is a need for a theoretical framework allowing for understanding the Mott transition for arbitrary degeneracy and density. This paper is aimed at providing such a technique and applying it to a variety of quantities that cannot be obtained easily using alternative approaches. Most of the results are obtained in a closed analytical form, allowing for a qualitative understanding of the physical situation.

In this work we investigate the effect of strong Coulomb interaction in systems with *orbital degeneracy*. Such a situation is realized in virtually all transition-metals and transition metal oxides. These systems contain d electrons in cubic or trigonal environments. The crystal field can only lift partially the degeneracy of the d bands, down to two as is the case of V_2O_3 (Ref. 5) or three as in $LaTiO_3$. Our goal is to understand how degeneracy affects the behavior of the different physical quantities near the Mott transition. To carry out the investigation we extend the slave-boson technique, which has been very successful in the study of the Mott transition, to the orbitally degenerate case.

A remarkable feature of the dynamical mean-field solution to the large-dimension limit of the Hubbard model is the metal-to-insulator transition that occurs in the vicinity of the Mott transition under an increase of the temperature.[3] In the metallic phase the spectrum of the one-electron Green's function consists of two incoherent excitation branches and one coherent quasiparticle peak, which is precisely absent in the insulating state. There is thus a coherence temperature $T_{\rm coh}$ at which the coherence of the interacting system giving rise to the Fermi liquid disappears. Such a coherent-incoherent transition is observed experimentally in V_2O_3 (Refs. 6 and 7) and can also be obtained out of the slave-boson mean-field theory.[8]

Compared to the variational wave-function approach[9,10] our formalism is more flexible since, as we demonstrate in this paper, it allows us to calculate a variety of quantities that are not easily accessible to the variational approach, as a function of the correlation strength and doping. It can also be improved systematically by performing a loop expansion around the saddle point. Our main results are as follows:

(a) Low-energy single-particle quantities such as the critical value of the interaction strength of the transition, the quasiparticle residue, and the single-particle Mott-Hubbard gap depend only weakly on degeneracy. This justifies the agreement between theory of Rozenberg *et al.*[11] and experiment on orbitally degenerate systems.

(b) The relative weights of the Hubbard bands depend strongly on degeneracy, in agreement with other methods.[12]

(c) The coherence temperature decreases with increasing band degeneracy.

(d) The magnetic properties, in particular the magnetic susceptibility and its associated Landau parameter in the paramagnetic phase and the magnetic phase diagram, are strongly modified with respect to the one-band case.

The Hamiltonian describing the low-energy properties of these systems is commonly written as

$$H=\sum_{i,j,\sigma,\rho} t_{i,j} c^{\dagger}_{i,\rho,\sigma} c_{j,\rho,\sigma} + U_3 \sum_{i,\rho} n_{i,\rho,\uparrow} n_{i,\rho,\downarrow} + U_1 \sum_{i,\rho'\neq\rho} n_{i,\rho,\uparrow} n_{i,\rho',\downarrow} + U \sum_{i,\sigma,\rho'<\rho} n_{i,\rho,\sigma} n_{i,\rho',\sigma}, \tag{1}$$

where σ is a spin index for the up and down states while ρ is labeling the M bands. U_3 describes the on-site interaction term between two particles in the same band but with opposite spin. U_1 relates to a pair of particles with opposite spin and different band index. U finally concerns the case of

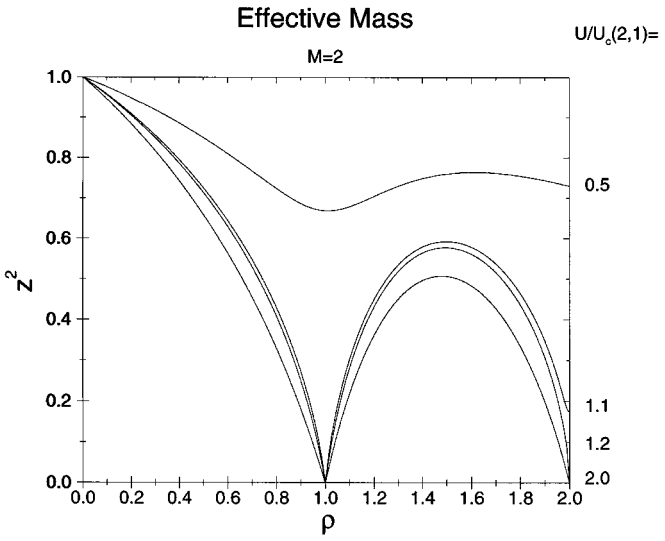

FIG. 1. Inverse effective mass in the two-band model as a function of density for several values of U.

equal spin. In the two-band model rotational symmetry requires $U_n = U + nJ$.[13] The relationship between the couplings is derived and discussed in the Appendix for a model that is relevant to the titanates. The description with only three different interaction strengths is a simplified version of the full problem with completely general exchange interaction. In that case the coupling constants would not be completely independent from one another, and relationships between them would follow from rotational symmetry as well. Here we consider a generic model where the number of independent parameters is kept small for simplicity. Taking J finite accounts for the Hund's rule coupling.

As for any model with on-site interaction, a slave-boson representation can be introduced, mapping all the degrees of freedom onto bosons. We can rewrite any atomic state with the help of a set of pseudofermions $\{f_\alpha\}$ and slave bosons $\{\psi^{(m)}_{\alpha_1,\ldots,\alpha_m}\}$ $(0 \leqslant m \leqslant 2M)$. $\psi^{(m)}_{\alpha_1,\ldots,\alpha_m}$ is the slave boson associated with the atomic state consisting of m electrons in states $|\alpha_1,\ldots,\alpha_m\rangle$ where α is a composite spin and band index. By construction it is symmetric under any permutation of two indices, and zero if any two indices are equal. We can now write the creation operator of a physical electron in terms of the slave particles as

$$c^\dagger_\alpha = \tilde{z}^\dagger_\alpha f^\dagger_\alpha . \tag{2}$$

$\tilde{z}^\dagger_\alpha$ describes the change in the boson occupation numbers when an electron in state α is created as

$$\tilde{z}^\dagger_\alpha = \sum_{m=1}^{2M} \sum_{\alpha_1 < \cdots < \alpha_{m-1}} \psi^{\dagger(m)}_{\alpha,\alpha_1,\ldots,\alpha_{m-1}} \psi^{(m-1)}_{\alpha_1,\ldots,\alpha_{m-1}},$$

$$\alpha_i \neq \alpha. \tag{3}$$

The operators $\tilde{z}^\dagger_\alpha$ in Eq. (3) describe the change in the slave-boson occupation as a many-channel process. In order to recover the correct noninteracting limit at mean-field level, one has to observe that the classical probability for these processes to happen is not simply given by taking the Bose fields in (3) to be given by their classical values, but by introducing normalization factors L_α and R_α (Refs. 14 and 2) as

$$z^\dagger_\alpha = \sum_{m=1}^{2M} \sum_{\alpha_1 < \cdots < \alpha_{m-1}} \times \psi^{\dagger(m)}_{\alpha,\alpha_1,\ldots,\alpha_{m-1}} L_\alpha R_\alpha \psi^{(m-1)}_{\alpha_1,\ldots,\alpha_{m-1}},$$

$$\alpha_i \neq \alpha, \tag{4}$$

where

$$R_\alpha = \left[1 - \sum_{m=0}^{2M-1} \sum_{\alpha_1 < \cdots < \alpha_m} \psi^{\dagger(m)}_{\alpha_1,\ldots,\alpha_m} \psi^{(m)}_{\alpha_1,\ldots,\alpha_m} \right]^{-1/2},$$

$$\alpha_i \neq \alpha,$$

$$L_\alpha = \left[1 - \sum_{m=1}^{2M} \times \sum_{\alpha_1 < \cdots < \alpha_{m-1}} \psi^{\dagger(m)}_{\alpha,\alpha_1,\ldots,\alpha_{m-1}} \psi^{(m)}_{\alpha,\alpha_1,\ldots,\alpha_{m-1}} \right]^{-1/2}. \tag{5}$$

Namely, L_α normalizes to one the probability that no electron in state $|\alpha\rangle$ is present on a site before one such electron hops on that particular site, and R_α makes sure that it happened. Clearly the eigenvalues of the operators L_α and R_α are one in the physical subspace. Now, the redundant degrees of freedom are projected out with the constraints

$$f^\dagger_\alpha f_\alpha - \sum_{m=1}^{2M} \sum_{\alpha_1 < \cdots < \alpha_{m-1}} \psi^{\dagger(m)}_{\alpha,\alpha_1,\ldots,\alpha_{m-1}} \psi^{(m)}_{\alpha,\alpha_1,\ldots,\alpha_{m-1}} = 0,$$

$$\sum_{m=0}^{2M} \sum_{\alpha_1 < \cdots < \alpha_m} \psi^{\dagger(m)}_{\alpha_1,\ldots,\alpha_m} \psi^{(m)}_{\alpha_1,\ldots,\alpha_m} - 1 = 0. \tag{6}$$

We obtain the Lagrangian at $J = 0$ as

$$L = \sum_{i,\alpha} f^\dagger_{i,\alpha} (\partial_\tau - \mu + i\lambda_{i,\alpha}) f_{i,\alpha} - i\Lambda_i + \sum_{i,m} \sum_{\alpha_1 < \cdots < \alpha_m} \psi^{\dagger(m)}_{i,\alpha_1,\ldots,\alpha_m} \left[\partial_\tau + i\Lambda_i + U\binom{m}{2} - i\sum_{j=1}^{m} \lambda_{i,\alpha_j} \right] \psi^{(m)}_{i,\alpha_1,\cdots,\alpha_m} + \sum_{i,j,\alpha} t_{i,j} z^\dagger_{i,\alpha} f^\dagger_{i,\alpha} z_{j,\alpha} f_{j,\alpha}. \tag{7}$$

We now proceed to the mean-field theory, and we investigate the paramagnetic, paraorbital saddle point. The latter is obtained after integrating out the fermions, and setting all bosonic fields to their classical value. The Mott transition that occurs at commensurate density n is best discussed by projecting out occupancies that are larger than $n+1$ and smaller than $n-1$ (if any). The constraints allows for eliminating the variables $\psi^{(n-1)}$ and $\psi^{(n)}$ to obtain the grand potential at n as

$$\Omega(D)=(1-2D^2)D^2(\sqrt{b_{n,M}}+\sqrt{c_n})^2\epsilon_0 + U\left[D^2+\binom{n}{2}\right]-\mu\rho, \tag{8}$$

with $\epsilon_0\equiv 2M\int d\epsilon\epsilon\rho(\epsilon)f_F(z^2\epsilon+\lambda_0-\mu)$, $D^2\equiv\binom{2M}{n+1}\psi^{(n+1)2}$, $b_{n,M}\equiv(2M-n+1)/(2M-n)$, and $c_n\equiv(n+1)/n$. Minimizing Eq. (8) with respect to D yields a critical interaction strength at which D vanishes. It reads

$$U_c^{(n,M)}=-\epsilon_0(\sqrt{b_{n,M}}+\sqrt{c_n})^2, \tag{9}$$

which reproduces the results of the Gutzwiller approximation.[9,10] This locates the Mott transition. Restricting ourselves to a flat density of states we can relate the critical interaction strength to the band width W. We obtain

$$U_c^{(n,M)}=\frac{nW}{4M}(2M-n)(\sqrt{b_{n,M}}+\sqrt{c_n})^2. \tag{10}$$

Its band-degeneracy dependence is fairly weak.[10] The effective mass of the quasiparticles diverges at the Mott transition. We obtain

$$\frac{m}{m^*}=z^2=\frac{(\sqrt{b_{n,M}}+\sqrt{c_n})^2}{8}\,\frac{U_c^{(n,M)2}-U^2}{U_c^{(n,M)2}}. \tag{11}$$

Due to the particular form of the coefficients b and c the dependence on the band degeneracy is weak. The critical interaction strength increases with M so the quasiparticle residue Z increases slightly with M. For small values of U (which we treated without projecting out higher occupancies), Z decreases with increasing M. So there is a crossover value of the interaction strength beyond which the system becomes more metallic with increasing M.[15] As a function of the hole doping δ, the quasiparticle residue vanishes for δ going to 0 above $U_c^{(n,M)}$ as

$$Z=\frac{\delta}{2}(b_{n,M}-c_n)+\frac{|\delta|}{2}[(b_{n,M}+c_n)\sqrt{1+4\varphi_{n,M}} +4\sqrt{b_{n,M}c_n\varphi_{n,M}}], \tag{12}$$

where we introduced

$$\varphi_{n,M}\equiv\frac{U_c^{(n,M)2}b_{n,M}c_n/(\sqrt{b_{n,M}}+\sqrt{c_n})^4}{(U-U_c^{(n,M)})(U-U_c^{(n,M)}[(\sqrt{b_{n,M}}-\sqrt{c_n})/(\sqrt{b_{n,M}}+\sqrt{c_n})^2])}. \tag{13}$$

The expression of the quasiparticle residue consists of two contributions that are either symmetric or antisymmetric with respect to particle or hole doping. The antisymmetric contribution vanishes for $n=M$ as a consequence of the particle-hole symmetry. The asymmetry of Z on particle or hole doping is seen to increase under an increase of $|n-M|$. For $n<M$, $Z(\delta)$ vanishes more slowly for hole doping than for particle doping. Increasing the degeneracy for fixed n, or increasing the degeneracy at $n=M$, makes the rate at which $Z(\delta)$ vanishes smaller. Increasing the interaction strength has the same consequence. As an example we calculate the effective mass for the two-band model without projecting out higher occupancies and show it on Fig. 1.

Interestingly we also obtain a Mott gap. Indeed the number of quasiparticles is a continuous function of their chemical potential $\mu-\lambda_0/2$. However, the saddle-point equations show that the Lagrange multiplier Λ jumps when going through the Mott gap, which implies that λ is going to jump as well, and so does μ. As a result we obtain the Mott gap $\Delta\equiv\lim_{\delta\to 0^-}\mu(\delta)-\lim_{\delta\to 0^+}\mu(\delta)$ as

$$\Delta=\sqrt{(U-U_c^{(n,M)})\{U-U_c^{(n,M)}[(\sqrt{b_{n,M}}-\sqrt{c_n})/(\sqrt{b_{n,M}}+\sqrt{c_n})]^2\}}. \tag{14}$$

In the limit of $U\gg U_c^{(n,M)}$, the Mott gap is given by U, while it closes at $U_c^{(n,M)}$ as $\Delta\sim U_c^{(n,M)}\sqrt{U/U_c^{(n,M)}-1}$, the square-root behavior being typical of slave-boson mean-field theories. It can be read from Fig. 2 where it is compared to the one-band case as obtained by Lavagna.[16] Clearly going from one band to two bands does not imply a big difference in the Mott gap. Indeed we obtain that $\Delta/U_c^{(n,M)}$ is independent of M at $n=M$, while for fixed n it depends very weakly on M.

Our result can be compared to experimental data. For the series $La_xY_{1-x}TiO_3$, Okimoto *et al.*[17] measured how the gap depends on the bandwidth. Assuming (for large ratio U/W) $\Delta\sim U-W$ we obtain out of their data $U=3.2$ eV. Inserting this and the experimental value of $(U/W)_c\sim 1.3$ into Eq. (14) we can compute Δ/W for $M=3$ as a function of W/U and compare it with experiment on Fig. 3. The experimental trend is clearly reproduced and the quantitative agreement is very satisfactory. According to the above discussion, including the threefold degeneracy of the d band in order to account for the experimental situation[17] only makes a small difference as compared to the nondegenerate case.

We now turn to the Hund's rule coupling dependence and treat as an example the two-band model around the $n=1$ Mott insulating lobe. At $\rho=1$ the grand potential at the saddle point reads

$$\Omega=\frac{4}{3}\epsilon_0(1-2r^2)[r+(d_0+d_x+\Delta_0)/\sqrt{2}]^2+(U+3J)\Delta_0^2 +(U+J)d_x^2+Ud_0^2-\mu\rho, \tag{15}$$

with $d_0\equiv(\psi^{(2)}_{\uparrow,\uparrow}+\psi^{(2)}_{\downarrow,\downarrow})/\sqrt{2}$, $d_x\equiv(\psi^{(2)}_{\uparrow,\downarrow}+\psi^{(2)}_{\downarrow,\uparrow})/\sqrt{2}$, $\Delta_0\equiv(\psi^{(2)}_{\uparrow\downarrow,0}+\psi^{(2)}_{0,\uparrow\downarrow})/\sqrt{2}$, $r^2\equiv d_0^2+d_x^2+\Delta_0^2$, and $\lambda\equiv\Sigma_\alpha\lambda_\alpha/2$,

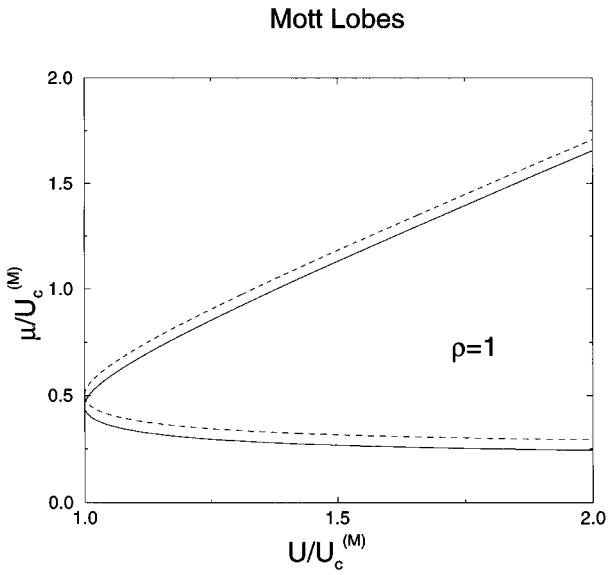

FIG. 2. Chemical potential for $n=1$ for the one-band (dashed line) and two-band (full line) models.

and we have used the constraints to remove the variables $\psi^{(0)}$ and $\psi^{(1)}$.

Such an expression differs from an ordinary Ginzburg-Landau free energy in the respect that it cannot be written as a fourth-order polynomial in the variables d_0, d_x, and Δ_0. As a result, if there were to be a critical point for one field, it would be critical for the other ones as well. For small J we obtain the location of the Mott transition as

$$U^{(2)}_{c,(J)}=U^{(2)}_{c,(0)}\left(1-\frac{4}{3}\frac{J}{U}+O(J/U)^2\right). \tag{16}$$

Another regime of interest is the large-J regime. There we obtain the location of the Mott transition as

$$U^{(2)}_c=-\frac{2}{3}\epsilon_0(3+2\sqrt{2})\left(1-\frac{8}{9}\frac{\epsilon_0}{J}\right)+O\left(\left(\frac{\epsilon_0}{J}\right)^2\right) \tag{17}$$

and thus decreasing J from infinity leads to an increase of the critical interaction.

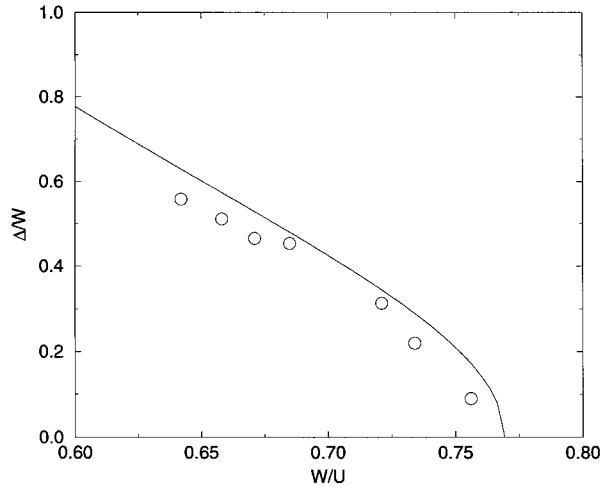

FIG. 3. Dependence of the Mott gap on the bandwidth for $n=1$ and $M=3$. Circles: experimental data of Okimoto *et al.*[17]

Another intriguing feature of transition-metal oxides such as V_2O_3 is the metal-to-insulator transition that occurs in the vicinity of the tricritical point under an increase of temperature.[6,7] It has recently been interpreted[11] as the transition from a Fermi liquid with finite quasiparticle residue Z to an insulator with $Z=0$. This interpretation has been obtained in the framework of the dynamical mean-field approximation, which yields equations that have two different solutions, one that resembles a Fermi liquid with a finite Z and the other, which is totally incoherent. In the slave-boson mean-field theory and at zero temperature, the quasiparticle residue Z vanishes continuously as U approaches $U_c^{(M)}$, as given by Eq. (11). In contrast this behavior does not hold at finite temperature[8] where the saddle-point equations acquire a higher degree of nonlinearity since ε_0 becomes a function of Z. Thus, for given U, they admit two solutions for $U<U_{c2}$, and only one for $U>U_{c2}$. Among the two solutions, one closely resembles the metallic solution with finite Z of the large d. The second one, characterized by a strongly renormalized effective mass, is not really a good description of the insulator because it does not have the incoherent parts. Nevertheless that is really the best mean-field theory can do. Given the resemblance of one of the slave-boson solutions to the metallic large-d solution it makes sense to ask at which temperature that solution ceases to exist, that is, our calculated $T_{\rm coh}$. When both solutions become degenerate there is a first-order metal-to-insulator transition at a critical $U_c^{(M)}(T)$:

$$U_c^{(M)}(T)=U_c^{(M)}(0)-\sqrt{8U_c^{(M)}(0)T\ln(2M)}. \tag{18}$$

Thus an increase in temperature may produce a metal-to-insulator transition, which is consistent with the experimental situation in V_2O_3. Here $T_{\rm coh}$ is given by

$$T_{\rm coh}=\frac{[U-U_c^{(M)}(0)]^2}{8U_c^{(M)}(0)\ln(2M)} \tag{19}$$

and thus decreases under an increase of M. In the dynamical mean-field approximation at finite temperature there is an interaction strength $U_{c2}(T)$ at which the metallic solution ceases to exist. This quantity can also be evaluated in our slave-boson scheme and, at $n=1$, is given by

$$U_{c2}^{(M)}(T)=U_c^{(M)}(0)[1-\alpha_M(T/W)^{2/3}], \tag{20}$$

with $\alpha_1\sim 2.53$ and $\alpha_2\sim 3.32$.

We now turn to the calculation of the magnetic susceptibility. Here we generalize the calculation of Li *et al.*[18] to the two-band model. The linear response to an external magnetic field is obtained as a one-loop calculation of the correlation function of the slave-boson fields in the spin-antisymmetric band-symmetric channel. Three fields couple in this channel:[15] $\chi_-\equiv\frac{1}{2}\Sigma_\alpha\sigma\psi^{(1)}_\alpha$, $\chi_+\equiv 1/\sqrt{2}(\psi^{(2)}_{\uparrow,\uparrow}-\psi^{(2)}_{\downarrow,\downarrow})$, and $\kappa\equiv\frac{1}{2}\Sigma_\alpha\sigma\lambda_\alpha$, and the magnetization is expressed in terms of slave bosons as $\mathcal{M}=4d_0\chi_++2\psi^{(1)}\chi_-$. The resulting susceptibility arises as a random-phase approximation form[15]

$$\chi_S=\frac{\chi_0}{1+F_0^a\chi_0/N(E_F)}. \tag{21}$$

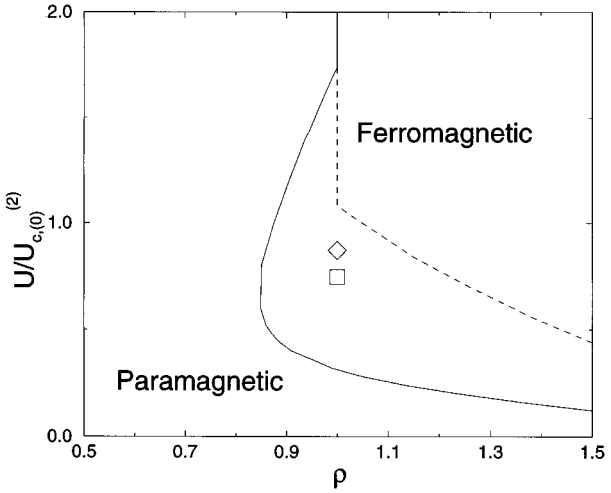

FIG. 4. Instability line of the paramagnetic phase for $U/J=10$ (dashed line) and $U/J=5$ (solid line). The diamond (square) indicates the position of the Mott transition for $U/J=10$ ($U/J=5$).

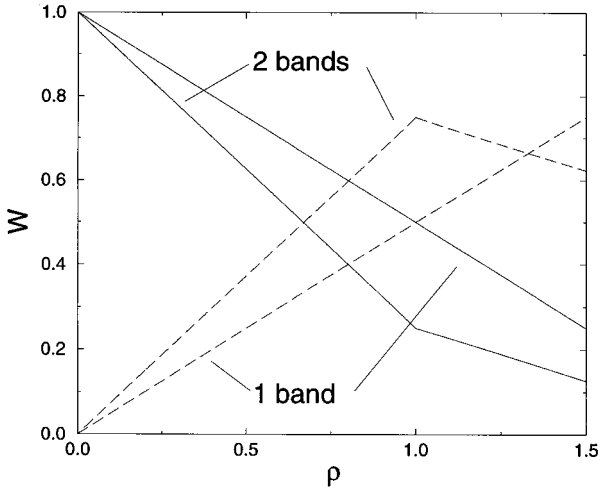

FIG. 5. Spectral weight of the upper (dashed lines) and lower (solid lines) Hubbard bands for the 1 band and 2 band models, at $U=2U_c^{(M)}$.

We now determine the instability line of the paramagnetic phase with respect to ferromagnetism. For $J=0$ we find no ferromagnetic instability even near the Mott transition, while for finite J we find that the Mott metal-to-insulator transition may be preempted by the appearance of a ferromagnetic phase. In other words, a sufficiently strong Hund's rule coupling turns a Mott insulator into a ferromagnet. Originally the Hubbard model was introduced in order to describe ferromagnetism in narrow-band systems, but it has been recently established that the ground state is not ferromagnetic for any reasonable values of the parameters on the square lattice.[19,20] Introducing a next-nearest-neighbor hopping term in the Hamiltonian,[21–24] which has the effect of shifting the van Hove singularity of the non-interacting system away from the center of the band, may lead to a ferromagnetic ground state in the vicinity of the van Hove singularity, even for realistic values of the coupling strength. We find that the ground state is much more likely to be ferromagnetic in the degenerate model for finite J, as shown in Fig. 4.

Our method can be applied to the calculation of dynamical quantities too. In the slave-boson method,[25] the Green's function that one obtains closely resembles the exact large-d result. It namely consists of a quasiparticle resonance and two Hubbard bands, which can be clearly separated. However, the sum rules are not quite satisfied for $N=2$. Here we use a decomposition that is more closely related to the Hubbard operator algebra treatment, and the idea is to calculate the spectral weights of the Hubbard operator Green's functions. We really do not know how to separate that weight into a lower band and a quasiparticle piece, but near half-filling the resonance has a small weight, and we can identify the weight in the Hubbard bands with the spectral weight of the corresponding Hubbard operator Green's functions. In the strong coupling regime the one-particle excitation spectrum is split off into several pieces, each of them carrying some fraction of the spectral weight (which are adding up to 1 so as to fulfill the sum rule). The various pieces follow from the discrete atomic levels, which are well separated by multiples of U, broadened by exchange processes. Let us now determine the fraction of the spectral weight carried by each sub-band. In our language the low-energy excitations are involving the field $\psi^{(1)}$, and the high-energy excitations centered around U the field $\psi^{(2)}$. Higher-energy excitations involving higher local occupancies are left out. We obtain the spectral weights in both bands by evaluating explicitly the anticommutator $\langle\{c_\alpha,c_\alpha^\dagger\}\rangle$ using the decomposition of the physical electron operator [Eqs. (2) and (3)]. Accordingly the spectral weight of the Green's function $T\langle c_\alpha(\tau)c_\alpha^\dagger(0)\rangle$ in the lower Hubbard band ($W_{\mathrm{LHB}}=\langle\{c_{L\alpha},c_{L\alpha}^\dagger\}\rangle$) and the upper Hubbard band ($W_{\mathrm{UHB}}\langle\{c_{U\alpha},c_{U\alpha}^\dagger\}\rangle$), where $c_{L\alpha}^\dagger$ ($c_{U\alpha}^\dagger$) is the contribution to $c_\alpha^\dagger$, which is involving the field $\psi_\alpha^{\dagger(1)}$ ($\psi_{\alpha,\alpha_1}^{\dagger(2)}$) in Eq. (3), are given by

$$W_{\mathrm{LHB}}=\langle\psi^{\dagger(0)}\psi^{(0)}+\psi_\alpha^{\dagger(1)}\psi_\alpha^{(1)}\rangle,$$

$$W_{\mathrm{UHB}}=\sum_{\beta\neq\alpha}\langle\psi_\beta^{\dagger(1)}\psi_\beta^{(1)}+\psi_{\alpha\beta}^{\dagger(2)}\psi_{\alpha\beta}^{(2)}\rangle \tag{22}$$

and are shown in Fig. 5. Here the weights do not quite add up to 1 in the two-band case because we projected out occupations larger than 2. In other words, on top of the two subbands that are considered here, there appears a second upper Hubbard band (centered around $3U-3\mu$, corresponding to triple occupancy) that is becoming relevant in the particle doped domain. To a very good accuracy its contribution to the spectral weight is given by $1-W_{\mathrm{LHB}}-W_{\mathrm{UHB}}$. Clearly the degeneracy plays an important role as the weight of the upper band at $n=1$ in the strong coupling regime is given by $(2M-1)/2M$.

In summary we introduced a slave-boson representation of the degenerate Hubbard model. We obtained that the band degeneracy has a weak influence on the location of the Mott transition, while the degeneracy temperature and the dynamical and magnetic properties strongly depend on it. We also showed that no ferromagnetic instability occurs unless the Hund's rule coupling becomes sizable, yielding a generic scenario for ferromagnetism in transition metals and transition-metal oxides. In that case a ferromagnetic instability may even shadow the Mott transition.

Note added. After this work was completed we became aware of related work by H. Hasegawa [cond-mat/9612142 (unpublished); cond-mat/9704168 (unpublished)].

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APPENDIX

In this appendix we derive the Hamiltonian that is relevant to the titanates, Eq. (1). In a cubic environment, the crystal field is partially lifting the degeneracy of the d band, by lowering the energy of the threefold degenerate T_{2g} orbital, and by raising the energy of the twofold degenerate e_g orbital. Here we concentrate on the T_{2g} electrons, for which the interacting part of the Hamiltonian is given by

$$H_{\rm int}=\sum_{\sigma,\sigma'}\sum_{\alpha,\beta,\gamma,\delta}\langle\alpha\beta|\,e^2/r\,|\gamma\delta\rangle c^\dagger_{\alpha,\sigma}c^\dagger_{\beta,\sigma'}c_{\delta,\sigma'}c_{\gamma,\sigma}, \tag{A1}$$

where the indices $\alpha,\beta,\gamma,\delta$ label the d_{xy}, d_{xz}, and d_{yz} orbitals. The nonvanishing matrix elements of the Coulomb interaction are grouped into direct and exchange interactions. There is a diagonal direct coupling:

$$u=\langle\alpha\alpha|e^2/r\,|\alpha\alpha\rangle, \tag{A2}$$

an off-diagonal direct coupling

$$u'=\langle\alpha\beta|\,e^2/r\,|\alpha\beta\rangle, \tag{A3}$$

and two exchange couplings

$$J=\langle\alpha\beta|\,e^2/r\,|\beta\alpha\rangle,$$

$$a=\langle\alpha\alpha|\,e^2/r\,|\beta\beta\rangle. \tag{A4}$$

Explicitly, introducing the Wannier real wave functions $\varphi_\alpha(\mathbf{r})$, we find for J:

$$J=\int d\mathbf{r}d\mathbf{r}'\varphi^\dagger_\alpha(\mathbf{r})\varphi^\dagger_\beta(\mathbf{r}')\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\varphi_\beta(\mathbf{r})\varphi_\alpha(\mathbf{r}'). \tag{A5}$$

The reality of the wave functions implies

$$a=J. \tag{A6}$$

Using the partial wave expansion of the Coulomb potential one obtains

$$J=\sum_{k,m}\int r^2drr'^2dr'\frac{r^k_<}{r^{k+1}_<}R(r)^2R(r')^2,$$

$$\int d\mathbf{\Omega}\varphi_\alpha(\mathbf{\Omega})Y^k_m(\mathbf{\Omega})\varphi_\beta(\mathbf{\Omega})$$

$$\times\int d\mathbf{\Omega}'\varphi_\beta(\mathbf{\Omega}')Y^k_m(\mathbf{\Omega}')\varphi_\alpha(\mathbf{\Omega}'), \tag{A7}$$

where $R(r)$ and $\varphi_\alpha(\mathbf{\Omega})$ are respectively the radial and angular part of the wave function $\varphi_\alpha(\mathbf{r})$. As usual, using, for instance, density-functional theory, the computation of the matrix elements can be brought down to the computation of three numbers, F_0, F_2, and F_4. They are defined as

$$F_0=\int r^2drr'^2dr'\frac{1}{r_>}R(r)^2R(r')^2,$$

$$F_2=\frac{1}{49}\int r^2drr'^2dr'\frac{r^2_<}{r^3_>}R(r)^2R(r')^2, \tag{A8}$$

$$F_4=\frac{1}{441}\int r^2drr'^2dr'\frac{r^4_<}{r^5_>}R(r)^2R(r')^2$$

and one obtains

$$u=F_0+4F_2+36F_4,$$

$$u'=F_0-F_2-4F_4, \tag{A9}$$

$$J=\frac{5}{2}F_2+\frac{45}{2}F_4.$$

In the limit where $F_4\ll F_2$, we obtain

$$2J=u-u'. \tag{A10}$$

Setting

$$U\equiv u-3J, \tag{A11}$$

and inserting the above-found matrix elements of the Coulomb interaction in Eq. (A1) we obtain the Hamiltonian Eq. (1) provided one neglects the two following small terms:

$$H_{\rm neg}=J\sum_{\alpha\neq\beta}\sum_{\sigma\neq\sigma'}c^\dagger_{\alpha\sigma}c^\dagger_{\alpha\sigma'}c_{\beta\sigma'}c_{\beta\sigma}$$

$$+J\sum_{\alpha\neq\beta}\sum_{\sigma\neq\sigma'}c^\dagger_{\alpha\sigma}c^\dagger_{\beta\sigma'}c_{\alpha\sigma'}c_{\beta\sigma}. \tag{A12}$$

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