Slave-boson mean-field theory of the Anderson lattice with finite U and orbital degeneracy

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We consider a stoichiometric metallic Anderson lattice with orbital degeneracy and finite U. The correlations in the f shell are formulated in terms of a complete set of "auxiliary bosons," generalizing in this way Kotliar and Ruckenstein's approach for the Hubbard model to arbitrary electronic configurations. A Gutzwiller type of mean-field approximation is introduced for the case where the occupancy of the f^n configurations for $n > 2$ is excluded. The occupation probabilities are discussed as a function of U and the f-level position. For sufficiently large U the paramagnetic solution becomes unstable towards ferromagnetism. This instability is suppressed with increasing orbital degeneracy. The case of a Kondo insulator with electron-hole symmetry is also discussed in mean-field theory.

I. INTRODUCTION

The unusual low-temperature properties of heavy-electron systems, in particular the development of *coherence* in stoichiometric compounds, has received a large amount of attention in recent years.[1,2] The coherence manifests itself most dramatically in the low-temperature resistivity and magnetoresistivity. At high temperatures (compared to the Kondo temperature T_K), the properties of a metallic system are similar to that of dilute impurity systems.[3] The scattering of the electrons is said to be *incoherent,* i.e., independent from site to site, giving rise to a large resistivity. At zero temperature, on the other hand, as a consequence of the translational invariance of the lattice, there is effectively no scattering (Bloch theorem) and the resistivity is then ideally zero for a heavy fermion metal.

The formation of the coherent state in the Kondo lattice can also be studied by introducing disorder into the system,[4] i.e., by alloying nonmagnetic impurities (Kondo holes) substituting for the rare earth or actinide ions. Adding impurities to a Kondo lattice breaks the translational invariance and gradually destroys the coherence of the heavy-fermion ground state. In recent publications[5,6] we reported a simple microscopic theory of the Kondo hole, for both the metallic and the insulating situations, and on the formation of impurity bands in Kondo insulators.

Antiferromagnetic long-range order in heavy-fermion metals has been a subject of intensive theoretical studies.[7–11] Experimentally a faint antiferromagnetic order has been observed in several heavy-fermion metals at low temperatures. The ordered magnetic moment is very small due to the competition between the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction with the Kondo effect. For small Kondo coupling antiferromagnetic order is expected, while if J is large the groundstate is paramagnetic. In a recent paper we studied the instabilities of the orbitally nondegenerate Kondo insulator to ferro- and antiferromagnetic long-range order[12] using a Gutzwiller type of mean-field approximation formulated in terms of four slave bosons per site in analogy to Kotliar and Ruckenstein's approach[13] for the Hubbard model.

In this paper we extend our analysis of the ferromagnetic instability for the Kondo insulator to the metallic situation and to orbital degeneracy for the f electrons. The possible multiple occupancy of the f level and the degeneracy of the f^n configurations require a large number of "auxiliary bosons" to describe all the correlations in the system. The model and its "slave-boson" variant are introduced in Sec. II. In Sec. III we discuss the mean-field (saddle-point) approximation for the case in which only the $4f^0$, $4f^1$, and $4f^2$ configurations have a nonzero probability of occupation. In mean field the boson operators are replaced by their expectation values, which are then determined by minimization of the total energy of the system. The limit $U \rightarrow \infty$ is also explicitly treated in this section. The extension to the electron-hole symmetric situation of a Kondo insulator with orbital degeneracy is derived in Sec. IV. In Sec. V we present the numerical solution of the mean-field equations derived in Secs. III and IV and discuss the ferromagnetic instability. Conclusions are drawn in Sec. VI.

For sufficiently small U the ground state is paramagnetic. The ferromagnetic instability occurs when the $4f^1$ configuration is sufficiently stable and becomes the dominant one, i.e., with increasing U or with decreasing f-level energy. An external magnetic field favors the ferromagnetic long-range order. Quantum fluctuations about the mean-field solution are believed to reduce the magnetic order; this probably shifts the paramagnetic to ferromagnetic boundary to larger U values. Although the mean-field approximation already introduces precursors of antiferromagnetic correlations among the f electrons at different sites, the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction mediated by the conduction electrons is expected to be the responsible one for antiferromagnetism. Since the RKKY interaction is not explicitly incorporated into our approach, we do not consider the instability towards antiferromagnetism in this paper.

The definition of the projectors renormalizing the hybridization is not unique. There are several possible

choices for the normalization of the projection operators that reproduce all matrix elements correctly. The one used here is associated with the Gutzwiller approximation and reproduces the $U=0$ limit correctly in mean field, although the approach is actually intended for highly correlated states. Within the mean-field approximation it gives a collective enhancement of the Kondo temperature and a tendency towards magnetic long-range order. This is very different from the $1/N$ slave-boson approach,[14–16] which in mean field and with Gaussian fluctuations about the mean field, shows no collective enhancement nor magnetic order, and yields universal properties as a function of one energy scale.[17,18] In both approaches fluctuations play a fundamental role: Within the Gutzwiller approximation the tendency towards magnetic order and the energy scale are expected to diminish, while within the $1/N$ expansion magnetic order has to be induced (probably to order N^{-2}).

A possible motivation to study the ferromagnetic instability as a function of magnetic field is the metamagnetic transition observed in several heavy-fermion compounds, e.g., UPt_3 and $CeRu_2Si_2$.[19] A magnetic field suppresses the antiferromagnetic correlations (not appropriately included in our approach) and induces a rapid increase in the magnetization at a characteristic field H^*. This metamagnetic transition correlates[19] with a peak in the susceptibility at T^*, so that $\mu H^* \sim k_B T^*$. The width of the transition increases with temperature and also the specific heat γ is maximum for $H \sim H^*$. A sharp peak is also observed in the magnetorestriction, $d(\ln V)/dH$. The strong sensitivity of $M(H)$ to alloying impurities into the system suggests that frustration of predominantly antiferromagnetic correlations could play an important role in this transition.

Within the mean-field approximation the low T specific heat is proportional to T with the γ coefficient given by the density of states of f electrons at the Fermi level. In the paramagnetic heavy-fermion situation the γ coefficient is large corresponding to a heavy effective mass. Its dependence with the magnetic field is difficult to estimate except in the $U \to \infty$ limit. With increasing field or magnetization the system undergoes a metamagnetic transition. A peak in the specific heat as a function of T is expected due to this transition. The density of states and hence the effective mass is reduced in the ferromagnetic phase, since the Kondo peak of the majority band is considerably broadened, while the width of the minority band remains roughly unchanged. In addition the peaks for both bands are off resonance with the Fermi level. The orbital degeneracy strongly reduces this change in the effective mass.

II. MODEL AND AUXILIARY BOSON FORMULATION

We consider the Anderson lattice with orbital degeneracy, on-site hybridization V and Coulomb repulsion U,

$$H = \sum_{\mathbf{k}m\sigma} \epsilon_k c^\dagger_{\mathbf{k}m\sigma} c_{\mathbf{k}m\sigma} + \epsilon_f \sum_{im\sigma} f^\dagger_{im\sigma} f_{im\sigma} + V \sum_{im\sigma} (c^\dagger_{im\sigma} f_{im\sigma} + f^\dagger_{im\sigma} c_{im\sigma}) + U \sum_{i,(m\sigma)\neq(m'\sigma')} f^\dagger_{im\sigma} f_{im\sigma} f^\dagger_{im'\sigma'} f_{im'\sigma'} , \tag{2.1}$$

where ϵ_f is the f-level energy, $c^\dagger_{im\sigma}(f^\dagger_{im\sigma})$ creates a conduction electron (f electron) with orbital index $m, |m| \le L$ and spin σ at the site $\mathbf{R}_i$ and $c^\dagger_{\mathbf{k}m\sigma}$ is the corresponding Bloch state with momentum $\mathbf{k}$. For simplicity we consider decoupled spin and orbital degrees of freedom, with the magnetic field only coupling to the spin.

The constraints on the f occupation of the sites caused by the Coulomb repulsion U leads to a complicated many-body problem, which can be reformulated in terms of "auxiliary bosons."[13,20,21] The slave-boson method has been extensively used for the $U \to \infty$ limit in terms of one "slave boson" per site. Within the saddle-point approximation and Gaussian fluctuations about the mean field one obtains universal Fermi-liquid properties in terms of a single energy scale, T_K.[17,18] The method has been extended by Kotliar and Ruckenstein[13] to the finite U situation without orbital degeneracy by introducing four "slave bosons" per site. They studied the Hubbard model with this approach, and later Balseiro *et al.*[20,21] applied this slave-boson technique to a model for highly correlated bands of hybridized Cu $3d$ and O $2p$ orbitals. The slave-boson approach has been formulated with spin-rotational invariance,[22] but this does not affect the mean-field results.

In this paper we generalize the non-spin-rotationally-invariant formulation of Kotliar and Ruckenstein for finite U to include orbital degeneracy. As already stated it is assumed that spin and orbital degrees of freedom are not coupled (no spin-orbit interaction) and that the magnetic field couples to the spin via the Zeeman effect, but not to the orbital moment. We introduce 2^{2N} Bose annihilation operators for each site ($N=2L+1$):

$$b^{(l)}_{i;m_1\sigma_1,m_2\sigma_2,\ldots,m_l\sigma_l} \tag{2.2}$$

and the corresponding creation operators. Here all the index pairs $m\sigma$ have to be different, otherwise the operator is identically zero. The supraindex l determines the configuration onto which the slave-boson projects, i.e., for $l=0$ there is only one operator corresponding to the f^0 configuration (no f electron); $l=1$ represents the f^1 states and there are $2N$ such operators; the operators for $l=2$ form a symmetric second rank tensor of order $2N$ and zero diagonal which describe the f^2 states; etc. In general the slave-boson operators can be represented by a tensor of rank l and order $2N$, which is symmetric in its arguments and has all diagonal elements equal to zero, $\underline{b}^{(l)}_i$.

To simplify the notation we introduce the following product operations between the tensors.

(i) A *full contraction* (scalar product) is defined as

$$\underline{b}^{(l)\dagger}_i \cdot \underline{b}^{(l)}_i \equiv \sum_{m_1\sigma_1,m_2\sigma_2,\ldots,m_l\sigma_l} b^{(l)\dagger}_{i;m_1\sigma_1,m_2\sigma_2,\ldots,m_l\sigma_l} b^{(l)}_{i;m_1\sigma_1,m_2\sigma_2,\ldots,m_l\sigma_l} . \tag{2.3}$$

(ii) For $l \geq 1$ we define a *partial contraction* where $m_n\sigma_n$ is kept fixed as

$$(\underline{b}_i^{(l)\dagger}\cdot\underline{b}_i^{(l)})_{m_n\sigma_n} \equiv \sum_{m_1\sigma_1,\ldots,m_{n-1}\sigma_{n-1},m_{n+1}\sigma_{n+1},\ldots,m_l\sigma_l} b^{(l)\dagger}_{i;m_1\sigma_1,m_2\sigma_2,\ldots,m_l\sigma_l} b^{(l)}_{i;m_1\sigma_1,m_2\sigma_2,\ldots,m_l\sigma_l} \ . \tag{2.4}$$

In terms of these operations the completeness relation takes the form

$$\sum_{l=0}^{2N} \underline{b}_i^{(l)\dagger}\cdot\underline{b}_i^{(l)} = 1 \ , \tag{2.5a}$$

and the correspondence between bosons and fermions is established via

$$f^\dagger_{im\sigma} f_{im\sigma} = \sum_{l=1}^{2N} (\underline{b}_i^{(l)\dagger}\cdot\underline{b}_i^{(l)})_{m\sigma} \equiv h_{im\sigma} \ . \tag{2.5b}$$

These bosons act as projectors onto the corresponding electronic states. In the physical subspace defined by Eqs. (2.5) the operators $f^\dagger_{im\sigma}$ and $f_{im\sigma}$ are replaced by

$$Z^\dagger_{im\sigma} f^\dagger_{im\sigma}, \quad f_{im\sigma} Z_{im\sigma} \ , \tag{2.6}$$

so that the matrix elements are invariant in the combined fermion-boson Hilbert space. The constraints (2.5) are incorporated into the Hamiltonian via Lagrange multipliers, $\lambda_i^{(1)}$ and $\lambda^{(2)}_{im\sigma}$, respectively, and

$$\begin{aligned} H = & \sum_{\mathbf{k}m\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}m\sigma} c_{\mathbf{k}m\sigma} + \epsilon_f \sum_{im\sigma} f^\dagger_{im\sigma} f_{im\sigma} + U \sum_{i,l=2}^{2N} C_2^l (\underline{b}_i^{(l)\dagger}\cdot\underline{b}_i^{(l)}) \\ & + V \sum_{im\sigma} (c^\dagger_{im\sigma} f_{im\sigma} Z_{im\sigma} + Z^\dagger_{im\sigma} f^\dagger_{im\sigma} c_{im\sigma}) + \sum_i \lambda_i^{(1)} \left[\sum_{l=0}^{2N} \underline{b}_i^{(l)\dagger}\cdot\underline{b}_i^{(l)} - 1 \right] + \sum_{im\sigma} \lambda^{(2)}_{im\sigma} (f^\dagger_{im\sigma} f_{im\sigma} - h_{im\sigma}) \ , \end{aligned} \tag{2.7}$$

where C_k^l is the number of possible combinations to choose k electrons out of l ($l \geq k$), i.e.,

$$C_k^l = \begin{bmatrix} l \\ k \end{bmatrix} .$$

As shown by Kotliar and Ruckenstein[13] the definition of the operators $Z_{im\sigma}$ is not unique, but the following choice yields the correct matrix elements *and* the correct expectation value of $\langle Z^\dagger_{im\sigma} Z_{im\sigma} \rangle$ within the mean-field approximation as $U \to 0$,

$$Z_{im\sigma} = (1 - h_{im\sigma})^{-1/2} \sum_{l=1}^{2N} \left[\underline{b}_i^{(l-1)+}\cdot\underline{b}_i^{(l)} \right]_{m\sigma} (h_{im\sigma})^{-1/2} \ , \tag{2.8}$$

where the partial contraction is defined as a summation over $(l-1)$ pairs of indices, while $m\sigma$ in $\underline{b}_i^{(l)}$ is kept fixed. In the Appendix we show that the above choice of normalization correctly reproduces the $U \to 0$ limit.

In the next section we apply the mean-field approximation, in which the boson operators are replaced by their expectation values, first to the general situation and then to the case where only three f-electron configurations are allowed, namely f^n with $n = 0, 1, 2$, while configurations with $n > 2$ are excluded by a very large Coulomb repulsion. This includes as a special case the $U \to \infty$ situation, which has previously been discussed within the saddle-point approximation in Refs. 23 and 24. The electron-hole symmetric Kondo insulator with orbital degeneracy is treated in Sec. IV.

III. MEAN-FIELD APPROXIMATION

To calculate observable quantities we express the partition function $\mathcal{Z}$ of model (2.7) as a functional integral over coherent states of Fermi and Bose fields. The constraints (2.5) commute with the Hamiltonian, so that the Lagrange multipliers are time independent and the physical Hilbert space is invariant under time evolution. The procedure is standard[13] and we obtain

$$\mathcal{Z} = \int [D\underline{b}^{(l)}] \int [D\lambda^{(1)}] \int [D\lambda^{(2)}] \exp\left[-\int_0^\beta d\tau L_{\text{eff}}(\tau) \right] \ , \tag{3.1}$$

where β is the inverse temperature and the site, spin, orbital, and l indices are implicit in the integration variables. The effective action can be written as the sum of two terms, $L_{\text{eff}} = L^B + L^F_{\text{eff}}$, where the first term involves only boson fields, while the second term also contains the Grassmann variables associated with the Fermi fields,

$$L^B = \sum_i \left[\sum_{l=0}^{2N} \underline{b}_i^{(l)\dagger} \left[\frac{\partial}{\partial\tau} + \lambda_i^{(1)} \right] \underline{b}_i^{(l)} - \sum_{m\sigma} \sum_{l=1}^{2N} \lambda^{(2)}_{im\sigma} (\underline{b}_i^{(l)\dagger}\cdot\underline{b}_i^{(l)})_{m\sigma} \right] + U \sum_i \sum_{l=2}^{2N} C_2^l (\underline{b}_i^{(l)\dagger}\cdot\underline{b}_i^{(l)}) \ , \tag{3.2}$$

$$\exp\left[-\int_0^\beta d\tau L^F_{\rm eff}(\tau)\right]=\int [Df][Dc]\exp\left[-\int_0^\beta d\tau L^F(\tau)\right], \tag{3.3}$$

$$L^F(\tau)=\sum_{im\sigma}\left[c^\dagger_{im\sigma}\left(\frac{\partial}{\partial\tau}-\mu\right)c_{im\sigma}+f^\dagger_{im\sigma}\left(\frac{\partial}{\partial\tau}+\epsilon_f-\mu+\lambda^{(2)}_{im\sigma}\right)f_{im\sigma}\right]$$
$$+V\sum_{im\sigma}(c^\dagger_{im\sigma}f_{im\sigma}Z_{im\sigma}+\text{h.c.})+\sum_{\mathbf{k}m\sigma}\epsilon_k c^\dagger_{\mathbf{k}m\sigma}c_{\mathbf{k}m\sigma}, \tag{3.4}$$

where μ is the chemical potential. The chemical potential adjusts the total number of electrons in the system.

The resulting saddle-point free energy functional, $F=-T\ln Z$, is obtained by minimizing the free energy. For the paramagnetic phase it is given by

$$F=-2T\sum_{\alpha,\mathbf{k}}\ln(1+\exp\{-\beta[E_\alpha(\mathbf{k})-\mu]\})+UN_s\sum_{l=2}^{2N}C^{2N}_l C^l_2 b_l^2+\lambda^{(1)}N_s\left[\sum_{l=0}^{2N}C^{2N}_l b_l^2-1\right]-2N\lambda^{(2)}N_s\sum_{l=1}^{2N}C^{2N-1}_{l-1}b_l^2, \tag{3.5}$$

where N_s is the number of sites, $\alpha=1,2$ and

$$E_\alpha(\mathbf{k})=\tfrac{1}{2}\{\epsilon_f+\lambda^{(2)}+\epsilon_k+(-1)^\alpha[(\epsilon_f+\lambda^{(2)}-\epsilon_k)^2+4Z^2V^2]^{1/2}\} \tag{3.6}$$

is the effective dispersion relation of the hybridized states. The minimization of (3.5) with respect to $b_l,\lambda^{(1)}$ and $\lambda^{(2)}$ leads to the set of equations for these parameters.

This approach is equivalent to the mean-field approximation in which all boson operators are replaced by their expectation value. The effective Hamiltonian is then bilinear in Fermi operators and the expectation value for the mean-field groundstate energy can straightforwardly be obtained via the one-particle Green's function. The Hellmann-Feynman theorem is then used to derive the mean-field equations.

In the remainder of this section we consider the metallic situation involving only the $4f^0,4f^1$, and $4f^2$ configurations. We assume that the occupations of the configurations $4f^n$ with $n>2$ can be neglected due to a large Coulomb energy. Projecting out these states corresponds to equating $b_l=0$ for $l>2$. In mean field the Hamiltonian takes the form $(N=2L+1)$

$$H=\sum_{\mathbf{k}m\sigma}\epsilon_k c^\dagger_{\mathbf{k}m\sigma}c_{\mathbf{k}m\sigma}+\sum_{im\sigma}\bar\epsilon_{f\sigma}f^\dagger_{im\sigma}f_{im\sigma}+V\sum_{im\sigma}Z_\sigma(c^\dagger_{im\sigma}f_{im\sigma}+f^\dagger_{im\sigma}c_{im\sigma})$$
$$+N_s\lambda^{(1)}\left[e^2+N\sum_\sigma p_\sigma^2+\frac{N(N-1)}{2}\sum_\sigma d_\sigma^2+N^2d_0^2-1\right]$$
$$-N_sN\sum_\sigma\lambda^{(2)}_\sigma[p_\sigma^2+(N-1)d_\sigma^2+Nd_0^2]+N_sNU\left[\frac{N-1}{2}\sum_\sigma d_\sigma^2+Nd_0^2\right], \tag{3.7}$$

where $\bar\epsilon_{f\sigma}=\epsilon_f+\lambda^{(2)}_\sigma-\sigma B$ is the renormalized f-level energy and B is the Zeeman splitting. Here we used the following notation for the slave-boson expectation values: e corresponds to $b^{(0)}$, i.e., the empty f configuration, p_σ to the $4f^1$ states with spin σ, i.e., bosons with index $l=1$, d_σ to a doubly occupied f state $(l=2)$ with both electrons having spin σ and d_0 to a doubly occupied f state $(l=2)$ with one electron having spin up and the other spin down. We do not distinguish between the spin-singlet and zero-component spin-triplet states, since the formulation is not spin rotationally invariant from the beginning.

We impose another simplifying assumption to reduce the rather large number of parameters to be determined self-consistently, namely, we approximate

$$d_\sigma^2=p_\sigma^2d^2,\quad d_0^2=p_\uparrow p_\downarrow d^2 \tag{3.8}$$

in terms of only one d parameter. With this simplification Z_σ in mean field takes the following form

$$Z_\sigma=\{p_\sigma[e+(N-1)p_\sigma d]+Np_\sigma^{1/2}p_{-\sigma}^{3/2}d\}[A_\sigma(1-A_\sigma)]^{-1/2},$$
$$A_\sigma=p_\sigma^2[1+(N-1)d^2]+Np_\sigma p_{-\sigma}d^2. \tag{3.9}$$

The parameters $\bar\epsilon_{f\sigma},\lambda^{(1)},e,p_\uparrow,p_\downarrow$, and d are obtained by minimization of the ground-state energy of (3.7) with respect to these parameters,

$$\langle f^{\dagger}_{im\sigma} f_{im\sigma}\rangle = p_\sigma^2 + (N-1)p_\sigma^2 d^2 + N p_\sigma p_{-\sigma} d^2 = A_\sigma \ ,$$

$$e^2 + N\left[1+\frac{N-1}{2}d^2\right]\sum_\sigma p_\sigma^2 + N^2 p_\downarrow p_\uparrow d^2 = 1 \ ,$$

$$NV\sum_\sigma \frac{\partial Z_\sigma}{\partial e}\langle f^{\dagger}_{im\sigma} c_{im\sigma}\rangle + \lambda^{(1)} e = 0 \ ,$$

$$V\sum_{\sigma'}\left[2\frac{\partial Z_{\sigma'}}{\partial p_\sigma} - \frac{N}{e}\frac{\partial Z_{\sigma'}}{\partial e}\{2p_\sigma + [(N-1)p_\sigma + Np_{-\sigma}]d^2\}\right]\langle f^{\dagger}_{im\sigma'} c_{im\sigma'}\rangle$$
$$+ U[(N-1)p_\sigma + Np_{-\sigma}]d^2 = \lambda^{(2)}_{-\sigma} N p_{-\sigma} d^2 + \lambda^{(2)}_\sigma\{2p_\sigma[1+(N-1)d^2] + Np_{-\sigma}d^2\} \ ,$$

$$V\sum_\sigma\left[\frac{\partial Z_\sigma}{\partial d} - \frac{Nd}{e}\frac{\partial Z_\sigma}{\partial e}\left[\frac{N-1}{2}\sum_{\sigma'} p_{\sigma'}^2 + Np_\sigma p_{-\sigma}\right]\right]\langle f^{\dagger}_{im\sigma} c_{im\sigma}\rangle$$
$$+ Ud\left[\frac{N-1}{2}\sum_\sigma p_\sigma^2 + Np_\sigma p_{-\sigma}\right] = d\sum_\sigma \lambda^{(2)}_\sigma [Np_{-\sigma} + (N-1)p_\sigma] \ . \quad (3.10)$$

The expectation values $\langle f^{\dagger}_{im\sigma} f_{im\sigma}\rangle$ and $\langle f^{\dagger}_{im\sigma} c_{im\sigma}\rangle$ are obtained from the one-particle Green's functions. We assume a flat density of states for the conduction electrons in the energy interval $(-D,+D)$. Note that in the $U\to 0$ limit for $N>1$ we still have highly correlated states (rather than noninteracting electrons) in view of the excluded occupancy of configurations with more than two f electrons. Below we discuss the solution for some special cases.

A. Paramagnetic solution in zero field

In the paramagnetic phase and for $B=0$ we have that

$$p_\sigma = p_{-\sigma}, \quad \tilde{\epsilon}_{f\sigma} = \tilde{\epsilon}_{f-\sigma} = \tilde{\epsilon}_f \ ,$$
$$Z_\sigma = Z_{-\sigma} = Z, \quad A_\sigma = A_{-\sigma} = A \ , \quad (3.11)$$

and the self-consistency equations (3.10) are reduced to

$$e^2 + Np^2[2+(2N-1)d^2] = 1 \ ,$$
$$A = p^2[1+(2N-1)d^2] \ ,$$
$$\tilde{\epsilon}_f = \mu + \frac{Z^2V^2}{2DA}, \quad \mu = D\left[\frac{n}{N} - 1 - 2A\right] \ , \quad (3.12)$$
$$\lambda^{(2)} = V\left[\frac{1}{p}\frac{\partial Z}{\partial p} - \frac{d}{p^2}\frac{\partial Z}{\partial d} - \frac{2N}{e}\frac{\partial Z}{\partial e}\right]\langle f^{\dagger}_{im\sigma} c_{im\sigma}\rangle$$
$$U = 2V\left[\frac{N}{e}\frac{\partial Z}{\partial e} - \frac{1}{(2N-1)p^2 d}\frac{\partial Z}{\partial d}\right]\langle f^{\dagger}_{im\sigma} c_{im\sigma}\rangle + 2\lambda^{(2)} \ ,$$
$$\langle f^{\dagger}_{im\sigma} c_{im\sigma}\rangle = -\frac{ZV}{2D}\ln\left[\frac{D+\tilde{\epsilon}_f}{\tilde{\epsilon}_f - \mu}\right] \ .$$

Here n is the number of electrons per site. The numerical solution of the above equations is presented in Sec. V.

B. Paramagnetic and ferromagnetic solution in the $U\to\infty$ limit

In the $U\to\infty$ limit only two configurations, namely, $4f^0$ and $4f^1$, play a role and the above equations simplify considerably.[24] Only three slave-boson operator expectation values have to be taken into account, $e, p_\uparrow$, and $p_\downarrow$, while d is identically zero. After some algebra the self-consistency equations can be reduced to

$$\frac{V^2}{2D}[1-N(p_\uparrow^2+p_\downarrow^2)]\left[\frac{1}{(1-p_\uparrow^2)^2}\ln(F_\uparrow) - \frac{1}{(1-p_\downarrow^2)^2}\ln(F_\downarrow)\right] = \tilde{\epsilon}_{f\downarrow} - \tilde{\epsilon}_{f\uparrow} - 2B \ , \quad (3.13a)$$

$$\frac{V^2}{2D}\left[\frac{2N-1+N(p_\downarrow^2-p_\uparrow^2)}{(1-p_\uparrow^2)^2}\ln(F_\uparrow) + \frac{2N-1+N(p_\uparrow^2-p_\downarrow^2)}{(1-p_\downarrow^2)^2}\ln(F_\downarrow)\right] = \tilde{\epsilon}_{f\downarrow} + \tilde{\epsilon}_{f\uparrow} - 2\epsilon_f \ . \quad (3.13b)$$

When we evaluate the integrals contained in F_σ we have to distinguish three situations depending on the position of the chemical potential, $\mu = D(n/N - 1 - p_\uparrow^2 - p_\downarrow^2)$, relative to the gaps in the mean-field density of states. Considering the paramagnetic and ferromagnetic solutions, in general, $p_\uparrow \geq p_\downarrow$, so that there are majority and minority bands for the hybridized conduction and f bands. Considering a bandfilling of less than two electrons per site the lower minority band is always partially filled, while the upper one is empty. On the other hand, the Fermi level can lie in the upper or lower majority band or in the gap.

(i) If μ is below the gap we obtain that

$$F_\sigma = \frac{D + \tilde{\epsilon}_{f\sigma}}{\tilde{\epsilon}_{f\sigma} - \mu}, \quad \tilde{\epsilon}_{f\sigma} = \mu + \frac{1 - N(p_\uparrow^2 + p_\downarrow^2)}{p_\sigma^2 (1 - p_\sigma^2)} \frac{V^2}{2D} . \tag{3.14a}$$

This result holds in general for the minority band, i.e., $\sigma = \downarrow$.

(ii) If μ lies in the gap between the two majority bands, we have

$$F_\uparrow = \frac{1 - p_\uparrow^2}{1 - N(p_\uparrow^2 + p_\downarrow^2)} \frac{D^2 - \tilde{\epsilon}_{f\uparrow}^2}{V^2}, \quad \tilde{\epsilon}_{f\uparrow} = D(1 - 2p_\uparrow^2) . \tag{3.14b}$$

(iii) for μ above the gap between the two majority bands, we have

$$F_\uparrow = \frac{D - \tilde{\epsilon}_{f\uparrow}}{\mu - \tilde{\epsilon}_{f\uparrow}}, \quad \epsilon_{f\uparrow} = \mu - \frac{1 - N(p_\uparrow^2 + p_\downarrow^2)}{(1 - p_\uparrow^2)^2} \frac{V^2}{2D} . \tag{3.14c}$$

The self-consistent solution of Eqs. (3.13) and (3.14) then determines the p_σ and $\tilde{\epsilon}_{f\sigma}$. The numerical solution of these equations for various fields B is presented in Sec. V.

C. Phase diagram for the ferromagnetic instability

The approximations introduced in (3.8) to reduce the total number of independent parameters are strictly valid within the saddle-point approximation only for small magnetizations, but they represent further approximations if $p_\uparrow$ and $p_\downarrow$ are substantially different. Equations (3.10) yield then the correct mean-field phase diagram for the ferromagnetic instability. The numerical solution of Eqs. (3.10) for $B = 0$ and several N is presented in Sec. V.

IV. SYMMETRIC KONDO INSULATOR

In this section we generalize our previous calculation for the symmetric nondegenerate Kondo insulator[12] to include orbital degeneracy. For the sake of simplicity we restrict ourselves to two situations with electron-hole symmetry: (a) $N = 2$ and (b) arbitrary N but by keeping only the three most relevant configurations, i.e., f^N, f^{N-1}, and f^{N+1}.

A. $N = 2$ with electron-hole symmetry

The five f configurations that play a role in this case are the $4f^0$ and $4f^4$ which are both singlets and have the same atomic energies, the $4f^1$ and $4f^3$ that are both fourfold multiplets which are degenerate with each other, and the $4f^2$ states which are the ones with lowest energy (sixfold degenerate atomic groundstate). The symmetric situation is realized for $\epsilon_f = -3U/2$. $N = 2$ could correspond to a crystal-field ground doublet with all other orbital states having large excitation energies. In the paramagnetic phase all matrix elements of the slave-boson operators are independent of spin indices and only depend on l. Hence, only three independent boson expectation values have to be considered, i.e., e for the empty and f^4 configurations, p for the f^1 and f^3 states and d for the configuration with double occupancy.

With the above notation the Hamiltonian reads

$$\begin{aligned} H = & \sum_{\mathbf{k}m\sigma} \epsilon_k c_{\mathbf{k}m\sigma}^\dagger c_{\mathbf{k}m\sigma} + \tilde{\epsilon}_f \sum_{im\sigma} f_{im\sigma}^\dagger f_{im\sigma} \\ & + VZ \sum_{im\sigma} (c_{im\sigma}^\dagger f_{im\sigma} + f_{im\sigma}^\dagger c_{im\sigma}) \\ & + N_s \lambda^{(1)} (2e^2 + 8p^2 + 6d^2 - 1) - 2N_s \lambda^{(2)} \\ & + 6N_s U(e^2 + 2p^2 + d^2) , \end{aligned} \tag{4.1}$$

where $Z = 4p(e + 3d)$. The minimization of the free energy with respect to the five parameters $e, p, d, \lambda^{(1)}$, and $\lambda^{(2)}$ leads to the following set of self-consistency equations

$$\begin{aligned} & 2V \langle f_{im\sigma}^\dagger c_{im\sigma} \rangle \frac{1}{e} \frac{\partial Z}{\partial e} + 3U + \lambda^{(1)} = 0 , \\ & V \langle f_{im\sigma}^\dagger c_{im\sigma} \rangle \frac{1}{p} \frac{\partial Z}{\partial p} + 3U + 2\lambda^{(1)} = 0 , \\ & 2V \langle f_{im\sigma}^\dagger c_{im\sigma} \rangle \frac{1}{d} \frac{\partial Z}{\partial d} + 3U + 3\lambda^{(1)} = 0 , \\ & e^2 + 4p^2 + 3d^2 = \tfrac{1}{2}, \quad \langle f_{im\sigma}^\dagger f_{im\sigma} \rangle = \tfrac{1}{2} . \end{aligned} \tag{4.2}$$

For a half-full flat density of states of the conduction electrons we obtain

$$\langle f_{im\sigma}^\dagger c_{im\sigma} \rangle = -\frac{ZV}{D} \ln \left[\frac{D}{ZV} \right] . \tag{4.3}$$

Eliminating $\lambda^{(1)}$ from the above equations we arrive at

$$\begin{aligned} & p^2 = \tfrac{1}{8}(1 - 6d^2 - 2e^2) , \\ & 4d(1 - 6d^2 - 4e^2 - 6ed) = 3(d - e)(1 - 6d^2 - 2e^2) , \\ & \frac{(d - e)(e + 3d)(1 - 6d^2 - 2e^2)}{ed} \\ & \quad \times \ln \left[\frac{D^2}{2(e + 3d)^2 (1 - 6d^2 - e^2) V^2} \right] = \frac{UD}{V^2} . \end{aligned} \tag{4.4}$$

Next we discuss these equations in two limiting cases: (i) $U = 0$ and (ii) the very large U limit. If $U = 0$ we straightforwardly obtain $d = e = p = \frac{1}{4}$, which corre-

sponds to noninteracting electrons. The Fermi level lies in the gap, $E_{\rm gap}=2V^2/D$. If $U \gg V$, on the other hand, we have that $d \gg e,p$ and

$$E_{\rm gap}=2D\exp\left[-\frac{UD}{12V^2}\right],$$
$$1-6d^2=8p^2=4\sqrt{2}e=\frac{1}{3}\left[\frac{D}{V}\right]^2\exp\left[-\frac{UD}{12V^2}\right]. \tag{4.5}$$

The characteristic energy scale for the paramagnetic phase then decreases exponentially with U. This result is an expected Kondo feature, consequence of the infrared logarithmic singularities caused by electron-hole excitations of arbitrarily energy which are implicit in the formulation. The exponent itself, however, differs from the usual Kondo exponential for an impurity. This is characteristic of Gutzwiller type of approximations and is known as the "lattice enhancement of the Kondo effect"[11,23] believed to arise from the "coherence" in the lattice. The numerical solution of Eqs. (4.4) is presented in Sec. V.

B. Excluded occupation for configurations other than f^N, f^{N-1}, and f^{N+1} for arbitrary N

We consider the totally symmetric situation with arbitrary orbital degeneracy N, i.e., $\epsilon_f=-(N-1/2)U$. If in addition electron-hole symmetry is assumed for the conduction band we have that $b_l=b_{2N-l}$ in the paramagnetic phase. For finite U the states with lowest energy are those of the f^N configuration. The two configurations next in the hierarchy are the f^{N-1} and f^{N+1}. The occupancy of all other configurations is assumed to be negligible and so that these states can be projected out. This means that even in the $U\to 0$ limit for $N>1$ the states are highly correlated. Hence, only three slave-boson expectation values are nonzero, which we denote by $b_N \equiv p$ and $b_{N-1}=b_{N+1}\equiv d$, and

$$H=\sum_{\mathbf{k}m\sigma}\epsilon_k c^\dagger_{\mathbf{k}m\sigma}c_{\mathbf{k}m\sigma}+\bar{\epsilon}_f\sum_{im\sigma}f^\dagger_{im\sigma}f_{im\sigma}+VZ\sum_{im\sigma}(c^\dagger_{im\sigma}f_{im\sigma}+f^\dagger_{im\sigma}c_{im\sigma})$$
$$+N_s\lambda^{(1)}\left[C_N^{2N}\left[p^2+\frac{2N}{N+1}d^2\right]-1\right]-N_sN\lambda^{(2)}+N_sNU\left[\frac{N^2-N+1}{N+1}d^2+\frac{N-1}{2}p^2\right]C_N^{2N}, \tag{4.6}$$

where $Z=2C_N^{2N}pd$. The minimization of the free energy with respect to the four parameters $p,d,\lambda^{(1)}$, and $\lambda^{(2)}$ leads to the following set of self-consistency equations

$$2NV\langle f^\dagger_{im\sigma}c_{im\sigma}\rangle\frac{1}{p}\frac{\partial Z}{\partial p}+\frac{N(N-1)}{2}C_N^{2N}U+C_N^{2N}\lambda^{(1)}=0,$$
$$2(N+1)V\langle f^\dagger_{im\sigma}c_{im\sigma}\rangle\frac{1}{d}\frac{\partial Z}{\partial d}+(N^2-N+1)C_N^{2N}U+2C_N^{2N}\lambda^{(1)}=0, \tag{4.7}$$
$$C_N^{2N}[(N+1)p^2+2Nd^2]=N+1,\quad \langle f^\dagger_{im\sigma}f_{im\sigma}\rangle=1/2.$$

For a half-full flat density of states of the conduction electrons we obtain

$$\langle f^\dagger_{im\sigma}c_{im\sigma}\rangle=-\frac{ZV}{2D}\ln\left[\frac{2D}{E_{\rm gap}}\right],\quad E_{\rm gap}=2\frac{Z^2V^2}{D}. \tag{4.8}$$

Eliminating $\lambda^{(1)}$ from the first two equations of the set (4.7) we arrive at

$$4C_N^{2N}[(N+1)p^2-2Nd^2]\ln\left[\frac{2D}{E_{\rm gap}}\right]=\frac{UD}{V^2}. \tag{4.9}$$

We now discuss the asymptotic solution of (4.9) for arbitrary N in the limit of large U. This equation yields the energy gap (about the Fermi level) within the paramagnetic phase. For large $U,d \ll p$ and $p^2\sim[C_N^{2N}]^{-1}$, so that

$$E_{\rm gap}=2D\exp\left[-\frac{UD}{4(N+1)V^2}\right], \tag{4.10}$$
$$1-C_N^{2N}p^2=\frac{2N}{N+1}C_N^{2N}d^2=\frac{N}{2(N+1)}\left[\frac{D}{V}\right]^2\exp\left[-\frac{UD}{4(N+1)V^2}\right],$$

which correctly reproduces the results for the orbitally nondegenerate ($N=1$) (Ref. 12) and the $N=2$ [Eq. (4.5)] cases.

V. RESULTS

Below we present the solution of the mean-field equations derived in the previous two sections.

A. Kondo insulator: $N=2$ with electron-hole symmetry

We now consider the situation of the orbitally degenerate Kondo insulator with electron-hole symmetry discussed in Sec. IV A. For the insulator the Fermi level lies in the energy gap, $E_{\rm gap}$. The corresponding mean-field equations for $N=2$ are given by (4.4). $N=2$ could represent a ground doublet caused by a large crystal field splitting. The numerical solution of these equations for $D=10$ V and as a function of U/V is shown in Fig. 1(a).

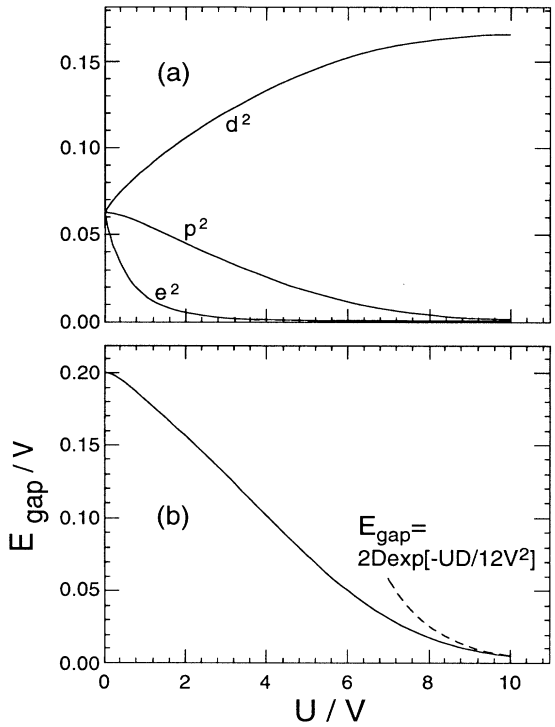

FIG. 1. Paramagnetic solution for the electron-hole symmetric Kondo insulator for $N=2$ and $D=10$ V. (a) Occupation probabilities for the f^n configurations: e^2 for $n=0$ and 4, p^2 for $n=1$ and 3, and d^2 for $n=2$, and (b) the energy gap $E_{\rm gap}$ normalized to V, as a function of U/V.

As expected for $U=0$ we obtain $e=p=d=\frac{1}{4}$. As a function of U, d^2 increases monotonically and asymptotically reaches the value $\frac{1}{6}$ for very large U. p^2 and e^2, which represent the occupation probabilities of the $4f^1$ and $4f^0$ configurations, decrease exponentially for sufficiently large U. Note that for large U the U dependence approximately follows $p^2/e \sim$ const. The magnitude of the energy gap, normalized to V, is displayed in Fig. 1(b). The exponential form given by Eq. (4.5) is approached asymptotically for large U.

B. Paramagnetic and ferromagnetic solution for the metal in the $U \to \infty$ limit

Next we present the numerical solution of the mean-field equations (3.13) and (3.14) as a function of the bare f-level position for the paramagnetic and ferromagnetic phases. Here we consider the orbitally nondegenerate case, i.e., $N=1$, with 1.8 electrons per site and $D/V=10$. The results are displayed in Figs. 2(a) and 2(b). For a sufficiently large ϵ_f there is only the paramagnetic solution, i.e., $p_\uparrow = p_\downarrow$, and the zero-field magnetization is zero. When ϵ_f is reduced to about 3.8 V a second solution with $p_\uparrow \neq p_\downarrow$ with lower energy than the paramagnetic one appears [see Fig. 2(a)]. The system undergoes a second-order phase transition to a ferromagnetic state. The magnetization grows monotonically when ϵ_f is decreased further until the lower majority band is filled. At this point the increase of the magnetization with decreasing ϵ_f becomes flat until the upper majority band starts to be occupied. Energy calculations show that this transition is of first order and occurs at about $\epsilon_f \sim -1.1$ V. The small variation of m with ϵ_f is due to the dependence of $p_\uparrow$ and $p_\downarrow$ on ϵ_f. Asymptotically as $\epsilon_f \to -\infty$ the system is fully polarized. An external magnetic field shifts the threshold of the paramagnetic to ferromagnetic transition to larger values of ϵ_f. The range of the flat region due to the gap in the majority band decreases with an external magnetic field and the first-order transition as a function of ϵ_f becomes continuous for $B > 0.05$ V.

In Fig. 2(b) we show the magnetization as a function of the field for various values of ϵ_f representing four different situations. If $\epsilon_f < 3.8$ V we obtain a spontaneous magnetization in zero field. The magnetization is always an increasing function of the magnetic field. The discontinuous transition shown for $\epsilon_f = 1.5$ V arises again from the upper majority band which at that field starts to get filled. This transition is continuous for $\epsilon_f = 3$ V. For $\epsilon_f = 4$ V and for small fields the paramagnetic

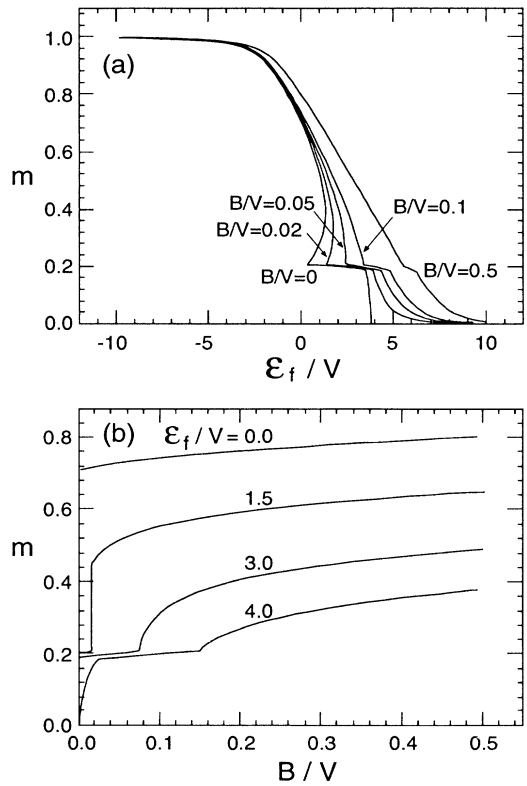

FIG. 2. Magnetization m of the paramagnetic and ferromagnetic phases for the metal in the $U \to \infty$ limit for $N=1$, $D=10$ V and 1.8 electrons per site. (a) m as a function of ϵ_f normalized to V for various fields B. The field is in units of V. There is a second- and a first-order transition if $B=0$; the discontinuous transition becomes continuous for $B > 0.05$ V. (b) m as a function of B/V for representative values of ϵ_f, which show the four different situations that may occur.

solution is the stable one.

Asymptotically as ϵ_f becomes very negative, the valence, $v = e^2$, of the paramagnetic state for arbitrary N is given by

$$v = 1 - n_f = \frac{(2N-1)(D+\epsilon_f+\lambda^{(2)})D}{2N^2V^2} \times \exp\left[-\frac{(2N-1)\lambda^{(2)}D}{2N^2V^2}\right] . \quad (5.1)$$

In this limit also $\epsilon_f + \lambda^{(2)} \sim \mu$, so that this expression agrees with the one derived previously by Ueda and Rice[23,24] within the Gutzwiller approximation. It should be pointed out that the exponential dependence for large ϵ_f in (5.1) differs from the usual Kondo exponential. This different exponential dependence is characteristic of Gutzwiller type of approximations and is known as the "lattice enhancement of the Kondo effect,"[11,23] which increases the ground-state Kondo-boundstate energy of the lattice with respect to that of the impurity. This difference is believed to arise due to the "coherence" in the lattice. For $N \to \infty$ the energy scale agrees with the corresponding one for the one slave-boson treatment.[15,16]

The orbitally degenerate situation has been discussed in more detail in a previous report.[24] There is only one second-order transition if $N > 1$, since the lower majority band can never be completely filled if the total number of electrons is kept constant at $n = 1.8$.

C. Paramagnetic solution for the metal in zerofield

We now present the numerical solution of Eqs. (3.12), which refer to the metallic paramagnet for arbitrary N and involving only the $4f^0, 4f^1$, and $4f^2$ configurations. All other configurations are projected out. The results are displayed in Figs. 3 and 4 for $D = 10$ V, $n = 1.8$ and $U = V$. In Figs. 3(a)–3(c) e^2, p^2, and d^2 are shown as a function of ϵ_f / V for $N = 1$, 3 and 5, respectively. e^2 (d^2) monotonically increases (decreases) with ϵ_f, while p^2 shows a maximum as a function of ϵ_f. This behavior can be understood in terms of the ionic energies of the three configurations, which are $E(f^0) = 0$, $E(f^1) = \epsilon_f$ and $E(f^2) = 2\epsilon_f + U$, respectively. There are crossovers of the levels when $\epsilon_f = 0$, $\epsilon_f = -U$, and $\epsilon_f = -U/2$. The former two level crossovers separate three regimes with different ground states. The hybridization smears out the sharp transitions between the ionic states and shifts the level crossovers to lower values of ϵ_f. The degeneracy introduces a strong asymmetry in the curves, since the number of states of the three configuration differs considerably, in particular, the degeneracy of the f^2 configuration grows rapidly with N, while the f^0 is always a singlet.[25]

In Fig. 4(a) the probability of occupation of the f^2 configuration is shown as a function of f-level position for $N = 1$, 3, and 5 and the same parameters as above. This occupation, of course, decreases with ϵ_f and strongly depends on the orbital degeneracy. A similar behavior is observed for the total number of f electrons [see Fig. 4(b)].

D. Phase diagram for the ferromagnetic instability

In Figs. 5(a)–5(c) we present the mean-field phase diagram for the magnetic instability in the metallic situation, i.e., the numerical solution of Eqs. (3.10) for $B = 0$ and $N = 1$, 3, and 5, respectively. The phase corresponding to the larger values of ϵ_f is the paramagnetic one. If ϵ_f is more negative than the paramagnetic to ferromagnetic boundary, the localized moment character is higher and there is the tendency towards magnetic order. As expected magnetic order becomes more unlikely with in-

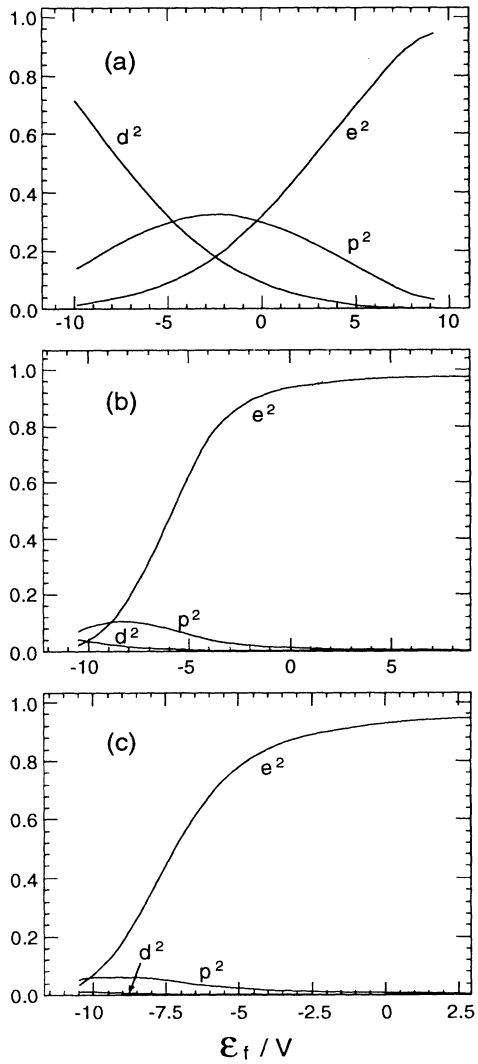

FIG. 3. Paramagnetic solution for the metal in zero field, $D = 10$ V, $n = 1.8$ and $U = V$. Shown are the occupation probabilities for the f^l configurations as a function of ϵ_f: e^2 for $l = 0$, p^2 for $l = 1$, and d^2 for $l = 2$, all other configurations are excluded by a large Coulomb repulsion: (a) $N = 1$, (b) $N = 3$, and (c) $N = 5$.

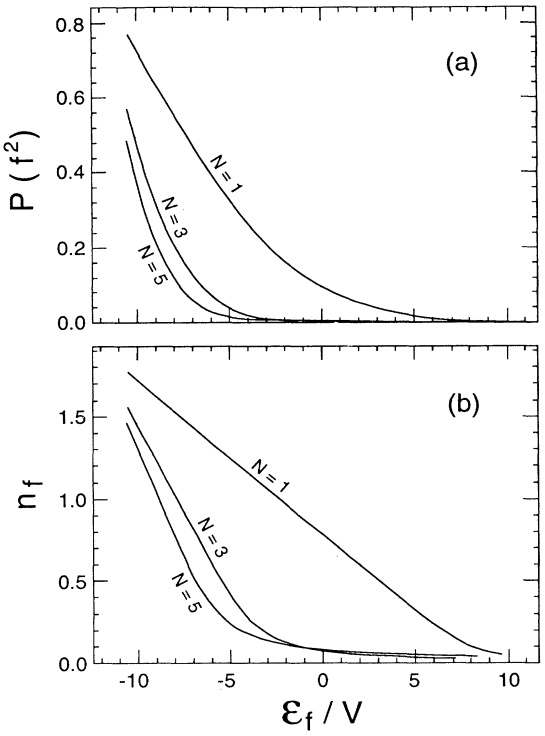

FIG. 4. (a) Probability of occupation of the f^2 configuration and (b) total number of f electrons, n_f, as a function of ϵ_f in the paramagnetic phase for the metal in zero field, $D=10$ V, $n=1.8$, $U=V$, and $N=1$, 3, and 5.

creasing N. For instance, since $D=10$ V, if $N=5$ the ferromagnetic boundary already lies outside the original conduction band.

The Gutzwiller saddle-point approximation is believed to overestimate the magnetic order. Quantum fluctuations about the mean-field solution will reduce the ferromagnetic long-range order. This would shift the paramagnetic and ferromagnetic boundary to larger U values.

VI. CONCLUSIONS

In order to treat the correlations within the f shell in a metallic Anderson lattice with orbital degeneracy adequately, we generalized Kotliar and Ruckenstein's treatment[13,20] of the Hubbard model and introduced a complete set of "slave"-boson operators, $b^{(l)}_{i,m_1\sigma_1,m_2\sigma_2,\ldots,m_l\sigma_l}$. These boson operators act as projectors onto the corresponding electronic states. In the physical subspace the fermion creation and annihilation operators are replaced by a product of a fermion operator and a function of Bose operators $Z_{im\sigma}$ so that the matrix elements are invariant in the combined fermion-boson Hilbert space. The constraints limiting the Hilbert space to the physical one are introduced via Lagrange parameters. Subsequently we performed the standard mean-field approximation and replaced the slave bosons by their expectation values. The boson expectation values and the Lagrange parameters are determined self-consistently by making use of the Hellmann-Feynman theorem and minimizing the ground-state energy.

We studied the $T=0$ properties of the paramagnetic and ferromagnetic states as a function of $N, \epsilon_f/V$, and U/V for the metallic situation (the Fermi level does not lie in the gap). For $U\to\infty$ the valence in the paramagnetic state has the characteristic exponential Kondo dependence, which includes the "lattice enhancement of the Kondo effect"[11,23] typical of Gutzwiller-type approximations and differs from the standard impurity Kondo temperature dependence, unless N is very large. For finite U and $N>1$ the role played by the f^0 and f^2 is different[25] and introduces a strong electron-hole asymmetry, as a consequence of the large difference in the degeneracies of the configurations. Note that for $U=0$ and $N>1$ this situation does not correspond to noninteract-

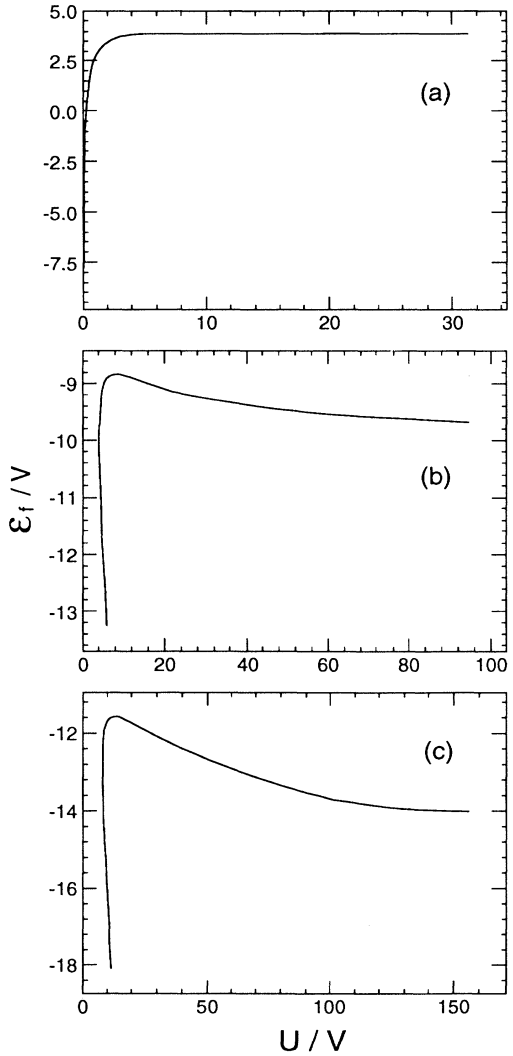

FIG. 5. (a) Mean-field phase diagram for the paramagnetic to ferromagnetic instability for the metallic situation in zero field, $D=10$ V, $n=1.8$ and (a) $N=1$, (b) $N=3$, and (c) $N=5$.

ing fermions.

Fluctuations about the mean field are expected to reduce the magnetic instability, in the same way as an increase in the orbital degeneracy for a given ϵ_f. In this sense we believe that the tendency towards ferromagnetic order is exaggerated within mean field. Fluctuations also will reduce or even smear the discontinuous transition shown in Fig. 1 for $N=1$ and $U\rightarrow\infty$. Since our approach does not generate the RKKY interaction between the rare-earth ions, which is a fundamental component possibly leading to antiferromagnetic order, we have not attempted to study this instability.

Finally, we extended our treatment of the Kondo insulator[12] to include orbital degeneracy. The paramagnetic phases of two cases have been discussed: (i) $N=2$ with electron-hole symmetry which involves five f configurations and (ii) the electron-hole symmetric situation for arbitrary N where only the three most important configurations are kept, while the occupation of all other configurations is assumed negligible in view of large Coulomb interactions within the f shell. The Fermi level lies in the gap, which in both cases has an exponential Kondo dependence.

ACKNOWLEDGMENT

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APPENDIX: NORMALIZATION OF THE OPERATORS $Z_{im\sigma}$

The physical subspace in which the "auxiliary bosons" represent the correlations among f electrons is restricted to the boson-occupation numbers zero and one. This is a consequence of the constraints (2.5). All the matrix elements of $\underline{b}_i^{(l)}$ become independent of $m\sigma$ in the limit $U\rightarrow 0$. In this limit the *full* and *partial contractions* simplify considerably. Within mean field we introduce expectation values of the boson operators, b_l, which are independent of the spin, the orbital momentum and the site, and obtain

$$\langle \underline{b}_i^{(l)\dagger}\cdot\underline{b}_i^{(l)}\rangle = C_l^{2N} b_l^2 , \tag{A1}$$

$$\langle (\underline{b}_i^{(l)\dagger}\cdot\underline{b}_i^{(l)})_{m\sigma}\rangle = C_{l-1}^{2N-1} b_l^2 . \tag{A2}$$

It is now straightforward to show that for $U=0$ and within the mean-field approximation the minimization of the groundstate energy is equivalent to maximize the expectation value of $Z_{im\sigma}^{\dagger}Z_{im\sigma}$, where $Z_{im\sigma}$ is defined by (2.8). In mean field this expectation value is given by

$$Z^2=\langle Z_{im\sigma}^{\dagger}Z_{im\sigma}\rangle = \frac{\left[\sum_{k=1}^{2N} C_{k-1}^{2N-1} b_{k-1}b_k\right]^2}{\left[\sum_{k=1}^{2N} C_{k-1}^{2N-1} b_k^2\right]\left[\sum_{k=1}^{2N} C_{k-1}^{2N-1} b_{k-1}^2\right]} \equiv \frac{C^2}{AB} , \tag{A3}$$

where A,B, and C are functions of the b_l defined by Eq. (A3). The function Z has its maximum with respect to the variables b_l when $\partial Z/\partial b_l=0$ for all l, i.e.,

$$[lb_{l-1}+(2N-1)b_{l+1}]AB = b_l[lB+(2N-l)A]C . \tag{A4}$$

Equation (A4) defines a set of recurrent relations, which has the following solution

$$b_k^2 = B^{2N-k}A^k . \tag{A5}$$

Inserting this solution into Eq. (A3) we obtain that $C^2=AB$, and consequently

$$Z=1 , \tag{A6}$$

which is the correct result in the absence of correlations. This extends the proof of Kotliar and Ruckenstein[13] to our more general case.

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