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The Gutzwiller approach to magnetic instabilities in heavy-fermion systems

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Abstract. Magnetic properties of the orbitally non-degenerate periodic Anderson model are investigated using Kotliar and Ruckenstein's slave-boson reformulation of the Gutzwiller variational method. The Gutzwiller approximation is reproduced at the saddle-point level for $T = 0$. This approach allows us to extend the analysis of Rice and Ueda to calculate the magnetization as a function of applied magnetic field. We find that a magnetic instability exists in the Kondo regime. Our findings suggest that the Gutzwiller approximation is too biased towards the magnetic state.

1. Introduction

Much progress has been made in understanding many of the low-temperature properties of heavy-fermion systems. Among the fundamental problems that remain, however, is an understanding of the instabilities in many of these systems at very low temperatures to various forms of magnetic order.

It is generally accepted that many of the properties of heavy-fermion systems can be understood on the basis of the periodic Anderson model (PAM). In this paper we investigate magnetic properties of the orbitally non-degenerate PAM using Kotliar and Ruckenstein's slave-boson reformulation of the Gutzwiller variational method (Kotliar and Ruckenstein 1986). For $T = 0$ the Gutzwiller approximation is reproduced at the saddle-point level. This approach allows us to extend the analysis of Rice and Ueda (1985, 1986) to calculate magnetization as a function of applied magnetic field.

In the Gutzwiller approach, correlations are treated by renormalizing all hopping processes by a factor $q(n_{f\uparrow}, n_{f\downarrow})$, where $n_{f\sigma}$ is the number of f electrons with spin σ. To make the calculation tractable one has to introduce the Gutzwiller approximation, which amounts to the neglect of intersite correlations. This additional approximation in using the Gutzwiller wavefunction has been shown to be exact in the limit of large dimensionality (Metzner and Vollhardt 1989, Gebhard 1991). Then for the strong-correlation limit (where the on-site Coulomb replusion between f electrons $U \rightarrow \infty$) , q is given by the ratio of occupation number factors for the correlated and uncorrelated wavefunctions. In the correlated wavefunction an f electron can hop onto another site only if it has no f electrons, while in the uncorrelated wavefunction the only requirement is that it does not have an f electron with the same quantum numbers, so that $q_\sigma = (1 - n_f)/(1 - n_{f\sigma})$.

Within the Gutzwiller approach a simple physical picture emerges for the existence of magnetic instabilites in the strong-correlation limit. In the PAM, hopping processes

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involve two factors of the hybridization V, and so V is renormalized by a factor $\sqrt{q_\sigma}$, $V_k \to \sqrt{q_\sigma} V_k$. It is the spin dependence of the effective hybridization which leads to a magnetic instability for a sufficiently small hybridization strength.

This paper is organized as follows. In section 2 we apply Kotliar and Ruckenstein's slave-boson reformulation of the Gutzwiller variational method to the orbitally non-degenerate PAM. In section 3 we present the results of numerically solving the saddle-point equations. Conclusions are presented in section 4.

2. Formulation

In this section we apply Kotliar and Ruckenstein's slave-boson reformulation of the Gutzwiller variational method to the orbitally non-degenerate PAM. Our analysis is carried out for the uniform magnetic states.

The orbitally non-degenerate periodic Anderson model is

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k\sigma} V_k f^\dagger_{k\sigma} c_{k\sigma} + V_k^* c^\dagger_{k\sigma} f_{k\sigma} + \sum_{i\sigma} E_f f^\dagger_{i\sigma} f_{i\sigma} + U \sum_i f^\dagger_{i\uparrow} f_{i\uparrow} f^\dagger_{i\downarrow} f_{i\downarrow} \tag{1}$$

where $c_{k\sigma}$ ($c^\dagger_{k\sigma}$) and $f_{k\sigma}$ ($f^\dagger_{k\sigma}$) are the conduction and f-electron annihilation (creation) operators, respectively. The position of the bare f level is given by $E_{f\sigma} = E_f + \sigma h$, where we have included an applied external magnetic field h, which couples only to the spin of the f electrons. For simplicity we take the hybridization-matrix element V_k for conduction and f electrons to be k-independent. The conduction-band dispersion is given by ϵ_k. To obtain a metal even in the presence of the hybridization gap we assume a non-integral number of electrons. This is achieved formally by introducing a second non-hybridized conduction band which acts merely as an electron reservoir.

To treat the effects of strong correlations we adopt Kotliar and Ruckenstein's slave-boson formulation of the Gutzwiller variational approach. They considered the one-band Hubbard model. To extend the method to the periodic Anderson model we need to project out the doubly occupied f orbitals, keeping fixed the number n_f of f electrons. To do this, we go over to a grand canonical ensemble and introduce an f-electron self-energy μ_σ, leading to the effective Hamiltonian for fixed n_f:

$$H_{\text{eff}} = H - \sum_{k\sigma} \mu_\sigma f^\dagger_{k\sigma} f_{k\sigma}. \tag{2}$$

Following Kotliar and Ruckenstein we enlarge the Fock space, to contain, in addition to the original fermions, a set of four bosons representing the creation (annihilation) of singly occupied f orbitals $p^\dagger_{i\sigma}$ ($p_{i\sigma}$), doubly occupied f orbitals $d^\dagger_{i\sigma}$ ($d_{i\sigma}$) and vacant f orbitals $e^\dagger_i$ (e_i). The f-electron operators are replaced by

$$f_{i\sigma} \to f_{i\sigma} z_{i\sigma} \tag{3}$$

with

$$z_{i\sigma} = e^\dagger_i p_{i\sigma} + p^\dagger_{i-\sigma} d_i \tag{4}$$

and we eliminate non-physical states by imposing the constraints,

$$\sum_\sigma p_{i\sigma}^\dagger p_{i\sigma} + e_i^\dagger e_i + d_i^\dagger d_i = 1 \qquad f_{i\sigma}^\dagger f_{i\sigma} = p_{i\sigma}^\dagger p_{i\sigma} + d_i^\dagger d_i \tag{5}$$

representing, respectively, the completeness (each f orbital is empty or singly or doubly occupied) and equality in the way f electrons are counted. The effective Hamiltonian becomes bilinear in creation and annihilation operators, and is given by

$$H_{\text{eff}} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{i,k\sigma} V_k \left(\mathrm{e}^{-\mathrm{i}kR_i} f_{i\sigma}^\dagger z_i^\dagger c_{k\sigma} + \mathrm{e}^{+\mathrm{i}kR_i} c_{k\sigma}^\dagger f_{i\sigma} z_i \right) + \sum_{i\sigma} (E_{f\sigma} - \mu_\sigma) f_{i\sigma}^\dagger f_{i\sigma} + U \sum_i d_i^\dagger d_i . \tag{6}$$

We obtain physical quantities from the partition function that we write as a functional integral over coherent states of Fermi and Bose fields with the constraints (equation (3)) enforced by Lagrange multipliers $\lambda_i^{(1)}$ and $\lambda_{i\sigma}^{(2)}$:

$$Z = \int [\mathcal{D}c][\mathcal{D}f][\mathcal{D}p][\mathcal{D}e] \prod_i \mathrm{d}\lambda_i^{(1)} \prod_i \mathrm{d}\lambda_{i\sigma}^{(2)} \exp\left(- \int_o^\beta \mathrm{d}\tau S(\tau) \right) \tag{7}$$

$$S = \sum_i e_i^\dagger \left(\partial + \lambda_i^{(1)} \right) e_i + \sum_\sigma p_{i\sigma}^\dagger \left(\partial + \lambda_i^{(1)} - \lambda_{i\sigma}^{(2)} \right) p_{i\sigma} + d_i^{(\dagger)} \left(\partial + U + \lambda_i^{(1)} - \lambda_{i\sigma}^{(2)} \right) d_i - \lambda_i^{(1)} + H_{\text{eff}} . \tag{8}$$

We formally integrate out the fermions and evaluate the resulting partition function in the saddle-point approximation, in which all Bose fields and Lagrange multipliers are taken to be independent of space and (imaginary) time.

Unfortunately, the resulting saddle-point equations lead to an incorrect result in the non-interacting limit (which occurs for $U = 0$ or in the case of fully spin-polarized f electrons). This is because in the saddle-point approximation the constraints are not satisfied explicitly at each lattice site but only on average.

To resolve this difficultly we note that the choice of $z_{i\sigma}$ is not unique and one can replace $z_{i\sigma}$ by any combination $U_{i\sigma} z_{i\sigma} V_{i\sigma}$ such that $U_{i\sigma} = 1$ when $e_i^\dagger e_i = 1$ or $p_{i-\sigma}^\dagger p_{i-\sigma} = 1$ and $V_{i\sigma} = 1$ when $p_{i\sigma}^\dagger p_{i\sigma} = 1$ or $d_i^\dagger d_i = 1$. All the choices are formally equivalent when the constraints are handled exactly. However, at the saddle-point level when the constraints are satisfied only on average, the results are dependent on the choice for $z_{i\sigma}$. We take advantage of this ambiguity to ensure that the non-interacting limit is correctly given in the saddle-point approximation. We choose, as did Kotliar and Ruckenstein,

$$z_{i\sigma} = \left(1 - d_i^\dagger d_i - p_{i\sigma}^\dagger p_{i\sigma} \right)^{-1/2} \left(e_i^\dagger p_{i\sigma} + p_{i-\sigma}^\dagger d_i \right) \left(1 - e_i^\dagger e_i - p_{i-\sigma}^\dagger p_{i-\sigma} \right)^{-1/2} . \tag{9}$$

This choice also reproduces the Gutzwiller approximation within the saddle-point approximation (Gebhard 1991).

The saddle-point free energy $F = -k_B T \ln Z$ can then be written as

$$F = Ud^2 + \sum_{\pm\sigma} \int \mathrm{d}k\, \rho \xi^{\pm}_{k\sigma} \ln[1 + \exp(-\beta \xi^{\pm}_{k\sigma})] + \lambda^{(1)} \left(\sum_{\sigma} p_\sigma^2 + e^2 + d^2 - 1 \right) - \sum_{\sigma} \lambda^{(2)} (p_\sigma^2 + d^2) \tag{10}$$

where $p_\sigma^2 = \langle p^+ p \rangle$ etc. The energy of the hybridized bands is

$$\xi^{\pm}_{k\sigma} = \tfrac{1}{2} \left[(\epsilon_k + E_{f\sigma} + \mu_\sigma) \pm \sqrt{(\epsilon_k - E_{f\sigma} - \mu_\sigma)^2 \pm 4 q_\sigma V^2} \right] \tag{11}$$

where

$$q_\sigma = \langle z_\sigma^\dagger z_\sigma \rangle \tag{12}$$

and the $+(-)$ label refers to the upper (lower) hybridized band. Minimizing the free energy (equation (10)) with respect to $\lambda^{(1)}, \lambda^{(2)}_\sigma, \mu_\sigma, p_\sigma$ and d gives integral equations for $n_{f\sigma}$, μ_σ and U

$$n_{f\sigma} = -\frac{1}{w} \int_{-w}^{w} A^+_{k\sigma} f(\xi^-_{k\sigma} - \mu) + A^-_{k\sigma} f(\xi^+_{k\sigma} - \mu)\, \mathrm{d}\epsilon_k \tag{13}$$

$$\mu_\sigma = -\sum_{\alpha} \frac{V^2}{2W} \frac{\partial q_\alpha}{\partial n_{f\sigma}} \int_{-w}^{w} \frac{f(\xi^-_{k\alpha} - \mu) - f(\xi^+_{k\alpha} - \mu)}{\xi^+_{k\alpha} - \xi^-_{k\alpha}}\, \mathrm{d}\epsilon_k \tag{14}$$

where

$$A^{\pm}_{k\sigma}(k) = -\tfrac{1}{2} \{ 1 \pm (\epsilon_k - E_f - \mu_\sigma) / [(\epsilon_k - E_f - \mu_\sigma)^2 + 4 q_\sigma V^2]^{1/2} \}. \tag{15}$$

We determine d from

$$U = \sum_{\alpha} \frac{V^2}{2W} \frac{\partial q_\alpha}{\partial d} \int_{-w}^{w} \frac{f(\xi^-_{k\alpha} - \mu) - f(\xi^+_{k\alpha} - \mu)}{\xi^+_{k\alpha} - \xi^-_{k\alpha}}\, \mathrm{d}\epsilon_k \tag{16}$$

and the chemical potential μ from the total electron density,

$$n_{e\sigma} = 2\rho \int_{-w}^{w} f(\xi^+_{k\sigma} - \mu) + f(\xi^-_{k\sigma} - \mu)\, \mathrm{d}\epsilon_k. \tag{17}$$

Here ρ_0 is the conduction-electron density of states and W is the conduction-electron bandwidth.

3. Results

In this section we present the results of numerically solving the saddle-point equations. We calculate the magnetization as a function of applied magnetic field for a variety of values of the on-site Coulomb repulsion between f electrons U, the bare hybridization V and the total electron density n_e.

We took the conduction-electron bandwidth to be $2W = 20\,\text{eV}$, the conduction-electron density of states was taken to be a constant, $\rho_0 = 1/2W$, and the bare f level was taken to be $E_f = -1.5\,\text{eV}$ below the middle of the conduction band.

In figure 1 we have plotted magnetization $m = n_{e\uparrow} - n_{e\downarrow}$ as a function of the on-site Coulomb repulsion between f electrons U for $n_e = 1.9$ and $n_e = 1.8$. For $U = 0$ we obtain the correct non-interacting limit with $q_\sigma = 1$ and with the double occupancy given by its Hartree–Fock value $d^2 = \langle n_{f\uparrow}\rangle\langle n_{f\downarrow}\rangle$, as it should be. With increasing U we find a crossover from paramagnetism to weak ferromagnetism corresponding to a full lower hybridized up-spin band. Here $n_{e\uparrow} = 1$, so the moment is $m = n_{e\uparrow} - n_{e\downarrow} = 1 - (n_e - 1) = 2 - n_e$. With a further increase in U there can be no further increase in the magnetization until electrons in the down-spin band can be transferred to the upper hybridized up-spin band. This occurs at much larger values of U when the Fermi level lies in the upper hybridized up-spin band. Then we find a crossover to strong ferromagnetism.

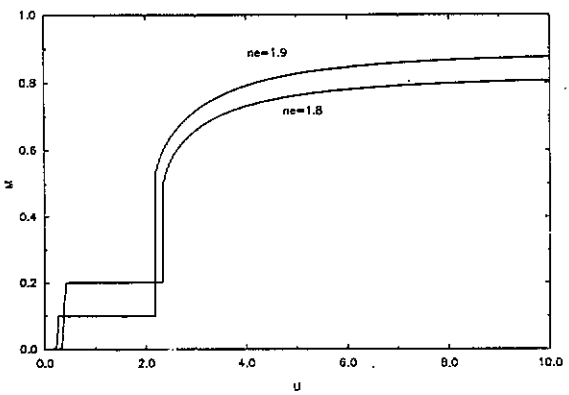

Figure 1. Magnetization as a function of the on-site Coulomb repulsion between f electrons U for the total electron density $n_e = 1.9$ and $n_e = 1.8$ and bare hybridization strength $V = 1.0$.

In figure 2, where we have plotted the hybridized bands $\xi_{k\sigma}$ as a function of the conduction band ϵ_k, the figure shows how the transition occurs from paramagnetism to ferromagnetism. We see in figure 2(*a*) (corresponding to $U = 0$ in figure 1) a paramagnet with magnetization $m = 0$, in figure 2(*b*) ($U = 1$) a weak ferromagnet with $m = 2 - n_e$ and in figure 2(*c*) ($U = 10$) a strong ferromagnet.

We have plotted in figure 3 the phase diagram in the U–n_e plane.

We now consider the strong-correlation limit ($U \to \infty$) in which double occupancy of f orbitals is forbidden ($d^2 = 0$). In figure 4 we show magnetization as a function of hybridization strength V for $n_e = 1.9$. We find strong ferromagnetism for a sufficiently low hybridization strength. With increasing hybridization strength, spin polarization decreases as f electrons are promoted to the Fermi level and delocalize. Then at a critical hybridization strength V_c there is a first-order transition to weak ferromagnetism, with the moment $m = 2 - n_e$.

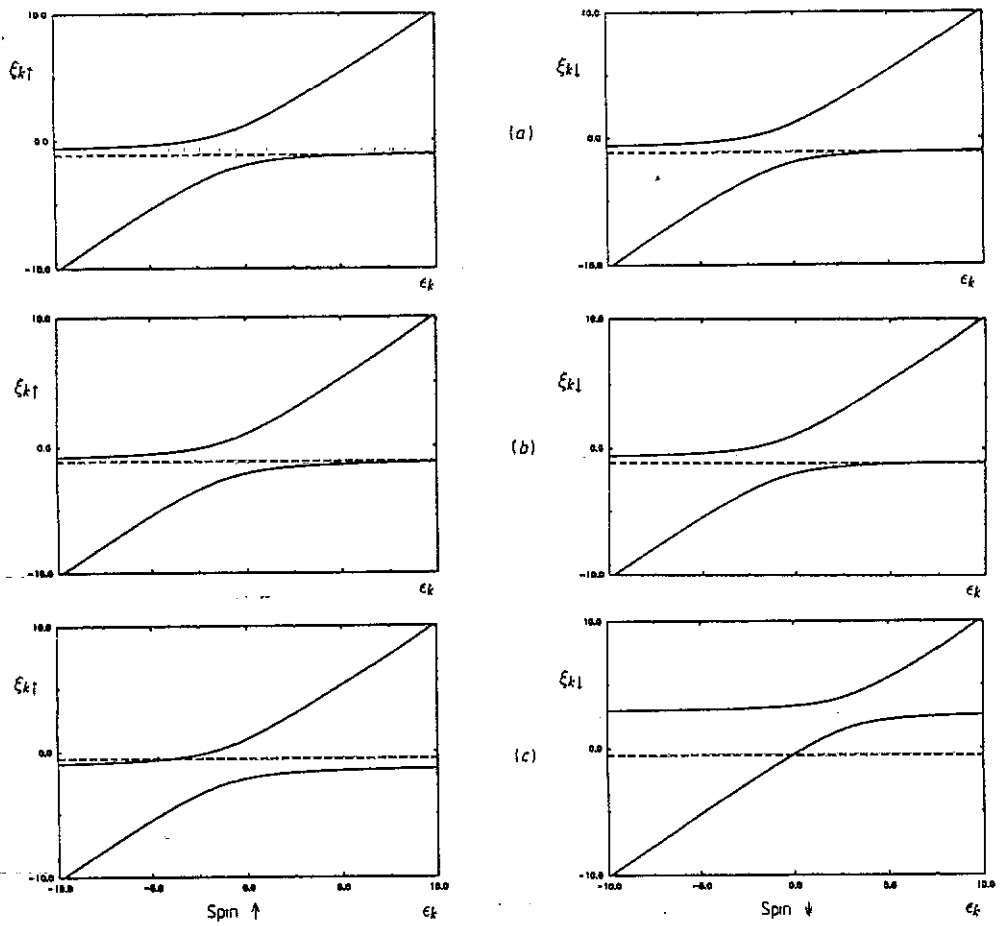

Figure 2. Hybridized band energy as a function of the conduction band energy. The transition from paramagnetism to ferromagnetism. (*a*) $U = 0$, paramagnetism; (*b*) $U = 1$, weak ferromagnetism with magnetization $m = 2 - n_e$; (*c*) $U = 10$, strong ferromagnetism. Bare hybridization strength $V = 1.0$.

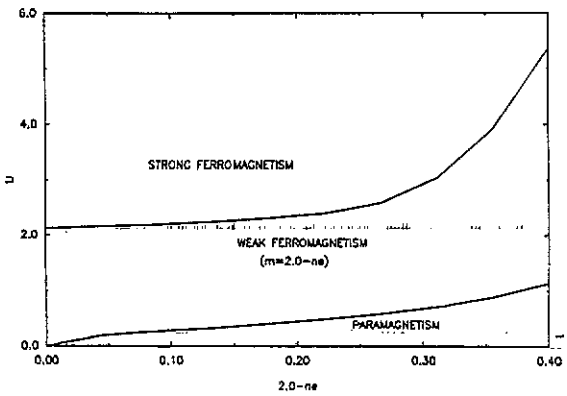

Figure 3. Phase diagram in the U–n_e plane for $E_f = -1.5$ and $V = 1.0$.

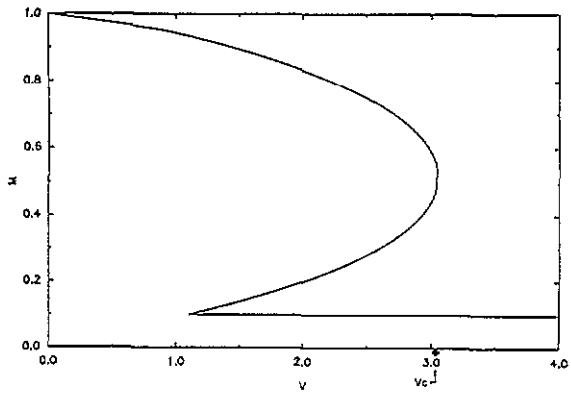

Figure 4. Magnetization as a function of the bare hybridization strength V for the total electron density $n_e = 1.9$ and $U \to \infty$. As V is increased, a first-order transition occurs from strong to weak ferromagnetism at $V = V_c$ (see text).

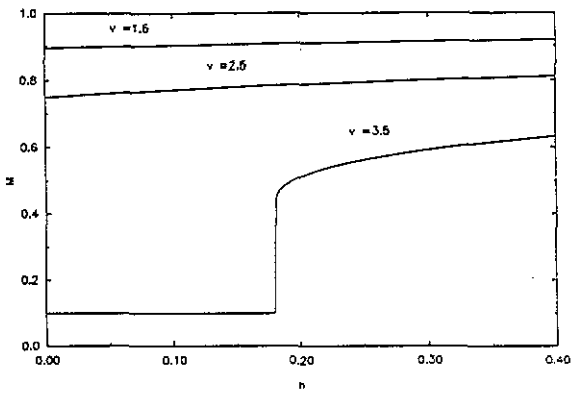

Figure 5. Magnetization as a function of applied magnetic field for several values of the bare hybridization strength V for $n_e = 2$, $U \to \infty$ and $E_f = -1.5$.

In figure 5 we have plotted magnetization against applied magnetic field h for several values of the hybridization strength V. For $V = 3.5\,\text{eV}$, we find weak ferromagnetism corresponding to a full lower hybridized up-spin band. As the strength of the applied magnetic field is increased, there can be no increase in the magnetization until the Fermi level lies in the upper hybridized up-spin band. Then we find a meta-magnetic-like transition. This is in contrast to the situation with the usual slave-boson approach (Rasul and Desgranges 1986) where $q = 1 - n_f$ and the crossover from the weak to strong magnetism is continuous (Evans 1991).

For $T = 0$ our results (figures 1–5) suggest that the Gutzwiller approximation for the strong-correlation limit is too biased towards the magnetic state. This problem might be rectified in one of two ways. First, it can be done by an alternative choice for the hybridization renormalization factor q_σ. The choice for q_σ is not unique and one could choose a form such that the spin dependence of the effective hybridization is reduced. This freedom to choose an alternative form for q_σ does not occur in the standard Gutzwiller approach. There q_σ is determined from statistical weighting factors. Our choice for q_σ (the one obtained from the standard Gutzwiller approach) ensured that the correct non-interacting limit was given in the saddle-point approximation. The sensitivity to the form of q_σ is demonstrated in figure 6 where we have introduced a parameter $0 \leqslant \alpha \leqslant 1$ and plotted magnetization against $q_\sigma = (1 - n_f)/(1 - \alpha n_{f\sigma})$. We find that for $q_\sigma = 1 - n_f$ the Kondo state is always stable with respect to magnetic ordering whilst for $q_\sigma = (1 - n_f)/(1 - n_{f\sigma})$

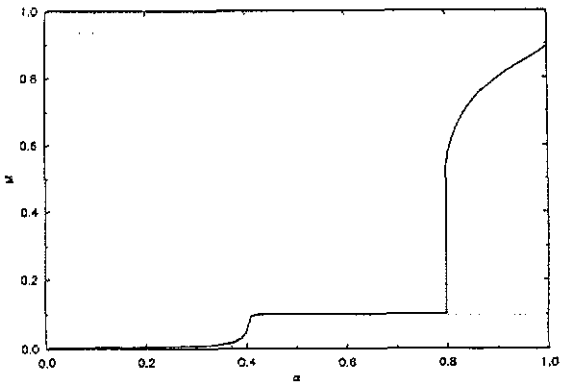

Figure 6. Magnetization as a function of α: $q_\sigma = (1 - n_f)/(1 - \alpha n_{f\sigma})$ for bare hybridization strength $V = 1.0$ and $U \to \infty$. Only for $q_\sigma = 1 - n_f$ (standard slave-boson approach) is the ground state always stable against magnetic ordering.

a magnetic instability persists over the entire Kondo regime. Alternatively, the non-magnetic state may be stabilized by going beyond the Gutzwiller approximation to include contributions from Gaussian (quantum) fluctuations to the free energy.

In making the saddle-point approximation, we have neglected thermal fluctuations so that magnetic ordering can only be destroyed by destruction of the f moments.

4. Conclusions

In this paper we have investigated magnetic properties of the orbitally non-degenerate periodic Anderson model using Kotliar and Ruckenstein's slave-boson reformulation of the Gutzwiller variational method. We worked within the saddle-point approximation, which for $T = 0$ reproduced the Gutzwiller approximation. With this approach we were able to extend the work of Rice and Ueda to the calculation of magnetization as a function of temperature and applied magnetic field.

Our findings suggest that for the strong-correlation limit ($U \to \infty$) the Gutzwiller approximation ($q_\sigma = (1 - n_f)/(1 - n_{f\sigma})$) is too biased towards the magnetic state. This is in contrast with the case for the standard slave-boson approach ($q = 1 - n_f$), where no magnetic instability has been found.

Finally we would like to mention two possible avenues for future work. The slave-boson reformulation of the Gutzwiller variational method reproduced the Gutzwiller approximation in the saddle-point approximation for $T = 0$. By including Gaussian fluctuations one could in principle go beyond the Gutzwiller approximation. A further development would be to extend our calculations to the case of antiferromagnetism.

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