

Quantum phase transitions in the extended periodic Anderson model

Akihisa Koga,^{1,2} Norio Kawakami,¹ Robert Peters,² and Thomas Pruschke²

¹*Department of Physics, Kyoto University, Kyoto 606-8502, Japan*

²*Institut für Theoretische Physik, Universität Göttingen, Göttingen D-37077, Germany*

(Received 31 July 2007; revised manuscript received 4 November 2007; published 15 January 2008)

We investigate quantum phase transitions in the extended periodic Anderson model, which includes electron correlations within and between itinerant and localized bands. We calculate zero and finite temperature properties of the system using the combination of dynamical mean-field theory and the numerical renormalization group. At half filling, a first-order phase transition between a Mott insulating state and a Kondo insulating state occurs in the strong-coupling regime. We furthermore find that a metallic state is stabilized in the weak-coupling regime. This state should be adiabatically connected to the orbital selective Mott state with one orbital-localized and the other itinerant. The effect of hole doping is also addressed.

DOI: [10.1103/PhysRevB.77.045120](https://doi.org/10.1103/PhysRevB.77.045120)

PACS number(s): 71.30.+h, 71.10.Fd, 71.27.+a

I. INTRODUCTION

Strongly correlated electron systems with orbital degeneracy have attracted considerable interest. One typical example is the transition metal oxide LiV_2O_4 . In this compound, unexpected heavy-fermion-like behavior was observed,¹ which is quite likely induced by an interplay between the geometrical frustration of the spinel structure and the orbital degeneracy of the d electrons.²⁻⁷ One particular scenario suggests that due to the V positions in the local trigonal crystal environment, the t_{2g} states at the Fermi energy are split into a_{1g} and e_g^π subbands, which then play different roles in stabilizing the heavy electron state.^{8,9} For example, due to different bandwidths of the a_{1g} and e_g^π bands, the local Coulomb correlations can induce a Mott insulating state in the former while the latter stay metallic.^{8,10} A hybridization between the two subshells on neighboring V atoms in the unit cell then can explain the observed heavy-fermion behavior. Other examples are the compounds $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ (Ref. 11) and $\text{La}_{n+1}\text{Ni}_n\text{O}_{3n+1}$,^{12,13} where a similar orbital-selective Mott transition¹⁴ is suggested to be induced by the chemical substitutions and the change of temperature, respectively. It was furthermore reported that a heavy-fermion state is realized in the former compound around $x \approx 0.2$,¹¹ while a bad metal with localized spins at low temperatures is characteristic of the latter.¹³ These observations stimulate further theoretical investigations on multiorbital systems.^{15-18,20,19}

A common feature of those interesting examples is that localized and itinerant electrons and their correlations in the multiorbital system seem to play an important role in the formation of heavy-fermion states in transition metal oxides. Motivated by this, we here investigate a multiorbital system with localized and itinerant bands. It is known that the hybridization together with local electron correlations leads to the Kondo effect and in turn to the large density of states at the Fermi level, which explains the heavy-fermion states observed in rare-earth compounds.²¹⁻²³ On the other hand, electron correlations in an itinerant band also yield a heavy mass and eventually induce a transition to the Mott insulating state.^{24,25} Thus the interesting question arises whether the heavy-fermion states originating from the Kondo effect and

close to the Mott transition can be distinguished from each other or not. This question has recently been discussed by several authors,^{15,16,26,27} but it was not clear how the heavy-fermion state is realized at low temperatures. In particular, the role of the Hund coupling needs to be clarified, which may be important in f -electron systems as well as transition metal oxides. Therefore, it is necessary to discuss low-temperature properties in correlated multiorbital electron systems with localized and itinerant bands systematically.

To this end, we investigate an extended version of the periodic Anderson model, where not only on-site Coulomb interactions in the localized and itinerant bands but also the interband Coulomb interaction and Hund coupling are taken into account. The properties we are interested in—heavy-fermion behavior and Mott transition—are well captured by the dynamical mean-field theory (DMFT),^{25,28-30} and furthermore do not depend critically on the details of the band structure. Thus we will discuss the low-temperature properties for a particle-hole symmetric system within DMFT. We will clarify that the Hund coupling between different orbitals plays an important role, leading to quantum phase transitions between a Kondo insulating phase, a Mott insulating phase, and the metallic phase. The Mott and Kondo insulators also behave differently when doping the system.

The paper is organized as follows. In Sec. II, we introduce the extended periodic Anderson model and briefly summarize DMFT and numerical techniques. The competition between some phases is discussed in Sec. III. We also discuss the effect of hole doping in Sec. IV. A brief summary is given in Sec. V.

II. MODEL AND METHOD

We consider a correlated electron system with orbital degeneracy described by the Hamiltonian

$$\mathcal{H} = H_t + \sum_i H_{local}^{(i)}, \quad (1)$$

$$H_t = \sum_{\langle ij \rangle \alpha \sigma} [t_{ij}^{(\alpha)} - \mu \delta_{ij}] c_{i\alpha\sigma}^\dagger c_{j\alpha\sigma}, \quad (2)$$

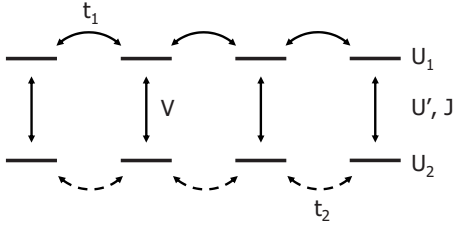


FIG. 1. Sketch of the structure of the model Hamiltonian.

$$\begin{aligned}
 H_{local}^{(i)} = & V \sum_{\sigma} (c_{i1\sigma}^{\dagger} c_{i2\sigma} + c_{i2\sigma}^{\dagger} c_{i1\sigma}) + \sum_{\alpha} U_{\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} \\
 & + \sum_{\sigma\sigma'} (U' - J\delta_{\sigma\sigma'}) n_{i1\sigma} n_{i2\sigma'} - J [(c_{i1\uparrow}^{\dagger} c_{i1\downarrow} c_{i2\downarrow}^{\dagger} c_{i2\uparrow} \\
 & + c_{i1\uparrow}^{\dagger} c_{i1\downarrow}^{\dagger} c_{i2\uparrow} c_{i2\downarrow}) + \text{H.c.}], \quad (3)
 \end{aligned}$$

where $c_{i\alpha\sigma}^{\dagger}$ ($c_{i\alpha\sigma}$) creates (annihilates) an electron with spin σ ($=\uparrow, \downarrow$) and orbital index α ($=1, 2$) at the i th site, and $n_{i\alpha\sigma} = c_{i\alpha\sigma}^{\dagger} c_{i\alpha\sigma}$. For orbital α , $t_{ij}^{(\alpha)}$ represents the transfer integral, V the hybridization between orbitals, U_{α} and U' the intra-orbital and interorbital Coulomb interactions, J the Hund coupling, and μ the chemical potential. The structure of the model Hamiltonian is schematically shown in Fig. 1. We note that the model is reduced to conventional systems in several limiting cases. For example, when $V=0$, the system becomes the two-orbital Hubbard model, where we expect a Mott transition to occur. On the other hand, when $t_{ij}^{(2)}=0$, we recover at $U_1=U'=J=0$ the conventional periodic Anderson model for heavy-fermion systems,²² while the choice $U_1=U_2=V=0$, $J>0$ leads to the double exchange model discussed in connection with magnetism in transition metal oxides.^{31–34}

In contrast to those limiting cases, there are few studies of the original model [Eq. (3)]. The ground state properties in the model were discussed by means of the slave-spin mean-field theory.¹⁶ Although this method is useful to clarify the second-order Mott transition, it is difficult to discuss how the metallic state is realized quantitatively. On the other hand, in the DMFT approach with quantum Monte Carlo (QMC) impurity solver,¹⁵ it was only possible to access high-temperature properties because of a serious sign problem at low temperatures. Therefore, it is desirable to discuss quantitatively how the metallic state is realized at low temperatures.

In this paper, we want to focus on the low-temperature properties of a system with one band localized and one kept itinerant, i.e., we choose the hopping integral for the $\alpha=2$ band as $t_{ij}^{(2)}=0$, but allow all other parameters to be finite. To treat the extended periodic Anderson model in this parameter regime, we use the DMFT. This method has been developed in several groups^{25,28–30} and has successfully been applied to correlated electron systems such as the single-band Hubbard model,^{35–39} the two-band Hubbard model,^{18,19,40–44} the periodic Anderson model,^{16,27,45–48} or the Kondo model.^{49,50} In the DMFT, a lattice model is mapped to an effective impurity model, where local electron correlations are taken into account precisely. The requirement that the site-diagonal lattice

Green function is equal to the one of the effective quantum impurity then leads to a self-consistency condition for the parameters entering the impurity problem. This treatment is formally exact for infinite spatial dimensions. If one is allowed to ignore nonlocal correlations, e.g., sufficiently far away from phase transitions with long-range order, the method can be used as a quite reliable and accurate approximation to three dimensional systems.

Within the DMFT, the lattice typically enters only via the density of states (DOS) of the system with vanishing two-particle interactions. Since we are interested in the generic features of the extended periodic Anderson model, we are free to choose a convenient lattice structure. Here, we use a Bethe lattice with infinite coordination,²⁵ for which the DMFT self-consistency equation is obtained as

$$[\hat{G}_0^{-1}(z)]_{11} = z + \mu - \left(\frac{D}{2}\right)^2 [\hat{G}_{loc}(z)]_{11}, \quad (4)$$

where \hat{G}_0 is the noninteracting Green function for the effective impurity model and \hat{G}_{loc} is the local Green function. Note that this simple equation follows from the lattice structure (Bethe lattice) including the local hybridization.^{26,27} Both are matrices with respect to the orbital index, but due to $t_{ij}^{(2)}=0$ only the (1, 1) element is needed. As is well known,²⁵ the relation (4) is equivalent to a semielliptic DOS for the itinerant band ($\alpha=1$) with half-bandwidth D .

Let us note that the localized band ($\alpha=2$) does not appear explicitly in the self-consistency condition Eq. (4). For the effective impurity model entering the DMFT, this means that only one of the impurity orbitals connects to the rest of the system through an effective hybridization function defined by $(\frac{D}{2})^2 [\hat{G}_{loc}(z)]_{11}$. In the following, this quantity is represented by an auxiliary set of dynamical degrees of freedom, which we will call an effective bath.

The Hamiltonian representing the effective impurity model can now be written as

$$\begin{aligned}
 H = & \sum_k \epsilon_k a_{k\sigma}^{\dagger} a_{k\sigma} + \sum_{k\sigma} \gamma_k (a_{k\sigma}^{\dagger} c_{1\sigma} + c_{1\sigma}^{\dagger} a_{k\sigma}) \\
 & + \sum_{\alpha\sigma} E_{\alpha} n_{\alpha\sigma} + H_{local}, \quad (5)
 \end{aligned}$$

where $a_{k\sigma}$ are the auxiliary annihilation operators with quantum number k and spin σ defining the effective bath, $E_{\alpha} = -\mu$ is the energy level for the impurity site, $n_{\alpha\sigma} = c_{\alpha\sigma}^{\dagger} c_{\alpha\sigma}$ and H_{local} the local interaction term as defined in Eq. (3). The set of parameters for the effective bath $\{\epsilon_k, \gamma_k\}$ must be determined self-consistently through the DMFT condition Eq. (4).

The Hamiltonian (5) represents a quantum impurity model, which is a challenging theoretical problem on its own account. Thus, to discuss the low-temperature properties of the extended periodic Anderson model in the DMFT, we need a tool to accurately solve such quantum impurity models. While applicable in the weak-coupling regime, perturbation theory in general fails in the strong-coupling regime, where, for example, the anticipated transition between Mott and Kondo physics should appear. Exact diagonalizations

and QMC simulations are known to be numerically exact methods, but both cannot properly resolve exponentially small energy scales, which again will play an important role in the interesting regime, where Kondo and Mott physics compete. In addition, due to the required computational resources, QMC simulations typically can access only a restricted window of the parameter space and can also be subject to a severe sign problem when applied to complex multi-orbital models.

Therefore, we here use Wilson's numerical renormalization group⁵¹ (NRG) to solve the effective impurity model.^{37-39,44,47,50} In the NRG, one discretizes the effective bath on a logarithmic mesh by introducing a discretization parameter $\Lambda > 1$. The resulting discrete system can be mapped to a semi-infinite chain with exponentially decreasing couplings,⁵¹ which allow us to access and discuss properties involving exponentially small energy scales quantitatively. To ensure that sum rules for dynamical quantities are fulfilled, we use the complete-basis-set algorithm proposed recently.⁵²⁻⁵⁴ We observe that obeying the sum rules is mandatory to properly describe the low energy properties of the system away from half filling. In the NRG calculations, we, in general, use a discretization parameter $\Lambda=2$ and keep $L=1600$ states at each step. In the vicinity of the critical point, values $\lambda=1.67$ and $L=3000$ have been used instead to increase the accuracy of the results here.

III. RESULTS AT HALF FILLING

In the following, we will present results calculated for $U=U_1=U_2$ with $J/U=0.1$ and $U'=U-2J$ fixed. The effect of Hund's coupling will be addressed later. Let us begin with the low-temperature properties of the extended periodic Anderson model at half filling, which is realized by fixing the chemical potential $\mu=\mu_0=U/2+U'-J/2$. For the conventional periodic Anderson model $U_1=U'=J=0$, it is known that the band insulator at ($V/D \gg 1$) is adiabatically connected to the Kondo insulator with $U_2/D \gg 1$. Furthermore, it was claimed that the introduction of a Coulomb interaction for the conduction band U_1 does not induce a transition to the Mott insulating state.^{26,27} Namely, in this case always antiferromagnetic spin correlations between the orbitals develop. However, in the presence of Hund's coupling J , which induces *ferromagnetic* spin correlations between the orbitals, one should expect a competition between the singlet formation due to the hybridization and a high spin formation due to the Hund coupling.

To discuss how spin correlations develop between the degenerate orbitals, we calculate the squared spin moment $\langle S_z^2 \rangle$, where $S_z = \sum_{\alpha} (n_{\alpha\uparrow} - n_{\alpha\downarrow})/2$, as shown in Fig. 2. When V/D is large, the local spin moment is strongly suppressed, $\langle S_z^2 \rangle \rightarrow 0$. In this regime, the hybridization together with the intra-orbital Coulomb interactions leads to the formation of an interorbital singlet, where the insulator (Kondo insulator) will be realized in the half-filled particle-hole symmetric system. On the other hand, different behavior occurs for small V/D , as shown in Fig. 2. Here we find that $\langle S_z^2 \rangle \rightarrow 2/3$ when $U/D \geq 2$, while $\langle S_z^2 \rangle \rightarrow 1/2$ in the other limit.

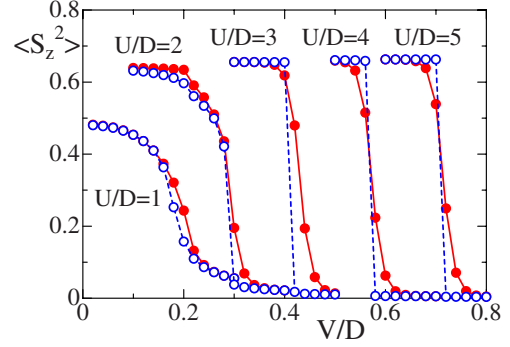


FIG. 2. (Color online) The local squared moment $\langle S_z^2 \rangle$ as a function of the hybridization V/D . Solid (open) circles represent the results at temperature $T/D=2.1 \times 10^{-2}$ (6.5×10^{-4}).

In the former case, strong correlations localize the electrons in band $\alpha=1$. Note that due to a finite Hund's coupling, the corresponding Mott transition will occur at a smaller value of U as compared to the one-band Hubbard model here.⁴⁴ Furthermore, for small V , the Hund's coupling will win over the effective antiferromagnetic exchange $\sim V^2/U$ generated by the hybridization and the Coulomb interaction, i.e., a spin triplet state $S=1$ is realized, which implies $\langle S_z^2 \rangle = 2/3$. Since for large V/D the ground state is a local singlet with $S=0$, we expect that at $T=0$ a phase transition from the Mott insulating state to the Kondo insulating state occurs as a function of V/D . In fact, the phase transition is clearly visible for the lower temperature, as shown in Fig. 2.

On the other hand, in the regime $U/D \leq 2$, we observe a smooth curve for $\langle S_z^2 \rangle$ as a function of V , which furthermore depends only little on temperature, except for a small region around the turning point. This behavior is shown in Fig. 2 for $U/D=1$ as example. For small V/D Hund's exchange will again dominate over the antiferromagnetic interorbital coupling generated by V . Thus we are effectively left with a Fermi liquid ferromagnetically coupled to a localized spin, i.e., a ferromagnetic Kondo model. As is well known, this model has a metallic ground state,²² where the local spin acts as a potential scatterer. The increase of V eventually leads to a dominance of the hybridization term and a Kondo screening of the local spin by the itinerant electrons. For finite temperatures one will observe a crossover, because only for $T_K \gg T$ a full singlet with $\langle S_z^2 \rangle = 0$ between local and band spins is realized. With decreasing temperature, the crossover becomes sharper and, because one now probes lower Kondo temperatures, shifts to the left, as seen in Fig. 2. Eventually it turns into a transition at $T=0$, where the Kondo state always leads to a singlet for arbitrary small antiferromagnetic coupling.

This qualitative discussion can be further substantiated by looking at the density of states for itinerant and localized orbitals in Fig. 3. We first focus on the case $U/D=1$. As anticipated before, for small V/D a metallic state is realized in the orbital $\alpha=1$. The orbital $\alpha=2$, on the other hand remains localized. To confirm the stability of the metallic state and support the qualitative discussion, we also show the density of states at a much lower temperature $T/D \approx 10^{-8}$ as the

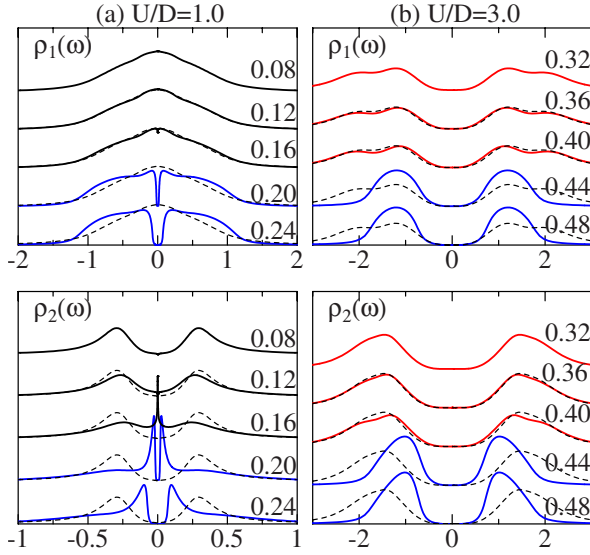


FIG. 3. (Color online) Density of states for the extended periodic Anderson model with fixed $U/D=1.0$ (a) and $U/D=3.0$ (b) at $T/D=6.5 \times 10^{-4}$. The numbers represent the values V/D . For comparison, we also show the density of states for $V/D=0.08(0.32)$ in (a) [(b)] as the dashed lines.

dashed lines in Fig. 4. As expected, we find that the metallic state is certainly the ground state for the $\alpha=1$ orbital, while a strongly suppressed DOS at Fermi level is seen in the other orbital. The NRG results are consistent with those obtained from a calculation using exact diagonalization,^{25,35} see full lines in Fig. 4. Further increase of the hybridization beyond the phase boundary $(V/D)_c \approx 0.14$ eventually leads to the appearance of a Kondo resonance in $\rho_2(\omega)$, as shown in Fig. 3(a), and a corresponding reduction of the DOS at the Fermi energy in $\rho_1(\omega)$. For even larger V , one then finds the structures known from Kondo insulators,^{45,47,55} i.e., a Kondo resonance split by a hybridization gap in $\rho_2(\omega)$ and a gap of the same width in $\rho_1(\omega)$. Note that one would actually expect a similar gap to appear in $\rho_2(\omega)$ at $V/D=0.16$. However, this gap appears only for $T \ll T_K$ and is thus not yet visible here.

When $U/D=3$, on the other hand, we always find an insulating state, which can be characterized as a Mott (Kondo)

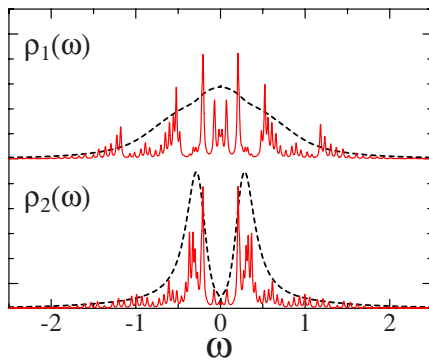


FIG. 4. (Color online) Solid and dashed lines represent the density of states obtained by exact diagonalization with 12 sites and the NRG method at $T/D \approx 10^{-8}$ for the metallic state with $U/D=1.0$ and $V/D=0.1$.

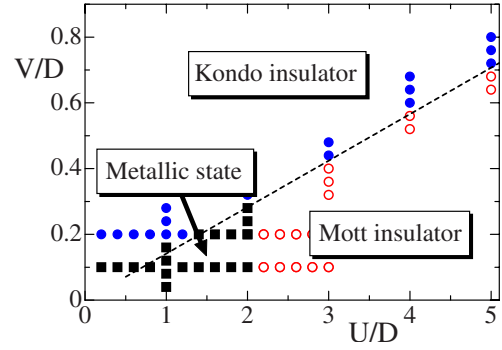


FIG. 5. (Color online) Finite temperature phase diagram for the extended periodic Anderson model with $J/U=0.1$ and $T/D=6.5 \times 10^{-4}$. Solid circles, open circles, and solid squares denote the Kondo insulator, the Mott insulator, and the metallic state, respectively. The dashed line is obtained from the simplified model (see text).

insulator with a charge gap in both orbitals for small (large) V/D . When V approaches the critical value $(V/D)_c \approx 0.42$ from below, the charge gap around the Fermi level decreases, but does not seem to vanish even at the critical point, which implies that the phase transition is of first order, in accordance with the behavior of $\langle S_z^2 \rangle$. The initial reduction of the charge gap with increasing V can be interpreted in the following way. For small V , the Mott state is stabilized at a lower critical U_c due to ferromagnetic Hund's coupling.^{41,42,44} With increasing V , the additionally generated antiferromagnetic exchange effectively reduces this effect, i.e., the orbital $\alpha=1$ is driven closer to its critical value and the charge gap decreases. As soon as the antiferromagnetic coupling dominates, the gap scale is set by the Kondo scale. The properties very close and at the critical point are thus determined by this subtle competition of energy scales. Whether the two regimes are separated by a quantum critical point or the transition is driven by a simple level crossing remains to be investigated.

By performing similar calculations for various parameter values, we obtain the phase diagram shown in Fig. 5. When V/D is large, the Kondo insulator prevails, where the spins for the localized band ($\alpha=2$) are screened by forming a singlet with the electrons in orbital $\alpha=1$. The increase of the Coulomb interaction U with fixed J/U decreases the hybridization gap characteristic of the Kondo insulating state. Finally, a phase transition occurs to the Mott insulating state with a local moment $S=1$. Note that in this regime the Kondo interaction is dominated by ferromagnetic Hund's exchange. The competition between these phases can be qualitatively described by a simplified local Hamiltonian for two orbitals H_{local} , since the bandwidth has a little effect on the phase transition. By examining the lowest state for this simplified model, we find a level crossing at $V/D = \sqrt{2}J/D$ between the singlet and the triplet states, which is shown as the dashed line in Fig. 5. Obviously, this line is in good agreement with the phase boundary obtained by DMFT. This result also suggests that the actual phase transition is of first order and not accompanied by a quantum critical point.

When the hybridization is small ($V/D < \sqrt{2}J/D$) and $U/D \lesssim 2$, a metallic state appears with orbital $\alpha=2$ almost

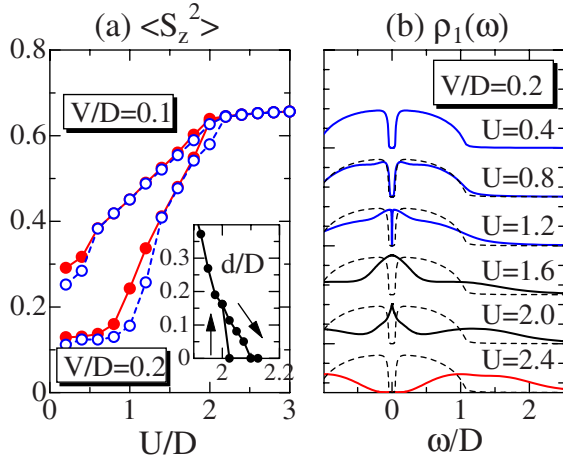


FIG. 6. (Color online) (a) Local moment as a function of the Coulomb interaction U for $V/D=0.1$ and 0.2 . Solid (open) circles are the results for $T/D=2.1 \times 10^{-2}$ (6.5×10^{-4}). The inset shows the width for the quasiparticle peak d as a function of U/D at the lower temperature. (b) Density of states for the orbital $\alpha=1$ and different values $U/D=0.4, 0.8, 1.2, 1.6, 2.0$, and 2.4 for $T/D=6.5 \times 10^{-4}$. The densities of states for $U/D=0.4$ are also shown as the dashed lines, for comparison.

localized and $\alpha=1$ itinerant. As the Coulomb interaction is increased for the metallic state, the quasiparticle peak becomes sharper for the itinerant orbital, as shown in Fig. 6. Finally the metal-insulator transition occurs to the Mott insulating state. The obtained phase boundary is consistent with the critical point $(U/D, V/D) \approx (2, 0)$ for the two-orbital Hubbard model with the large difference of the bandwidths.²⁰

What is the nature of the metal-insulator transitions? When $V/D = \sqrt{2}J/D$ and $U/D \leq 2$, a first-order transition between the Kondo insulating and the metallic state should occur at zero temperature. In fact, with decreasing temperature, the local moment is hardly changed in the metallic state, while it is screened in the Kondo insulating state, as shown in Fig. 6(a). This is consistent with the fact that in the vicinity of the transition point, no sharp quasiparticle peak appears in the metallic state, and a tiny hybridization gap in the Kondo insulating state, which is smeared at high temperatures, appears. Therefore, we can say that the first-order phase transition occurs only at zero temperature, being replaced by a crossover at finite temperatures. On the other hand, we encounter a different behavior at the other transition between the metallic and the Mott insulating states, as discussed above. Since there exists a hybridization between the orbitals in the model, the renormalization factor, which is obtained from the diagonal part of the self-energy, may not be a proper quantity to characterize the sharp quasiparticle peak in the density of states for the $\alpha=1$ orbital. Instead, we calculate its width d defined by $\rho_1(d/2) = (\pi D)^{-1}$, as shown in the inset of Fig. 6(a). We find a hysteresis appearing at low temperatures. Furthermore, the width is smoothly decreasing when the interactions increase. This behavior is similar to that found in the single-band Hubbard model.³⁹ Therefore, we believe that the second-(first-)order metal-insulator transition occurs at zero (finite) temperature.

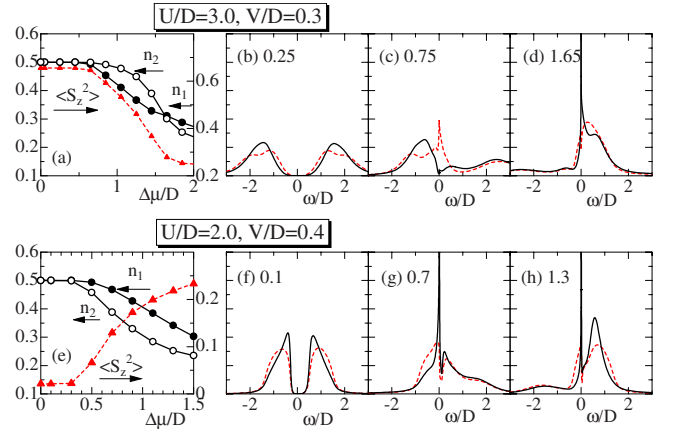


FIG. 7. (Color online) Occupancy $\langle n_\alpha \rangle$ and squared moment $\langle S_z^2 \rangle$ as a function of the chemical potential for $V/D=0.2$ (a) and $V/D=0.4$ (e). The densities of states for $\alpha=1(2)$ are shown as the dashed (solid) lines in the others. The numbers represent the values $\Delta\mu/D$.

Our results are in clear contrast to those for the conventional periodic Anderson model, where at half filling and particle-hole symmetry, no Mott transition occurs even in the large U_1 and U_2 case, but one always finds a Kondo insulator. Since this model is obtained in the limit Hund's exchange $J=0$ in our extended periodic Anderson model, we can therefore conclude that the competition between metallic and the insulating states originates from the Hund coupling. This observation may be relevant for the heavy-fermion behavior observed in transition metal oxides such as $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ ($0.2 < x < 0.5$) and $\text{La}_{n+1}\text{Ni}_n\text{O}_{3n+1}$, which is now under investigation.

IV. EFFECT OF HOLE DOPING

In this section, we discuss the effect of hole doping on the insulating states to clarify how the heavy-fermion behavior emerges. To this end, we introduce the parameter $\Delta\mu = \mu_0 - \mu$. In Fig. 7, we show occupancy, local moment, and density of states. For $(U/D, V/D) = (3.0, 0.3)$, the system is in the Mott insulating state at half filling $\Delta\mu = 0$, and the increase of $\Delta\mu$ has a little effect on the nature of the phase for $0.0 < \Delta\mu/D < 0.5$, as shown in Fig. 7(a). Further increase of the chemical potential eventually drives the system into a metallic state, where the local moment and the total occupancy $n_{\text{tot}} (= n_1 + n_2)$ both decrease. Note that most of the holes are doped in the $\alpha=1$ band while only a small amount of holes populates the other when $0.5 < \Delta\mu/D < 1.0$. This implies that the character of original orbitals still survives in the system with hybridization. This orbital-selective behavior is also found clearly in the density of states, as shown in Fig. 7(b). When $\Delta\mu/D > 1.3$, the behavior changes: the number of electrons for the $\alpha=2$ band deviates from the half filling, as shown in Fig. 7(a). Furthermore, we find that a sharp peak appears in the density of states characteristic of the doped Kondo insulator. This suggests that a crossover between different metallic states occurs around $\Delta\mu/D \approx 1.3$.

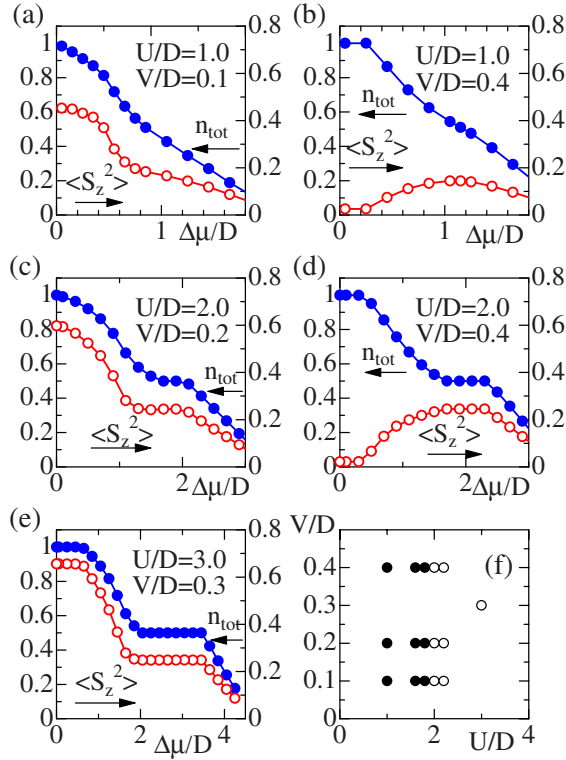


FIG. 8. (Color online) [(a)–(e)] The total number of electrons n_{tot} and local moment $\langle S_z^2 \rangle$ as a function of $\Delta\mu/D$ with fixed parameters at $T/D=6.5 \times 10^{-4}$. (f) Finite temperature phase diagram for the quarter filling at $T/D=6.5 \times 10^{-4}$. Solid (open) circles denote the metallic (Mott insulating) state.

On the other hand, when holes are doped into the Kondo insulating state at $(U/D, V/D)=(2.0, 0.4)$, monotonic behavior appears in the quantities in Fig. 7(c). In this case, a conventional heavy-fermion state, studied in detail in the conventional periodic Anderson model, is realized, as shown in Fig. 7(d).

Before closing this section, we briefly mention the Mott transitions at quarter filling, which should be induced by the intraorbital and the interorbital interactions. The results obtained for several choices of parameters are shown in Fig. 8. It is found that the ground state at quarter filling $n_{\text{tot}}=0.5$ strongly depends on the strength of the Coulomb interaction U . When U is small, no remarkable features are visible in the curve of the total occupancy, as shown in Figs. 8(a) and 8(b).

Therefore, we infer that the system is a metal state in the case. In the large U case, on the other hand, a plateau appears in the curve at quarter filling, as shown in Figs. 8(c)–8(e). In addition, one observes a local moment $\langle S_z^2 \rangle=1/4$ in this region, which suggests the existence of a Mott insulating state. Our results are similar to those for a two-orbital system without hybridization,^{43,56} which is a Mott insulator at quarter filling for large enough interaction parameters. We can therefore conclude that the hybridization has little effect on the phase diagram for the quarter filled system, as shown in Fig. 8(f), in contrast to that for the half-filled system (Fig. 5).

V. SUMMARY

We have investigated the extended periodic Anderson model within the dynamical mean-field theory with the numerical renormalization group as a solver for the effective quantum impurity problem. We have discussed the nature and physics of phase transitions between the metallic, Kondo insulating, and Mott insulating states. It has been clarified that the metallic and Mott insulating states are stabilized by the Hund exchange coupling between the localized and itinerant bands, which may be relevant to real materials, e.g., transition metal oxides that show heavy-fermion behavior under certain conditions.

Although we have restricted our discussion to the paramagnetic state in the paper, it is an interesting and instructive problem to discuss possible instabilities toward ordered states such as magnetic order, superconductivity, etc. In particular, an antiferromagnetic state induced by magnetic field^{48,57} can be of considerable interest in connection with various heavy-fermion compounds. These problems are currently under investigation.

ACKNOWLEDGMENTS

We would like to thank K. Inaba, S. Nakatsuji, M. Sigrüst, and Y. Maeno for useful discussions. This work was partly supported by a Grant-in-Aid from the Ministry of Education, Science, Sports and Culture of Japan [19014013 (N.K.) and 17740226 (A.K.)] and the German Science Foundation (DFG) through the collaborative research grant SFB 602 (T.P. and A.K.) and the project PR 298/10-1 (T.P.). A.K. would, in particular, like to thank the SFB 602 for its support and hospitality during his stays at the University of Göttingen. Part of the computations were done at the Supercomputer Center at the Institute for Solid State Physics, University of Tokyo and Yukawa Institute Computer Facility.

¹S. Kondo *et al.*, Phys. Rev. Lett. **78**, 3729 (1997).

²H. Kaps, N. Büttgen, W. Trinkl, A. Loidl, M. Klemm, and S. Horn, J. Phys.: Condens. Matter **13**, 8497 (2001).

³M. Isoda and S. Mori, J. Phys. Soc. Jpn. **69**, 1509 (2000).

⁴S. Fujimoto, Phys. Rev. B **64**, 085102 (2001).

⁵H. Tsunetsugu, J. Phys. Soc. Jpn. **71**, 1844 (2002).

⁶J. Hopkinson and P. Coleman, Phys. Rev. Lett. **89**, 267201 (2002).

⁷Y. Yamashita and K. Ueda, Phys. Rev. B **67**, 195107 (2003).

⁸V. I. Anisimov, M. A. Korotin, M. Zolff, T. Pruscheke, K. Le Hur, and T.-M. Rice, Phys. Rev. Lett. **83**, 364 (1999).

⁹H. Kusunose, S. Yotsuhashi, and K. Miyake, Phys. Rev. B **62**, 4403 (2000).

¹⁰R. Arita, K. Held, A. V. Lukoyanov, and V. I. Anisimov, Phys. Rev. Lett. **98**, 166402 (2007).

¹¹S. Nakatsuji, D. Hall, L. Balicas, Z. Fisk, K. Sugahara, M.

- Yoshioka, and Y. Maeno, Phys. Rev. Lett. **90**, 137202 (2003).
- ¹²K. Sreedhar, M. McElfresh, D. Perry, D. Kim, P. Metcalf, and J. M. Honig, J. Solid State Chem. **110**, 208 (1994); Z. Zhang, M. Greenblatt, and J. B. Goodenough, *ibid.* **108**, 402 (1994); Z. Zhang and M. Greenblatt, *ibid.* **117**, 236 (1994).
- ¹³Y. Kobayashi, S. Taniguchi, M. Kasai, M. Sato, T. Nishioka, and M. Kontani, J. Phys. Soc. Jpn. **65**, 3978 (1996).
- ¹⁴V. I. Anisimov, I. A. Nekrasov, D. E. Kondakov, T. M. Rice, and M. Sigrüst, Eur. Phys. J. B **25**, 191 (2002).
- ¹⁵A. Koga, N. Kawakami, T. M. Rice, and M. Sigrüst, Phys. Rev. B **72**, 045128 (2005).
- ¹⁶L. de' Medici, A. Georges, and S. Biermann, Phys. Rev. B **72**, 205124 (2005).
- ¹⁷A. Liebsch, Europhys. Lett. **63**, 97 (2003).
- ¹⁸A. Koga, N. Kawakami, T. M. Rice, and M. Sigrüst, Phys. Rev. Lett. **92**, 216402 (2004); A. Koga, K. Inaba, and N. Kawakami, Prog. Theor. Phys. Suppl. **160**, 253 (2005).
- ¹⁹A. Liebsch, Phys. Rev. Lett. **91**, 226401 (2003); C. Knecht, N. Blümer, and P. G. J. van Dongen, Phys. Rev. B **72**, 081103 (2005); A. Rüegg, M. Indergand, S. Pilgram, and M. Sigrüst, Eur. Phys. J. B **48**, 55 (2005); M. Ferrero, F. Becca, M. Fabrizio, and M. Capone, Phys. Rev. B **72**, 205126 (2005); R. Arita and K. Held, *ibid.* **72**, 201102(R) (2005); P. Werner and A. J. Millis, *ibid.* **74**, 155107 (2006).
- ²⁰K. Inaba, A. Koga, S. I. Suga, and N. Kawakami, Phys. Rev. B **72**, 085112 (2005); J. Phys. Soc. Jpn. **74**, 2393 (2005); K. Inaba and A. Koga, Phys. Rev. B **73**, 155106 (2006).
- ²¹N. Grewe and F. Steglich, in *Handbook on the Physics and Chemistry of Rare Earths*, edited by K. A. Gschneidner, Jr. and L. Eyring (North-Holland, Amsterdam, 1991), Vol. 14, p. 343.
- ²²A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, 1993).
- ²³K. Yamada, K. Yosida, and K. Hanzawa, Prog. Theor. Phys. Suppl. **108**, 141 (1992).
- ²⁴W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302 (1970).
- ²⁵A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
- ²⁶T. Schork and S. Blawid, Phys. Rev. B **56**, 6559 (1997).
- ²⁷R. Sato, T. Ohashi, A. Koga, and N. Kawakami, J. Phys. Soc. Jpn. **73**, 1864 (2004).
- ²⁸W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
- ²⁹E. Müller-Hartmann, Z. Phys. B: Condens. Matter **74**, 507 (1989).
- ³⁰T. Pruschke, M. Jarrell, and J. K. Freericks, Adv. Phys. **42**, 187 (1995).
- ³¹C. Zener, Phys. Rev. **82**, 403 (1951).
- ³²P. W. Anderson and H. Hasegawa, Phys. Rev. **100**, 675 (1955).
- ³³K. Kubo and N. Ohata, J. Phys. Soc. Jpn. **33**, 21 (1975).
- ³⁴N. Furukawa, J. Phys. Soc. Jpn. **64**, 2734 (1995).
- ³⁵M. Caffarel and W. Krauth, Phys. Rev. Lett. **72**, 1545 (1994).
- ³⁶Th. Pruschke, D. L. Cox, and M. Jarrell, Phys. Rev. B **47**, 3553 (1993).
- ³⁷O. Sakai and Y. Kuramoto, Solid State Commun. **89**, 307 (1994).
- ³⁸R. Bulla, Phys. Rev. Lett. **83**, 136 (1999).
- ³⁹R. Bulla, T. A. Costi, and D. Vollhardt, Phys. Rev. B **64**, 045103 (2001).
- ⁴⁰A. Georges, G. Kotliar, and W. Krauth, Z. Phys. B: Condens. Matter **92**, 313 (1993).
- ⁴¹Y. Ono, R. Bulla, and A. C. Hewson, Eur. Phys. J. B **19**, 375 (2001); Y. Ohashi and Y. Ono, J. Phys. Soc. Jpn. **70**, 2989 (2001).
- ⁴²A. Koga, Y. Imai, and N. Kawakami, Phys. Rev. B **66**, 165107 (2002); A. Koga, T. Ohashi, Y. Imai, S. Suga, and N. Kawakami, J. Phys. Soc. Jpn. **72**, 1306 (2003).
- ⁴³Y. Ono, M. Potthoff, and R. Bulla, Phys. Rev. B **67**, 035119 (2003).
- ⁴⁴Th. Pruschke and R. Bulla, Eur. Phys. J. B **44**, 217 (2005).
- ⁴⁵M. Jarrell, H. Akhlaghpour, and T. Pruschke, Phys. Rev. Lett. **70**, 1670 (1993).
- ⁴⁶T. Mutou and D. Hirashima, J. Phys. Soc. Jpn. **63**, 4475 (1994).
- ⁴⁷T. Pruschke, R. Bulla, and M. Jarrell, Phys. Rev. B **61**, 12799 (2000).
- ⁴⁸T. Ohashi, A. Koga, S. I. Suga, and N. Kawakami, Phys. Rev. B **70**, 245104 (2004).
- ⁴⁹N. Furukawa, J. Phys. Soc. Jpn. **63**, 3214 (1994).
- ⁵⁰R. Peters and Th. Pruschke, Phys. Rev. B **76**, 245101 (2007).
- ⁵¹R. Bulla, T. Costi, and T. Pruschke, arXiv:cond-mat/0701105 (unpublished).
- ⁵²F. B. Anders and A. Schiller, Phys. Rev. B **74**, 245113 (2006).
- ⁵³R. Peters, Th. Pruschke, and F. B. Anders, Phys. Rev. B **74**, 245114 (2006).
- ⁵⁴A. Weichselbaum and J. von Delft, Phys. Rev. Lett. **99**, 076402 (2007).
- ⁵⁵N. Grewe, Solid State Commun. **50**, 19 (1984); K. Yamada and K. Yoshida, in *Theory of Heavy Fermions and Valence Fluctuations*, edited by T. Kasuya and T. Saso (Springer, Berlin, 1985); Th. Pruschke and N. Grewe, Z. Phys. B: Condens. Matter **74**, 439 (1989).
- ⁵⁶K. Inaba and A. Koga, J. Phys. Soc. Jpn. **76**, 094712 (2007).
- ⁵⁷I. Milat, F. Assaad, and M. Sigrüst, Eur. Phys. J. B **38**, 571 (2004).