Antiferromagnetism versus Kondo screening in the two-dimensional periodic Anderson model at half filling: Variational cluster approach

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The variational cluster approach (VCA) based on the self-energy functional theory is applied to the two-dimensional symmetric periodic Anderson model at half filling. We calculate a variety of physical quantities including the staggered moments and single-particle spectra at zero temperature to show that the symmetry breaking due to antiferromagnetic ordering occurs in the strong coupling region, whereas in the weak-coupling region, the Kondo insulating state without symmetry breaking is realized. The critical interaction strength is estimated. We thus demonstrate that the phase transition due to competition between antiferromagnetism and Kondo screening in the model can be described quantitatively by VCA.

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I. INTRODUCTION

The two-dimensional (2D) heavy-fermion system has attracted much attention as a subsequent study of high-temperature superconductors and has recently been one of the central issues in the study of strongly correlated electron systems. For example, the heavy-fermion material $YbRh_2Si_2$ shows a rapid change in the Hall coefficient as a function of magnetic field at zero temperature, which is accompanied by the antiferromagnetic (AF) to paramagnetic (PM) phase transition.[1] Also, heavy-fermion-like behavior is observed in the system of ^{3}He bilayers adsorbed on graphite.[2] Generally speaking, competition between the magnetic ordering of localized spins through the Ruderman-Kittel-Kasuya-Yoshida (RKKY) (Ref. 3) interaction and the nonmagnetic states induced by the Kondo screening[4] brings about the observed anomalous behaviors in heavy-fermion materials. From the theoretical point of view, the periodic Anderson model (PAM) (Ref. 5) is one of the simplified models for heavy-fermion systems, which is believed to describe the competition between magnetic ordering and Kondo singlet formation observed in heavy-fermion materials.

In 2D quantum systems, the symmetry-broken magnetically ordered state can be realized in the ground state at zero temperature, and therefore, one needs a method of calculation appropriate for infinite-size systems in the thermodynamic limit. In this paper, we therefore use the variational cluster approach (VCA) (Refs. 6 and 7) based on the self-energy functional theory (SFT) (Ref. 8) to consider the 2D periodic Anderson model at half filling. Although the self-energies of the small clusters are used in the VCA calculations and thus the long-range spin fluctuations beyond the cluster size are not taken into account, the quantum fluctuations within the cluster are treated exactly in this approach. We may, therefore, expect that this approach should be applicable to describe the possible symmetry breaking of the model in the thermodynamic limit beyond the simple mean-field theory.

We will show that, by means of VCA, the symmetry breaking due to the AF ordering of localized spins occurs in the strong coupling region, whereas in the weak-coupling region, the Kondo insulator without symmetry breaking is realized. The critical interaction strength will thereby be determined. We will also calculate the staggered magnetic moment as a function of the interaction strength and show that the phase transition is of the second order. We will furthermore calculate the single-particle spectra and densities of states (DOSs) to discuss the effects of electron correlation on the quasiparticle band structure. We will, thus, show how the system changes from the AF insulator, Kondo insulator, to the band insulator, with decreasing the interaction strength.

This paper is organized as follows. In Sec. II, we present our model and method of calculation. In Sec. III, we present our results of calculations for the stability of the AF ordering, staggered magnetic moment, single-particle spectra, and DOS by VCA. We summarize our work in Sec. IV.

II. MODEL AND METHOD

A. Model

We consider the PAM defined on the 2D square lattice. The Hamiltonian is given by

$$H = -t\sum_{\langle ij\rangle}(c_{i\sigma}^{\dagger}c_{j\sigma} + \text{H.c.}) - V\sum_{i\sigma}(c_{i\sigma}^{\dagger}f_{i\sigma} + \text{H.c.}) + U\sum_{i} n_{i\uparrow}^{f}n_{i\downarrow}^{f} + \varepsilon_f\sum_{i\sigma} n_{i\sigma}^{f}, \quad (1)$$

where $c_{i\sigma}$ ($f_{i\sigma}$) is the annihilation operator of an electron at site i with spin σ in the conduction-electron c (f-electron f) orbital, and $n_{i\sigma}^{f}=f_{i\sigma}^{\dagger}f_{i\sigma}$ is the electron number operator in the f orbital. t is the hopping parameter between the nearest-neighbor c orbitals, V is the on-site hybridization parameter between the c and f orbitals, U is the on-site repulsion on the f orbital, and ε_f is the energy level of the f orbital with respect to that of the c orbital set to be the origin of energy. In the following calculations, we consider the symmetric case, i.e., the case with $\varepsilon_f=-U/2$. We also focus on the electron densities at half filling, i.e., $2N_s$ electrons in the N_s unit cells, where the unit cell contains one c and one f orbital. We hereafter set $t=V=1$ as the unit of energy, and we change the value of the interaction strength U.

B. Variational cluster approach

Let us first briefly review the formulation of SFT (Ref. 8) and present the method of calculation of the magnetic ordering by VCA (Refs. 6 and 7) in order to make our paper self-contained. We consider the system of the Hamiltonian $H=H_0(\boldsymbol{t})+H_1(\boldsymbol{U})$, where $\boldsymbol{t}$ and $\boldsymbol{U}$ denote the one-particle and interaction parameters of H, respectively. In general, the grand potential is given from the stationary point of the self-energy functional

$$\Omega[\Sigma] = F[\Sigma] + \mathrm{Tr}\ \ln[-(G_0^{-1} - \Sigma)^{-1}], \tag{2}$$

where $F[\Sigma]$ and G_0 are the Legendre transform of the Luttinger-Ward potential $\Phi[G]$ and the bare Green's function, respectively. The rigorous variational principle $\delta\Omega[\Sigma]/\delta\Sigma=0$ gives the Dyson equation $G^{-1}=G_0^{-1}-\Sigma$, where G is the physical Green's function.

In the above expression [Eq. (2)], $F[\Sigma]$ is a universal functional of the self-energy; i.e., $F[\Sigma]$ remains unchanged for an arbitrary reference system of the Hamiltonian $H'=H_0(\boldsymbol{t}')+H_1(\boldsymbol{U})$ that has the same interaction part as the original system has, but with modified one-particle parameters. We here introduce the restriction of the space of the exact self-energies of the original system to the set of exact self-energies of the reference system. Because of this restriction, the following procedure becomes approximate, but it enables us to obtain the grand potential of the original system from the stationary point of the $\Sigma(\boldsymbol{t}')$ functional

$$\Omega[\Sigma(\boldsymbol{t}')] = \Omega' + \mathrm{Tr}\ \ln\{-[G_0^{-1} - \Sigma(\boldsymbol{t}')]^{-1}\} - \mathrm{Tr}\ \ln\{-[G_0'^{-1} - \Sigma(\boldsymbol{t}')]^{-1}\}, \tag{3}$$

where Ω', $\Sigma(\boldsymbol{t}')$, and G_0' are the grand potential, exact self-energy, and bare Green's function of the reference system, respectively. The condition $\partial\Omega[\Sigma(\boldsymbol{t}')]/\partial\boldsymbol{t}'=0$ gives an appropriate reference system that describes the original system approximately.

In VCA, we first divide the original infinite lattice into the finite-size identical clusters. By switching off the hopping parameters between the identical clusters, we construct the reference system as an assembly of the exactly solvable finite-site clusters. One of the major advantages of VCA is its ability to describe the symmetry-breaking long-range order by introducing suitably chosen fictitious symmetry-breaking Weiss fields in the set of variational parameters $\boldsymbol{t}'$. In order to discuss the competition between the AF ordering and Kondo screening in the parameter space, we here introduce staggered magnetic field h' on the f orbitals in the cluster Hamiltonian as a variational parameter. We thus obtain the Hamiltonian of the reference system, H', which is given by

$$H' = \sum_{\boldsymbol{R}} H'_{\boldsymbol{R}}, \tag{4}$$

$$H'_{\boldsymbol{R}} = -t\sum_{\langle ij\rangle}(c_{i\sigma}^{\dagger}c_{j\sigma} + \mathrm{H.c.}) - V\sum_{i\sigma}(c_{i\sigma}^{\dagger}f_{i\sigma} + \mathrm{H.c.}) + U\sum_i n_{i\uparrow}^f n_{i\downarrow}^f + \varepsilon_f\sum_{i\sigma} n_{i\sigma}^f + h'\sum_i e^{i\boldsymbol{Q}\cdot\boldsymbol{r}_i}(n_{i\uparrow}^f - n_{i\downarrow}^f), \tag{5}$$

where $\boldsymbol{R}$ is the label of the clusters, i and j are the labels of the sites within the cluster $\boldsymbol{R}$, and $\boldsymbol{Q}=(\pi,\pi)$.

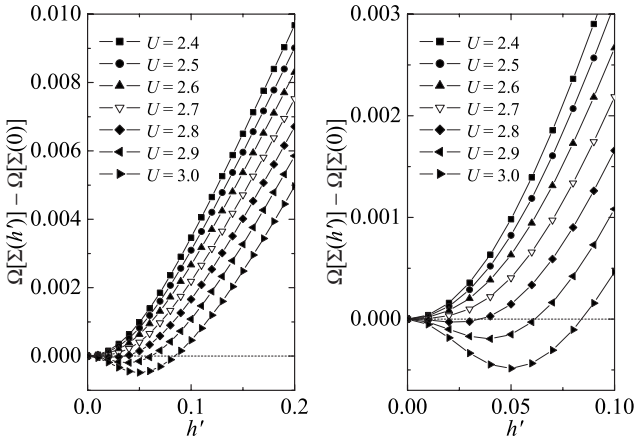

FIG. 1. Calculated results for $\Omega[\Sigma(h')]-\Omega[\Sigma(0)]$ (per site). The right panel shows an enlargement of the small h' region of the left panel. We show the results for several values of U near the phase transition. Dotted horizontal line is a guide for eyes.

In the present study, we use a six-site (2×3) cluster to search for the stationary point of $\Omega[\Sigma(h')]$ with a condition $\partial\Omega[\Sigma(h')]/\partial h'=0$ as discussed above. We should note that the shape of the cluster introduced as a reference system is not commensurate with the AF ordering. We therefore treat a 12-site (2×6) cluster as a supercell by combining the two six-site clusters. We treat the intercluster hopping elements, as well as the hopping elements between the supercells, "perturbatively";[9] i.e., we use the self-energies of the six-site clusters to calculate the Green's function of the original infinite system, as well as that of the reference systems (an assembly of the identical 12-site clusters) via the Dyson equation and obtain the values of $\Omega[\Sigma(h')]$ for various values of h' by using the Eq. (3).

III. RESULTS OF CALCULATIONS

A. Stability of the antiferromagnetic ordering

It is known that the AF ordering of the f electrons is realized in the ground state of the strong coupling region of PAM (as well as Kondo-lattice model) in 2D.[10–12] We demonstrate this in Fig. 1, where the calculated values of $\Omega[\Sigma(h')]-\Omega[\Sigma(0)]$ per site for several values of U near the critical point are shown. We find the following: (i) The value has a minimum at a finite value of h' for $U>U_{\mathrm{cr}}$, which indicates that the symmetry-broken AF ordering is stabilized for $U>U_{\mathrm{cr}}$. (ii) The value of h' at which $\Omega[\Sigma(h')]-\Omega[\Sigma(0)]$ has a minimum approaches 0 with decreasing U to $U\to U_{\mathrm{cr}}$. (iii) The critical value of U is determined as $U_{\mathrm{cr}}=2.7$. This value is comparable to (but is slightly smaller than) the result of the quantum Monte Carlo calculation,[10] where the value $U_{\mathrm{cr}}\simeq2.95$ is reported. The reason for the overestimation of the AF stability in VCA may be explained as follows: In the VCA calculation, we use the cluster representable self-energies, i.e., exact self-energies of small clusters, as the trial self-energies. Thus, the long wavelength spin fluctuations beyond the cluster size are not taken into account.[7] Also, we use the staggered magnetic field on the f

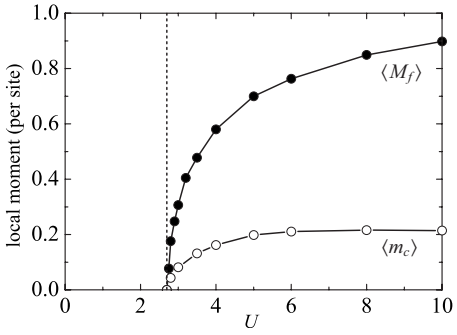

FIG. 2. Calculated results for the staggered magnetic moment of the f orbitals $\langle M_f \rangle$ and c orbitals $\langle m_c \rangle$ as a function of U. Dotted line represents the critical value $U_{\rm cr}=2.7$.

orbitals h' as a single variational parameter, which suppresses the quantum spin fluctuations. This may also be responsible for the overestimation. (iv) For $U<U_{\rm cr}$, we find the minimum at $h'=0$, which indicates that there is no long-range AF ordering in the system.

B. Staggered magnetic moment

In Fig. 2, we show calculated results for the staggered magnetic moment of the f orbitals $\langle M_f \rangle$ and c orbitals $\langle m_c \rangle$ per site at zero temperature, which are defined by

$$\langle M_f \rangle = -\lim_{h^f_{\rm ext}\to 0} \frac{\partial \Omega}{\partial h^f_{\rm ext}}, \tag{6a}$$

$$\langle m_c \rangle = -\lim_{h^c_{\rm ext}\to 0} \frac{\partial \Omega}{\partial h^c_{\rm ext}}, \tag{6b}$$

where Ω is the grand potential of the system per site and $h^f_{\rm ext}$ ($h^c_{\rm ext}$) is the external staggered magnetic field acting on the f (c) orbitals. We find the following: (i) The staggered magnetic moment of the f electrons decreases continuously to 0 when we decrease the value of U from the strong coupling region to $U_{\rm cr}$. Thus, the phase transition is of the second order. (ii) The staggered moment of the c electrons also shows the similar behavior but the polarization is of the opposite sign. (iii) The obtained staggered moments may be overestimated as in the case of the Hubbard model in 2D,[7] which is due again to the overestimation of the stability of the AF ordered state in VCA as discussed above.

We also point out that the calculated staggered moments $\langle M_f \rangle$ and $\langle m_c \rangle$ are found to show a power-law behavior in the vicinity of the transition point as $\sim(U-U_{\rm cr})^{\beta}$ with the exponent $\beta \simeq 0.5$, which is consistent with the mean-field value $\beta=0.5$ within the numerical accuracy. Thus, the VCA calculation, which neglects the long-range spin fluctuations beyond the cluster size, gives the results equivalent to those of the simple mean-field approximation at least in the description of the critical behaviors such as the critical exponent.

C. Single-particle spectra and densities of states

We then calculate the single-particle spectra[13] defined by the imaginary part of the "Fourier transform" of the optimized physical Green's function.[7] We also calculate the DOS from the $\boldsymbol{k}$-space integration of the imaginary part of the optimized physical Green's function. The results are shown in Fig. 3, where we use the AF Brillouin zone when the system is in the symmetry-broken AF state [see Figs. 3(a) and 3(b)], but for nonmagnetic states, we use the standard first Brillouin zone [see Fig. 3(c)].

In Fig. 3(a), i.e., for $U=10$, we can first identify the "upper and lower Hubbard bands" for the f electrons, which are almost dispersionless and are separated by an energy $\sim U$. We can also identify the lower-energy dispersive bands in Fig. 3(a). Here, we use the spin-density-wave (SDW) dispersion to fit the spectra. The SDW dispersion can be obtained by diagonalizing the SDW Hamiltonian $H_{\rm SDW}$ defined by

$$H_{\rm SDW} = \sum_{k\sigma} (c^{\dagger}_{{\rm A}k\sigma} c^{\dagger}_{{\rm B}k\sigma} f^{\dagger}_{{\rm A}k\sigma} f^{\dagger}_{{\rm B}k\sigma}) \times \begin{pmatrix} \sigma m_c & \varepsilon_{\boldsymbol{k}} & -\tilde{V} & 0 \\ \varepsilon_{\boldsymbol{k}} & -\sigma m_c & 0 & -\tilde{V} \\ -\tilde{V} & 0 & \tilde{E}_f - \sigma M_f & 0 \\ 0 & -\tilde{V} & 0 & \tilde{E}_f + \sigma M_f \end{pmatrix} \begin{pmatrix} c_{{\rm A}k\sigma} \\ c_{{\rm B}k\sigma} \\ f_{{\rm A}k\sigma} \\ f_{{\rm B}k\sigma} \end{pmatrix}, \tag{7}$$

where A and B are the sublattice indices, $\tilde{V}$ and $\tilde{E}_f$ are the effective hybridization parameter and effective energy level of the f orbital, respectively, M_f (m_c) is the staggered magnetic moment of the f (c) orbitals, and $\varepsilon_{\boldsymbol{k}}=-2t(\cos k_x + \cos k_y)$. We assume M_f and m_c to have the values obtained in Eqs. (6a) and (6b) and we fix $\tilde{E}_f$ to be 0. We determine the value of $\tilde{V}$ so as to reproduce the size of the SDW gap. We find that the fitting works well for the dispersions of the lower-energy bands but the spectral weight on the f orbital differs very much from that of the VCA calculations since the upper and lower Hubbard bands for the f electrons do not appear in the SDW spectral functions. We then find the value $\tilde{V} \simeq 0.35$ from the fitting, indicating that the quasiparticle is not quite heavy. In other words, with increasing U, the AF ordering occurs in 2D before the quasiparticle mass is strongly enhanced.

In Fig. 3(b), i.e., for $U=4$, we find that the localized energy level is not well defined but there is a band repulsion in the spectra at $\varepsilon_f = \pm U/2$. The spectral weight of the f electrons becomes large near the Fermi energy for all the momenta. Also, by comparing the results of the noninteracting case ($U=0$), the sharp peak just below the Fermi energy is observed in the partial DOS of the f orbital [see the right panel of Fig. 3(b)]. Thus, we conclude that this peak not only arises from the hybridization but is caused by the many-body resonance, which corresponds to the Kondo resonance peak in the metallic state.

In Fig. 3(c), i.e., for $U=2$, where there is no AF ordering in the system, we find that the spectra look very similar to the spectra of noninteracting case. However, we again find that the localized energy level is not well defined but there is a weak band repulsion in the spectra at $\varepsilon_f = \pm U/2$.

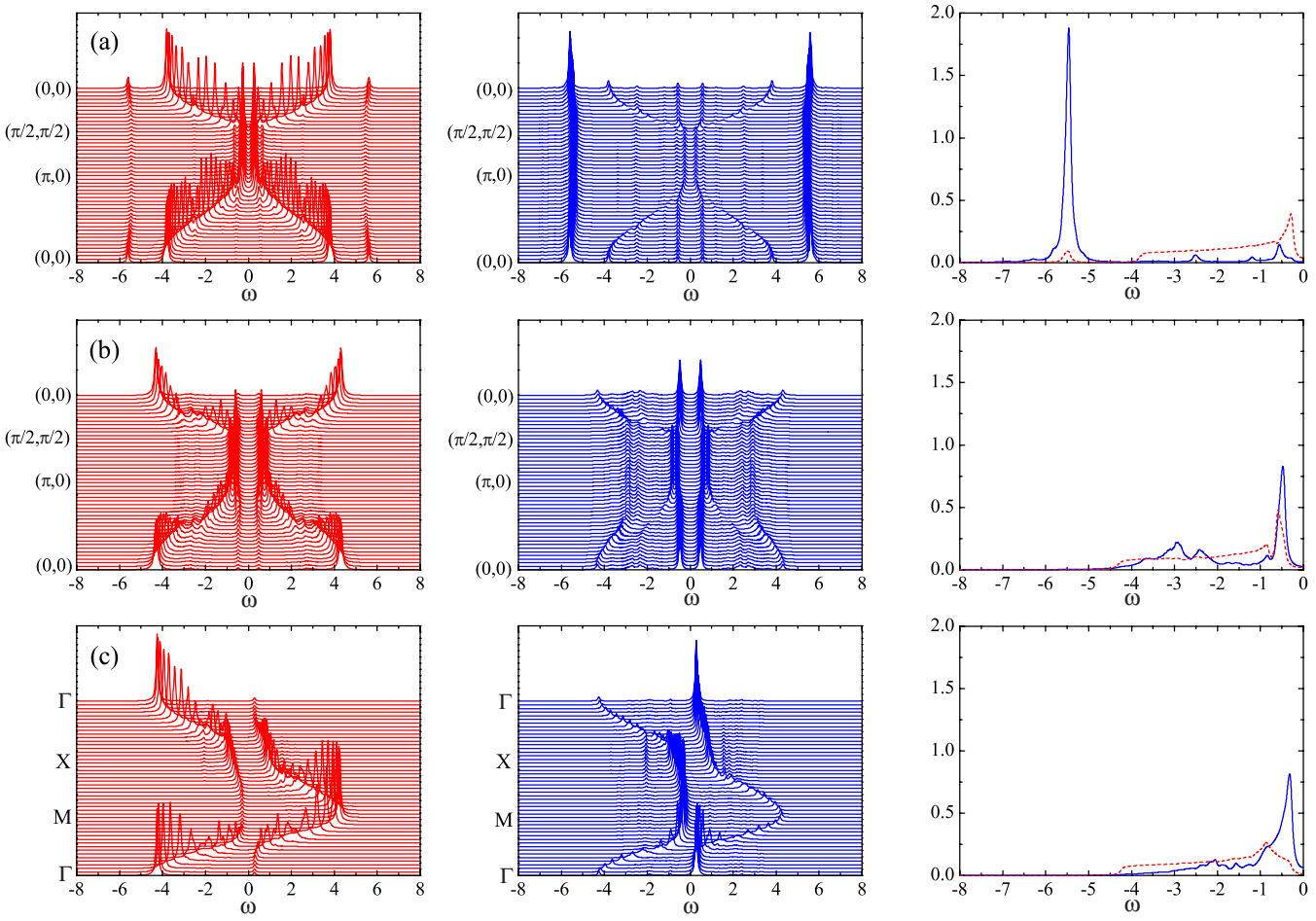

FIG. 3. (Color online) Calculated results for the single-particle spectra (left and middle panels) and DOS (right panels) for (a) $U=10$, (b) $U=4$, and (c) $U=2$, where $\omega=0$ corresponds to the Fermi energy. The left and middle panels show the spectra of the c and f electrons, respectively. In the right panel, the solid and dotted curves are the DOS for the f and c orbitals, respectively. The artificial Lorentzian broadening of $\eta=0.05$ is included.

D. Charge gap and spin gap

To clarify the behavior in the weak-coupling region, where there is no AF ordering, i.e., $U<U_{\mathrm{cr}}$, we calculate the spin and charge gaps defined as $\Delta_s=E_0(N_\uparrow+1,N_\downarrow-1)-E_0(N_\uparrow,N_\downarrow)$ and $\Delta_c=[E_0(N_\uparrow+1,N_\downarrow+1)+E_0(N_\uparrow-1,N_\downarrow-1)-2E_0(N_\uparrow,N_\downarrow)]/2$, respectively, where $E_0(N_\uparrow,N_\downarrow)$ is the ground-state energy of a cluster with $N_\uparrow$ up-spin and $N_\downarrow$ down-spin electrons. Because the two-particle Green's functions cannot be calculated directly from VCA, we here use an exact-diagonalization technique on small clusters. We use the eight-site, 16-orbital cluster with periodic boundary condition to calculate the ground-state energies and estimate the spin and charge gaps. In Fig. 4, we show the ratio of the spin gap to the charge gap Δ_s/Δ_c, thus, obtained as a function of U, where the result only at $U<U_{\mathrm{cr}}$ (with U_{cr} determined in Sec. III A) is shown because no phase transition occurs in finite-size systems. We find $\Delta_c>\Delta_s$ for all values of U ($<U_{\mathrm{cr}}$), indicating the system to be in the regime of the Kondo insulator;[10] i.e., there is no long-range AF ordering, where localized spins are screened by the formation of the Kondo singlet state. As U decreases to 0, we find that the two gaps tend smoothly to the same value, i.e., $\Delta_s/\Delta_c\to 1$, indicating the system tends to the noninteracting band insulator.

IV. SUMMARY

In summary, we have applied the VCA based on the SFT to consider the symmetric PAM at half filling in 2D. We

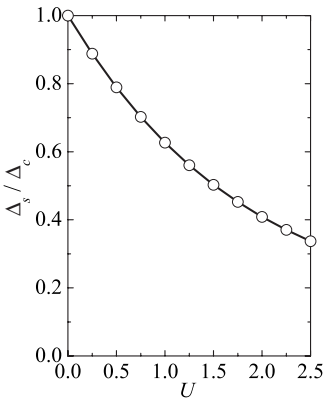

FIG. 4. Calculated result for the ratio of the spin gap to charge gap Δ_s/Δ_c as a function of U ($U<U_{\mathrm{cr}}$). The eight-site cluster is used.

have, thus, demonstrated the validity of the approach by discussing in particular the competition between antiferromagnetism and Kondo screening in the thermodynamic limit at zero temperature. We have shown that the symmetry-broken AF ordering of localized spins is realized in the strong coupling region $U > U_{cr}$, and the Kondo insulating behavior is realized in the weak-coupling region $U < U_{cr}$. We have determined the critical interaction strength as $U_{cr}=2.7$. We have calculated the staggered magnetic moment as a function of the interaction strength and have shown that the phase transition is of the second order. We have also calculated the single-particle spectra and density of states. We have thereby discussed the effect of electron correlations on the quasiparticle band structure. We have applied an exact-diagonalization technique on small clusters to calculate the ratio of the spin gap to charge gap in the weak-coupling region and found that the Kondo insulating state continuously tends to the noninteracting band insulator with decreasing the value of U to 0.

We thus have shown that the present approach is very useful for considering the electronic states of PAM in 2D. To improve the accuracy of our results, one may introduce additional variational parameters, such as the hopping terms, to take into account the quantum fluctuations more efficiently and suppress the overestimation of the stability of the AF ordering, which we want to leave for future studies.

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