Validity of the equation-of-motion approach to the Kondo problem in the large-*N* limit

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The Anderson impurity model for Kondo problem is investigated for arbitrary spin-orbital degeneracy N of the magnetic impurity by the equation-of-motion method (EOM). By employing a different decoupling scheme, a set of self-consistent equations for the one-particle Green's function is derived and numerically solved in the large-N approximation. For the particle-hole symmetric Anderson model with finite Coulomb interaction U, we show that the Kondo resonance at the impurity site exists for all $N \geq 2$. The approach removes the pathology in the standard EOM for $N=2$ and has the same level of applicability as noncrossing approximation. For $N=2$, an exchange field splits the Kondo resonance into only two peaks as predicted by a more rigorous numerical renormalization-group method. The temperature dependence of the Kondo resonance peak is also discussed.

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I. INTRODUCTION

The Kondo effect has been a subject of intensive investigation both experimentally and theoretically for many years. The Anderson impurity model[1] has been regarded as one of the successful models, which correctly describe the coupling between conduction electrons and local magnetic impurity. Although many techniques have been developed for solving this model,[2] it is desirable to have a semianalytic and more generic method that can treat the finite-U case at finite temperatures. It is believed that the effect due to finite U is important in determining spectroscopic, thermodynamics, and transport properties at finite temperature.[3,4]

The equation-of-motion method (EOM) (Refs. 5–9) might be such a candidate. This approach has been employed to derive an analytical expression for the single-particle Green's function of the local electron at the impurity site, and from which finite temperature properties of the system can be obtained. The EOM successfully yields approximate but correct behaviors for the resistivity,[10,11] the spin susceptibility,[10,12] and other transport properties.[13] Especially, when the temperature is above T_K, the results based on this approach agree well with those from perturbative calculations. However, the most serious weakness in the standard EOM is its failure to show the Kondo resonance peak at the Fermi energy for symmetric Anderson model with finite U for spin-orbital $N=2$. Recently, it has been correctly pointed out[14] that the particle-hole symmetric case is the singular point for the standard EOM. However, we note that the noncrossing approximation (NCA) method with large-N expansion,[15–20] when generalized to the finite-U cases,[21] is successful in producing a Kondo resonance peak at the Fermi energy for the particle-hole symmetric case. Therefore, it would be legitimate to ask whether one can develop a large-N EOM and the Kondo resonance peak can be recovered when $N=2$. Another important issue is whether this kind of method can describe the effect of applied exchange magnetic field correctly. By addressing these two important issues, this paper will establish the validity of the EOM for treating the Kondo problem in the large-N limit.

The outline of this paper is as follows. In Sec. II, we present the large-N-limit EOM approach to the Anderson impurity model. The main difference of the derived impurity Green's function from that based on the conventional EOM approach is discussed. In Sec. III, we present the numerical results for the impurity spectral density in the particle-hole symmetric case, which is the primary interest of this paper. The effects of both the temperature and an exchange magnetic field are also discussed. A conclusion is given in Sec. IV.

II. ANDERSON IMPURITY MODEL AND LARGE-*N* EQUATION-OF-MOTION APPROACH

We start with the Anderson impurity Hamiltonian with an arbitrary spin-orbital degeneracy N to study the Kondo problem. In this model, a single band for conduction electrons is adopted, and the magnetic impurity has $N/2$ degenerate localized orbitals plus each orbital carrying a spin degeneracy of 2. The Anderson Hamiltonian of a magnetic impurity with spin-orbital degeneracy N in metal has the following expression:

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \sum_\alpha^N \epsilon_\alpha f_\alpha^\dagger f_\alpha + \frac{U}{2} \sum_{\alpha \neq \beta}^N f_\alpha^\dagger f_\alpha f_\beta^\dagger f_\beta + \sum_{k,\alpha}^N [V_{k\alpha} c_k^\dagger f_\alpha + V_{k\alpha}^* f_\alpha^\dagger c_k], \quad (1)$$

where we have defined $k=(\vec{k},\sigma)$ for conduction-band indices. $c_k^\dagger$ and $f_\alpha^\dagger$ are, respectively, the creation operators for conduction and f electrons at the impurity site. The quantities ϵ_k and ϵ_α are the band energy of conduction electrons and energy of the local electron in the α orbital (spin index included) at the impurity site, respectively. For simplicity, a constant conduction electron density of states (DOS) is assumed, i.e., $\rho(\epsilon)=1/2D$ when $-D \leq \epsilon_k \leq D$, where D is the band half width. Here an SU(N)-type Coulomb interaction with strength U is assumed between electrons of different orbitals (or with opposite spins in the same orbital) at the

impurity site, and $V_{k\alpha}$ represents the s-f hybridization.

The decoupling scheme used in the original work of Appelbaum, Penn, and Lacroix (APL) (Refs. 5 and 6) has been regarded as standard in EOM. The "standard" scheme for the EOM starting from the local electron Green's function generates the higher-order Green's function, which have to be truncated. Thereby one obtains a closed set of equations to be solved self-consistently. However, a close look at the truncating approximation, certain higher order of the Green's function terms should not be simply discarded, and they need to be properly included since these terms are absent at $N=2$ and become important when N is larger than 2. We here generalize Lacroix's $N=2$ decoupling scheme to the large-N case and write the matrix element of the following higher-order Green's function as proposed by Czycholl[7] in the approximate form:

$$\langle\langle f_\alpha f_\gamma^\dagger f_\gamma c_k^\dagger f_{\alpha'} | f_\beta^\dagger \rangle\rangle = \langle c_k^\dagger f_{\alpha'}\rangle \langle\langle f_\alpha f_\gamma^\dagger f_\gamma | f_\beta^\dagger\rangle\rangle + \mathcal{O}(V^2). \quad (2)$$

Corrections to this decoupling scheme are of the order of V^2 and can be neglected in the limit of $V \to 0$, and the validity of this corrections has been discussed in Ref. 7. Adding the above terms to our work is necessary to make the local electron Green's functions satisfy a set of self-consistent equations and make the EOM more powerful as will be demonstrated below. After a complicated but straightforward derivation, the final expression for the matrix element of the impurity Green's function $G_{\alpha\beta} \overset{\text{def}}{=} \langle\langle f_\alpha | f_\beta^\dagger\rangle\rangle \equiv G_{\alpha\alpha}\delta_{\alpha\beta}$ in the large-N approximation is found to be

$$G_{\alpha\alpha} = \frac{1-\bar{n}_{\alpha'}(\omega)}{\omega - \epsilon_\alpha - \Sigma_{0,\alpha} + \dfrac{U\Sigma_{1,\alpha\alpha'}}{\omega - \epsilon_\alpha - U - \Sigma_{0,\alpha} - \Sigma_{3,\alpha\alpha'}}} + \frac{\bar{n}_{\alpha'}(\omega)}{\omega - \epsilon_\alpha - \Sigma_{0,\alpha} - U - \dfrac{U(\Sigma_{3,\alpha\alpha'} - \Sigma_{1,\alpha\alpha'})}{\omega - \epsilon_\alpha - \Sigma_{0,\alpha} - \Sigma_{3,\alpha\alpha'}}}. \quad (3)$$

Here the spin-orbital index $\alpha' \neq \alpha$, and we have defined several self-energies and functions. The variable $\bar{n}_{\alpha'}$ is defined as

$$\bar{n}_{\alpha'}(\omega) \overset{\text{def}}{=} (N-1)\left[\langle n_{\alpha'}\rangle + \sum_k \frac{V_{k\alpha'}\langle c_k^\dagger f_{\alpha'}\rangle}{D_{1,\alpha\alpha'}(k,\omega)} + \sum_k \frac{V_{k\alpha'}^*\langle f_{\alpha'}^\dagger c_k\rangle}{D_{2,\alpha\alpha'}(k,\omega)}\right], \quad (4)$$

where n_α is the occupation number of local electrons on spin-orbital α. The three self-energies are

$$\Sigma_{0,\alpha} \overset{\text{def}}{=} \sum_k \frac{|V_{k\alpha}|^2}{\omega - \epsilon_k}, \quad (5)$$

$$\Sigma_{1,\alpha\alpha'} \overset{\text{def}}{=} (N-1)\sum_k \frac{V_{k\alpha'}^*\left[\sum_q V_{q\alpha'}\langle c_q^\dagger c_k\rangle - \Sigma_{0,\alpha}\langle f_{\alpha'}^\dagger c_k\rangle\right]}{D_{2,\alpha\alpha'}(k,\omega)} + (N-1)\sum_k \frac{V_{k\alpha'}\left[\sum_q V_{q\alpha'}^*\langle c_k^\dagger c_q\rangle - \Sigma_{0,\alpha}\langle c_k^\dagger f_{\alpha'}\rangle\right]}{D_{1,\alpha\alpha'}(k,\omega)}, \quad (6)$$

and

$$\Sigma_{3,\alpha\alpha'} \overset{\text{def}}{=} \sum_k |V_{k\alpha'}|^2\left[\frac{1}{D_{1,\alpha\alpha'}(k,\omega)} + \frac{1}{D_{2,\alpha\alpha'}(k,\omega)}\right], \quad (7)$$

where we have defined two functions,

$$D_{1,\alpha\alpha'}(k,\omega) \overset{\text{def}}{=} \omega + \epsilon_k - \epsilon_\alpha - \epsilon_{\alpha'} - U \quad (8)$$

and

$$D_{2,\alpha\alpha'}(k,\omega) \overset{\text{def}}{=} \omega - \epsilon_k - \epsilon_\alpha + \epsilon_{\alpha'}. \quad (9)$$

The final expression of Eq. (3) is nontrivial and requires a delicate derivation. We can simply summarize our main results.

(1) The high-order Green's functions have been naturally included in our derivation, which enables us to truncate arbitrary order to close the coupling integral equations; (2) the higher-order decoupling scheme we have used in our derivation makes our formula be distinguished from the previous conventional $N=2$ results; (3) Eq. (3) is not an extension to APL (Refs. 5 and 6) but a different large-N decoupling scheme. It is due to the fact that all of the terms $N-1$, which are implicitly included in Eq. (3) and explicitly expressed in Eqs. (4) and (6), are absent if one takes the APL decoupling with the large-N EOM.

We shall illustrate the following features and ingredients of Eq. (3): (1) it includes a set of the $N \geq 2$ closed self-consistent integral equations, which can be numerically solved; (2) the effective occupancy is frequency dependent; (3) the higher-order self-energy contains the intermediate off-diagonal states in momentum space (e.g., $\langle c_k^\dagger c_q\rangle$) and charge fluctuations (e.g., $\langle f_\alpha^\dagger c_q\rangle$); (4) it reproduces the results from the standard $N=2$ EOM in the infinite-U limit,[8] and for the finite-U case, the formulation is different in essence than that from the standard decoupling approach[8] by noticing the sign change before the terms involving D_1 in Eq. (4) and Σ_0/D_1 in Eq. (6).

Before we proceed to carry out numerical calculations, we shall also point out that the expectation value of $\langle c_q^\dagger c_k\rangle$ and $\langle f_{\alpha'}^\dagger c_k\rangle$, which have been discarded in the EOM with the APL decoupling scheme, prove to be very important at low temperatures since they diverge logarithmically at the Fermi level as the temperature approaches zero. Their values should be self-consistently evaluated through the spectral densities between the conduction electron and the impurity Green's functions,

$$\langle c_q^\dagger c_k\rangle = -\frac{1}{\pi}\int f_{\rm FD}(\omega){\rm Im}\langle\langle c_k|c_q^\dagger\rangle\rangle d\omega, \tag{10}$$

where $f_{\rm FD}(\omega)=1/[\exp(\omega/k_BT)+1]$ is the Fermi-Dirac distribution function, and the Green's function $\langle\langle c_{k\bar\sigma}|c_{q\bar\sigma}^\dagger\rangle\rangle$ is

$$\langle\langle c_k|c_q^\dagger\rangle\rangle = \frac{\delta_{q,k}}{\omega-\epsilon_k}+\frac{V_{k\alpha'}V_{q\alpha'}^*\langle\langle f_{\alpha'}|f_{\alpha'}^\dagger\rangle\rangle}{(\omega-\epsilon_k)(\omega-\epsilon_q)}, \tag{11}$$

and similarly

$$\langle f_{\alpha'}^\dagger c_k\rangle = -\frac{1}{\pi}\int f(\omega){\rm Im}\langle\langle c_k|f_{\alpha'}^\dagger\rangle\rangle d\omega, \tag{12}$$

with

$$\langle\langle c_k|f_{\alpha'}^\dagger\rangle\rangle = \frac{V_{k\alpha'}\langle\langle f_{\alpha'}|f_{\alpha'}^\dagger\rangle\rangle}{(\omega-\epsilon_k)}. \tag{13}$$

Solving the coupled Eq. (3) not only yields the correct Kondo resonance at low temperatures but also allows us to explicitly include the logarithmic divergence in general. When the spin-dependent effect is taken into account, the significance of our present EOM approach is that it does not rely on the additional renormalization introduced in the previous EOM technique.[9] The purpose of the additional renormalization is to account for the spin-dependent level splitting and broadening.[22,23] The lack of rigorous justification for the existence of the additional renormalization has cast a doubt for the effectiveness of the EOM approach for the nonequilibrium Kondo problem. In our improved EOM formula, we find that the correct Kondo resonance can be derived without introducing the additional renormalization. Comparing with previous calculations, we have properly evaluated terms such as $\langle c_q^\dagger c_k\rangle$ and $\langle f_{\alpha'}^\dagger c_k\rangle$ through Eq. (6).[8] These terms make crucial contributions to the Kondo resonance peak at very low temperatures. Neglecting these terms will lead to severe errors, which has to be recovered by adding *ad hoc* an additional renormalization.

III. NUMERICAL RESULTS

A. Kondo resonance in the absence of a magnetic field

In order to demonstrate the power of our large-N EOM approach, we shall apply our present formulation to consider the Kondo impurity problem in the particle-hole symmetric case, where the standard $N=2$ EOM fails to show the Kondo resonance peaks. In this case, the incoherent peaks for $V_{k\alpha}=0$ are symmetrically placed about the Fermi level at $\epsilon=-U/2$ and $\epsilon=U/2$. If the model system has particle-hole symmetry, the impurity site is half filled and the average occupation of each spin-orbital $\langle n_\alpha\rangle=0.5$, for which the impurity bare level plays the role of Lagrange multiplier and should be adjusted within the method. This symmetric model can display the full range of behavior from nonmagnetic for $k_BT, U<\Delta_0$ to magnetic and Kondo behavior for $U\gg\Delta_0$, where $\Delta_0=-{\rm Im}[\Sigma_{0,\alpha}(\omega+i0^+)]$. We shall examine this well-studied case by numerically solving Eq. (3), and we choose the following parameters for our numerical calculation. The energy of the half width of the impurity resonance in a nonmagnetic metal, Δ_0, is taken to be 0.1 in the unit of conduction-band half width D unless specified otherwise. In this special case, the Coulomb interaction energy U has usually been taken as a parameter.

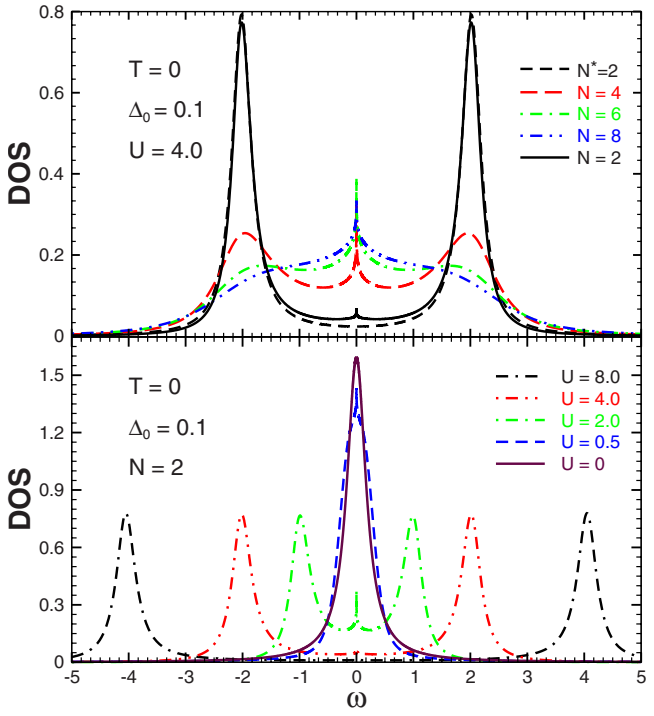

FIG. 1. (Color online) Top: spectral DOS calculated via the EOM method for particle-hole symmetric Anderson impurity model for different spin-orbital degeneracy N at zero temperature with Coulomb interaction $U=4$. The short dashed line as denoted by $N^*=2$ is the result from the standard EOM formulation while other lines correspond to our large-N (≥ 2) formulation. Bottom: results of spectral DOS via large-N limit EOM for $N=2$ particle-hole symmetric Anderson model with different Coulomb interaction U. The peak intensity at the Fermi energy decreases as U is increased.

The first illuminating example is the more familiar equilibrium Kondo problem where both the impurity bare level and the hybridization are spin-orbital degenerate. As shown on the top panel of Fig. 1, when one uses the formulation from the standard EOM for $N=2$,[8] there are no Kondo resonance peaks (dashed line). This result numerically confirms the analysis made by Kashcheyevs *et al.*[14] that the standard EOM technique, as a severe drawback, cannot produce the Kondo resonance at the particle-hole symmetric point. Interestingly, within our large-N EOM technique, the Kondo resonance peak at the Fermi energy is indeed obtained even for $N=2$. With an increase in the spin-orbital degeneracy N, the spectral weight is transferred more significantly from the virtual bound states toward the coherence region around the Fermi energy. This behavior is similar to the case, as demonstrated below, when the localized level is moved toward the Fermi energy within the energy region of bare resonance width Δ_0—mixed-valence region. Notice that, for $N\geq 4$, except those two peaks symmetrically placed around the Fermi energy, other high-energy atomic peaks, which are important at very high temperatures, are beyond the description of the

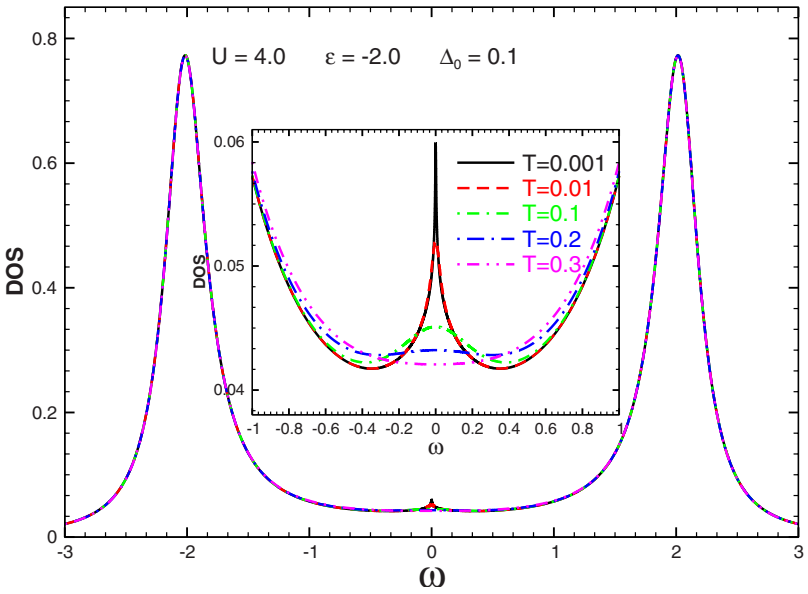

FIG. 2. (Color online) Spectral DOS calculated via the large-N limit EOM method $N=2$ for a finite-U particle-hole symmetric Anderson impurity model at various temperatures. The inset displays the zoom-in view of the Kondo resonance near the Fermi energy. The peak intensity at the Fermi energy decreases as the temperature is increased.

present EOM formulation. The bottom panel of the Fig. 1 shows the impurity spectral ($\rho_{f\uparrow}=\rho_{f\downarrow}$) DOS for different Coulomb energy U at zero temperature by using our large-N EOM formula. At small values of U, the DOS exhibits the two broad peaks at $\epsilon=-U/2$ and $\epsilon=U/2$, respectively, and a sharp Kondo resonance peak at the Fermi level. With the increased U, the Kondo resonance peak disappears gradually, evolving into a localized state. These well-known results agree with many various approaches, e.g., the scaling analysis,[24] the numerical renormalization-group (NRG) method, and NCA.[15] Throughout the calculations, it has also been observed that the impurity spectral density satisfies the sum rule $\int\rho_\sigma(\omega)d\omega=1$ reasonably well.

The temperature-dependent effect has been shown in Fig. 2. We find that the width and height of Kondo resonance peaks dramatically changed with increasing temperature. The inset displays the zoom-in view of the Kondo resonance near the Fermi energy. By further increasing the temperature, the Kondo resonance peaks disappear at a characteristic temperature (about 0.3 for the given parameter values). We should also mention but not show that the present large-N EOM technique can describe equally well the Kondo physics for an asymmetric Anderson impurity model.

B. Kondo Resonance in the presence of a magnetic field

We now consider another very interesting application of our large-N limit EOM technique to the Kondo impurity problem in the presence of external magnetic field. We show in Fig. 3 the spectral DOS for a finite-U particle-hole symmetric model at different exchange fields. A splitting of the Kondo resonances peaks for the spin-up and spin-down electrons is obtained at energy $\epsilon=\pm 2H_{\rm ex}$. There is no spurious peak but only a small bump showing up near the Fermi energy. This result is in reasonable agreement with that from the NRG calculations,[25,26] except for a small bump obtained here. However, the advantage of the present method is that the determination of the asymmetric peak form is free of

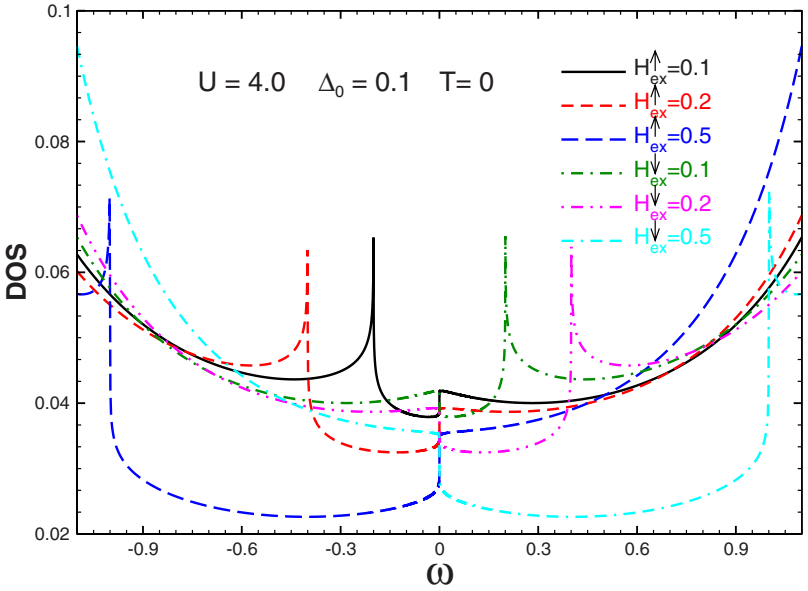

FIG. 3. (Color online) Spectral DOS calculated via the large-N limit EOM method $N=2$ for a finite-U particle-hole symmetric Anderson impurity model at different exchange fields.

such numerical uncertainty as the logarithmic broadening scheme used in the NRG approach, thus providing an updated result on the magnetic field effect.

IV. SUMMARY

In conclusion, we have developed a large-N EOM approach to the Kondo impurity problem for arbitrary Coulomb interaction U at finite temperatures. Numerical results are carried out for symmetric Anderson impurity model with finite U. We show that the Kondo resonance peak, which escapes from the standard EOM approach for the particle-hole symmetric point, can be restored in the present technique. Furthermore, we have also shown that the present technique describes reasonably well the field dependence of the Kondo effect. Both successes establish the power of this present EOM technique.

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