Kondo resonance in the presence of spin-polarized currents

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We propose an improved method of the equation of motion approach to study the Kondo problem in spin-dependent nonequilibrium conditions. We find that the previously introduced additional renormalization for nonequilibrium Kondo effects is not required when we use a proper decoupling scheme. Our improved formulation is then applied to address the spin-split Kondo peaks when a spin current injects into a Kondo system.

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I. INTRODUCTION

The Kondo effect¹ has been one of the central and challenging problems in condensed-matter physics for many years. In equilibrium, the Kondo peak formed at the Fermi level is degenerate with respect to spin degrees of freedom when a magnetic impurity is embedded in a nonmagnetic metal. By applying a magnetic field, the spin degeneracy of the Kondo peak can be lifted due to Zeeman splitting of the impurity level. For a mesoscopic system such as a quantum dot, one can also use ferromagnetic leads to lift the spin degeneracy; this is because the ferromagnetic leads provide the spin dependence of the interaction (or hybridization) between the conduction electrons of the leads and the localized state in the quantum dot.² To explain the above spindependent nonequilibrium phenomena, one frequently relies on the method of the equation of motion (EOM) where an additional renormalization in the self-energy is introduced without rigorous justification.

In this paper, we address two issues. First, we show that the nonequilibrium Kondo problem can be solved without the artificial additional renormalization as long as one correctly keeps the previously neglected terms in the EOM. We establish a general formulation for the case of finite and infinite U in the Anderson model. Second, we use the improved EOM method to predict spin-split Kondo peaks in the presence of a nonequilibrium spin accumulation. The spin accumulation has played a crucial role in the emerging field of spin electronics.^{3–5} Our prediction directly connects the separation of the Kondo peaks with the spin accumulation, and thus it provides a way to determine the spin accumulation in Kondo systems. We emphasize an important distinction of the present study from the previous one: the nonequilibrium condition generated by a voltage across the quantum dot and the ferromagnetic lead has a common chemical potential for spin-up and down electrons, while the spin accumulation generates spin-split chemical potentials.

The rest of the paper is outlined as follows. Section II presents a generic procedure of the EOM approach. In Sec. III, we consider the Kondo resonance in the limit of infinite Hubbard interaction. We benchmark the calculations in the cases where previous results by other authors are available. In Sec. IV, we consider an interesting setup and predict the

important consequence of spin accumulation on the Kondo effect. A summary is given in Sec. V.

II. TECHNICAL PROCEDURE

There are a number of methods to study the Kondo effect in the spin-dependent nonequilibrium condition. The EOM approach of the Anderson model has been used intensively in the past for treating both equilibrium and nonequilibrium Kondo physics at low temperatures.^{6–15} The EOM approach includes resummation of low-order hopping processes and needs a decoupling scheme in order to obtain a closed analytical form. We follow the procedure introduced by Appelbaum, Penn, and Lacroix,^{16,17} which is known to capture the right qualitative feature of physics at low temperatures. We note that other approaches, e.g., numerical renormalizationgroup (NRG) method, can also describe the low-temperature Kondo effect.^{18,19}

The Hamiltonian of the impurity Anderson model is

$$H = \sum_{k,\sigma} \epsilon_{k\sigma} c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} d^{\dagger}_{\sigma} d_{\sigma} + U d^{\dagger}_{\sigma} d_{\sigma} d^{\dagger}_{\overline{\sigma}} d_{\overline{\sigma}} + \sum_{k,\sigma} V_{k\sigma} [c^{\dagger}_{k\sigma} d_{\sigma} + d^{\dagger}_{\sigma} c_{k\sigma}].$$
(1)

Here $c_{k\sigma}^{\dagger}$ and d_{σ}^{\dagger} are, respectively, the creation operators for conduction and *d* electrons at the impurity site. The quantities $\epsilon_{k\sigma}$ and $\epsilon_{d\sigma}$ are the conduction-electron energy dispersion and the impurity energy, respectively. We assume that conduction-electron density of states (DOS) is constant but spin dependent, i.e., $\rho(\epsilon_{\sigma})=1/2D_{\sigma}$ when $-D_{\sigma} \leq \epsilon_{k\sigma} \leq D_{\sigma}$, *U* is the intra-atomic Coulomb interaction at the impurity site, and $V_{k\sigma}$ represents the *s*-*d* hybridization.

By using the standard procedure for the EOM, we obtain def

the impurity Green's function, $G_{d\sigma} = \langle \langle d_{\sigma} | d_{\sigma}^{\dagger} \rangle \rangle$,

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$$G_{d\sigma} = \frac{1 - \bar{n}_{d\bar{\sigma}}(\omega)}{\omega - \epsilon_{d\sigma} - \Sigma_{0\sigma} + \frac{U\Sigma_{1\sigma}}{\omega - \epsilon_{d\sigma} - U - \Sigma_{0\sigma} - \Sigma_{3\sigma}}} + \frac{\bar{n}_{d\bar{\sigma}}}{\omega - \epsilon_{d\sigma} - \Sigma_{0\sigma} - U - \frac{U[\Sigma_{3\sigma} - \Sigma_{1\sigma}]}{\omega - \epsilon_{d\sigma} - U - \Sigma_{0\sigma} - \Sigma_{3\sigma}}}.$$

$$(2)$$

To arrive at Eq. (2), we have made the decoupling approximation procedure shown below. The "dynamic" average occupation number (i.e., frequency dependence) of the impurity level is defined as

$$\bar{n}_{d\bar{\sigma}}(\omega) \stackrel{\text{def}}{=} \langle n_{d\bar{\sigma}} \rangle - \sum_{q} \frac{V_{q\bar{\sigma}} \langle c_{q\bar{\sigma}}^{\dagger} d_{\bar{\sigma}} \rangle}{D_{1\sigma}(\omega, q)} + \sum_{q} \frac{V_{q\bar{\sigma}}^{*} \langle d_{\bar{\sigma}}^{\dagger} c_{q\bar{\sigma}} \rangle}{D_{2\sigma}(\omega, q)}, \quad (3)$$

and the three self-energies are

$$\Sigma_{0\sigma} = \sum_{k} \frac{|V_{k\sigma}|^2}{\omega - \epsilon_{k\sigma}},\tag{4}$$

$$\Sigma_{1\sigma} = \sum_{k} \sum_{q} \left[\frac{V_{k\bar{\sigma}}^{*} V_{q\bar{\sigma}} \langle c_{q\bar{\sigma}}^{\dagger} c_{k\bar{\sigma}} \rangle}{D_{2\sigma}(\omega,k)} + \frac{V_{k\bar{\sigma}} V_{q\bar{\sigma}}^{*} \langle c_{k\bar{\sigma}}^{\dagger} c_{q\bar{\sigma}} \rangle}{D_{1\sigma}(\omega,k)} \right] + \sum_{k} \left[\frac{V_{k\bar{\sigma}}^{*} \langle c_{k\bar{\sigma}} d_{\bar{\sigma}}^{\dagger} \rangle}{D_{2\sigma}(\omega,k)} + \frac{V_{k\bar{\sigma}} \langle c_{k\bar{\sigma}}^{\dagger} d_{\bar{\sigma}} \rangle}{D_{1\sigma}(\omega,k)} \right] \Sigma_{0\sigma},$$
(5)

and

$$\Sigma_{3\sigma} = \sum_{k} \frac{|V_{k\overline{\sigma}}|^2}{D_{1\sigma}(\omega,k)} + \sum_{k} \frac{|V_{k\overline{\sigma}}|^2}{D_{2\sigma}(\omega,k)},\tag{6}$$

where

$$D_{1\sigma}(\omega,k) = \omega + \epsilon_{k\bar{\sigma}} - \epsilon_{d\sigma} - \epsilon_{d\bar{\sigma}} - U$$
(7)

and

$$D_{2\sigma}(\omega,k) = \omega - \epsilon_{k\bar{\sigma}} - \epsilon_{d\sigma} + \epsilon_{d\bar{\sigma}}.$$
 (8)

We shall point out that the expectation values of $\langle c_{q\bar{\sigma}}^{\dagger}c_{k\bar{\sigma}}\rangle$, $\langle d_{\bar{\sigma}}^{\dagger}c_{k\bar{\sigma}}\rangle$ which have been discarded in previous EOM studies are important at low temperatures since they diverge logarithmically at the Fermi level as the temperature approaches to zero. Their values should be self-consistently evaluated through the following identities:

$$\langle c_{q\bar{\sigma}}^{\dagger}c_{k\bar{\sigma}}\rangle = -\frac{1}{\pi} \int f_{\rm FD}(\omega) \mathrm{Im}\langle\langle c_{k\bar{\sigma}} | c_{q\bar{\sigma}}^{\dagger}\rangle\rangle d\omega, \qquad (9)$$

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

$$\langle\langle c_{k\bar{\sigma}} | c_{q\bar{\sigma}}^{\dagger} \rangle\rangle = \frac{\delta_{q,k}}{\omega - \epsilon_{k\bar{\sigma}}} + \frac{V_{k\bar{\sigma}} V_{q\bar{\sigma}}^* \langle\langle d_{\bar{\sigma}} | d_{\bar{\sigma}}^{\dagger} \rangle\rangle}{(\omega - \epsilon_{k\bar{\sigma}})(\omega - \epsilon_{q\bar{\sigma}})},$$
(10)

and similarly

$$\langle d_{\overline{\sigma}}^{\dagger} c_{k\overline{\sigma}} \rangle = -\frac{1}{\pi} \int f(\omega) \operatorname{Im} \langle \langle c_{k\overline{a}} | d_{\overline{\sigma}}^{\dagger} \rangle \rangle d\omega, \qquad (11)$$

with

$$\langle\langle c_{k\bar{\sigma}} | d_{\bar{\sigma}}^{\dagger} \rangle\rangle = \frac{V_{k\bar{\sigma}} \langle\langle d_{\bar{\sigma}} | d_{\bar{\sigma}}^{\dagger} \rangle\rangle}{(\omega - \epsilon_{k\bar{\sigma}})}.$$
(12)

Equation (2) is an extension to a similar result obtained by Meir *et al.*²⁰ Equations (2)–(10) constitute a set of the closed self-consistent equations which can be numerically solved. Before we carry out numerical calculations, we point out the key ingredients in our formula: (1) the effective occupancy is frequency dependent and (2) the higher-order self-energy contains the intermediate off-diagonal states in momentum space (e.g., $\langle c_{k\sigma}^{\dagger}c_{q\sigma} \rangle$) and charge fluctuations (e.g., $\langle d_{\sigma}^{\dagger}c_{q\sigma} \rangle$). Solving the coupled Eqs. (2)–(10) not only yields the Kondo resonance at low temperatures but also allows us to explicitly include the logarithmic divergence in general.

III. KONDO RESONANCE AT AN INFINITY U

For the case of an infinite U, Eq. (2) takes a simpler form,

$$G_{d\sigma} = \frac{1 - \langle n_{d\bar{\sigma}}(\omega) \rangle + \sum_{q} \frac{V_{q\bar{\sigma}} \langle d_{\bar{\sigma}}^{\dagger} c_{q\bar{\sigma}} \rangle}{D_{2\sigma}(\omega, q)}}{\omega - \epsilon_{d\sigma} - \alpha \Sigma_{0\sigma} - \sum_{k} \sum_{q} \frac{V_{k\bar{\sigma}}^{*} V_{q\bar{\sigma}} \langle c_{q\bar{\sigma}}^{\dagger} c_{k\bar{\sigma}} \rangle}{D_{2\sigma}(\omega, k)}}, \quad (13)$$

where the zero-ordered self-energy is renormalized by a factor

$$\alpha = 1 + \sum_{k} \frac{V_{k\bar{\sigma}}^* \langle c_{k\bar{\sigma}} d_{\bar{\sigma}}^{\bar{\tau}} \rangle}{D_{2\sigma}(\omega, k)}.$$
 (14)

Before we apply our formulation to discuss the Kondo resonance in the presence of the spin accumulation, we examine various well-studied cases by numerically solving Eq. (13). We choose the following parameters for our numerical calculation. The energy of the half-width of the impurity resonance in a nonmagnetic metal, $\Delta_0 = -\text{Im}[\Sigma_{0\sigma}(\omega+i0^+)]$, is taken to be 200 meV unless specified otherwise. The conduction-band half-width is $D=100\Delta_0$. The degenerate impurity level is $\epsilon_d = -6\Delta_0$.

The simplest case is the conventional equilibrium Kondo problem where neither impurity state nor hybridization is spin dependence. Figure 1 shows the impurity spectral density ($\rho_{d\uparrow} = \rho_{d\downarrow}$) for four temperatures. As expected, the virtual bound level with a broad spectrum and a sharp peak at the Fermi level known as the Kondo peak appears. The Kondo peak is suppressed and broadened when the temperature is increased. The Kondo temperature which is defined as the full width of the Kondo peak is $T_K \approx \exp[\pi \epsilon_d / 2\Delta_0]$. These well-known results agree with many various approaches, e.g., the scaling analysis²¹ and the noncrossing approximation.²² Meir *et al.*²³ and Martinek *et al.*²⁴ also used the EOM approach to derive these Kondo peaks in the absence of spin polarization.



FIG. 1. Spectral density $\rho_{d\sigma}$ calculated via the EOM method for an infinity U Anderson model for various temperatures in the absence of spin polarization. The inset displays the zoom-in view of the Kondo resonance near the Fermi energy.

We now turn on the spin polarization. In a quantum dot, the spin polarization is introduced via the coupling to a ferromagnetic lead. In this case, one can parametrize the spin dependence through the hybridization parameter, i.e., $\Delta_{\sigma} = \Delta_0(1-\sigma P)$, where the parameter 0 < P < 1 and $\sigma = \pm 1$ for spin up (+1) and down (-1). The results are shown in Fig. 2. When *P* is nonzero, the Kondo resonance splits [Figs. 2(a) and 2(b)], i.e., the peak for spin-up (down) spectral density shifts below (above) the Fermi energy. Note also that the intensity of the peak for spin up (down) is suppressed (enhanced) compared to the equilibrium Kondo peaks [see Figs. 2(a) and 2(b)]. These results are again consistent with those obtained by Martinek *et al.*²⁴ Another way of introducing the spin polarization is to apply a magnetic field. In this case, the Zeeman splitting of the impurity level becomes $\epsilon_{\sigma} = \epsilon_d + \sigma \mu_B B$, where *B* is the magnetic field. We find that the Kondo peaks for spin up and down are separated by $2\mu_B B$ (not shown), which agrees with that in Ref. 23.

The agreement of our results with other approaches validates the EOM approach in Eq. (2) or (13). The significance of our EOM approach is that it does not rely on the additional renormalization introduced in the previous EOM technique.²⁰ Note that dephasing broadening τ_{ϕ} was intro-duced by Meir *et al.*²⁰ and Martinek *et al.*²⁴ in a heuristic way to describe decoherence due to a finite bias voltage or impurity level splitting, which only take into account the real part of self-energy corrections. Since we can solve the improved EOM fully self-consistently, not only the real part but also the imaginary one of self-energy correction have been naturally included. The dephasing broadening and the Kondo resonance peak splitting have been automatically demonstrated here. It is unclear whether it is essential or necessary to introduce the dephasing broadening lifetime to study nonequilibrium Kondo problems. The purpose of the additional renormalization is to account for the spin-dependent level splitting and broadening.^{23,24} 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 have shown that the correct Kondo resonance can be derived without introducing the additional renormalization. Comparing with previous calculations, we have properly evaluated terms such as $\langle c_{a\bar{\sigma}}^{\dagger}c_{k\bar{\sigma}}\rangle$ and $\langle d_{\bar{\sigma}}^{\dagger}c_{k\bar{\sigma}}\rangle$



FIG. 2. Spectral density $\rho_{d\sigma}$ calculated via (a) and (b) the EOM method for an infinity U Anderson model for various temperatures for a fixed degree, P=0.5, of spin polarization, (c) the Kondo resonance splitting as a function of the degree of spin polarization, and (d) the hybridization strength at a fixed P=0.5.



FIG. 3. Schematic illustration of a spin current injected from a ferromagnetic layer to a nonmagnetic conductor containing a magnetic impurity.

through Eq. (5). These terms make crucial contributions to the Kondo resonance splitting at low temperatures. Neglecting these terms will lead to severe errors, which has to be recovered by the artificially adding an additional renormalization.

IV. APPLICATIONS AND DISCUSSIONS

We now apply the EOM to calculate the Kondo resonance in the presence of the spin accumulation. We consider a bilayer structure where a current flows from the ferromagnetic layer to the nonmagnetic layer containing Kondo impurities, as schematically shown in Fig. 3. When a spin-polarized current injects into the nonmagnetic conductor, a spin accumulation is build up near the interface. Assuming that the ferromagnetic layer carries a spin polarization of the current *P*, the spin accumulation is^{25,26} $\delta m = (Pj\lambda\mu_B/eD)\exp(-x/\lambda)$, where *j* is the current density, λ is the spin-diffusion length, μ_B is Bohr magneton, *D* is the diffusion constant, and *x* is the distance away from the interface. If we only consider the Kondo impurity sufficiently close to the interface, i.e., within the distance of λ , we can drop the spatial dependence of the spin accumulation, i.e., $\delta m = Pj\lambda\mu_B/eD$.

To calculate the Kondo resonance from Eq. (13), we specify the dependence of the parameters on the spin accumulation. First, the spin accumulation makes the chemicalpotential spin dependent.^{25,26} Specifically, the chemicalpotential splitting of spin-up and down conduction electron is $\mu^{\uparrow} - \mu^{\downarrow} = \delta m (eD\rho/\mu_B) = P j \rho \lambda$,²⁷ where ρ is the resistivity. Thus one should replace the Fermi level in Eq. (13) by the spin-dependent chemical potentials for the spin up and down $\mu^{\uparrow} = E_F + P j \rho \lambda/2$ and $\mu^{\downarrow} = E_F - P j \rho \lambda/2$, where E_F is the Fermi level. Second, the hybridization parameter Δ would also be spin dependent since the density of states of the conduction electrons is modified by the nonequilibrium electrons. However, the nonequilibrium electron density at very high current density (say 10^7 A/cm^2) is at least several orders of magnitude smaller than the equilibrium electron density, and thus the correction to Δ is very small and we will assume that Δ remains spin independent. Finally, the spin accumulation could lead to the spin-dependent energy shift of the impurity state. If one models the interaction between the spin accumulation and the impurity via a phenomenological exchange coupling, i.e., $H' = -J_{ex} \delta \mathbf{m} \cdot \mathbf{S}_i$, where $\delta \mathbf{m}$ is the spin accumulation and S_i is the impurity spin, the impurity level would be spin split; this will be equivalent to the case when the impurity is subject to an effective magnetic field $\mathbf{B}_{eff} = J_{ex} \delta \mathbf{m}$. Although the magnitude of the effective field could be respectable for a high current density, the local



FIG. 4. Spectral density $\rho_{d\sigma}$ calculated via the EOM method for an infinity U Anderson impurity for various temperatures in presence of spin accumulation with $\Delta \mu = 2$ meV.

level splitting by a magnetic field has already been thoroughly investigated and thus we neglect the effect of the direct coupling between the spin accumulation and the impurity. Therefore, we focus on the Kondo resonances due to spin-dependent Fermi levels. We should emphasis that Kondo problem due to the spin-dependent chemical potential has been recently investigated by Katsura.²⁸ However, this is very different from our considering in several aspects; First, when considering a quantum dot connected by the spindependent chemical potential, Katsura²⁸ started with Kondo Hamiltonian model and used the method of Bethe ansatz to exactly solve the nonequilibrium Kondo problem. The obtained results are thus limited to a special point in the parameter space of the model. Second, we focus on the single impurity Anderson model in a very interesting medium where spin accumulation is generated either by applying the spin-polarized current or by spin injection. Finally, by using our improved EOM approach, we can demonstrate more details about DOS spectrum at different temperatures.

In Fig. 4, we show the spectral density $\rho_{d\sigma}$ for various temperatures with a spin-current-induced chemical-potential shift. It is found that the spin-current influence on the Kondo resonance splitting is robust against temperatures. The more the amplitude of chemical-potential relative shift by spin current, the more pronounced the Kondo resonance splitting between two spin channels will be. Noticeably, the amplitude of the split Kondo peaks remains robust against the spininduced chemical-potential splitting (compare Fig. 4 with Fig. 1), which is different from the case of a ferromagnetic metal as discussed before [see Figs. 2(a) and 2(b)]. This observation is the hallmark of the Kondo resonance splitting from the spin accumulation—a purely nonequilibrium effect.

Advanced experimental techniques such as magnetic tunneling into quantum dots and STM measurement would be able to detect the spin-split Kondo peaks. This will provide a high-resolution detection of the spin accumulation. For example, for a relatively small current density of the order of 10^5 A/cm^2 , the Kondo peaks will be separated by about $\delta E = 0.02 \text{ meV}$ for a typical transition metal such as Fe (note that the width of the Kondo resonance, which is of the order of the Kondo temperature). In comparison, the reliable measurement of the spin accumulation based on the Johnson Silsbee-Johnson technique²⁵ usually requires the current density more than 10^7 A/cm² in order to derive sufficient large signals.

V. CONCLUSION

In conclusion, we have developed an improved decoupling scheme for the EOM approach in Kondo problems at zero and finite temperatures. We have shown Kondo resonance peak spin splitting by keeping the previously discarded terms in the EOM approach, which the dephasing broadening and the additional renormalization are naturally implemented. We then apply the improved EOM approach to study the Kondo effect in the presence of the spin-polarized current induced spin accumulation—this has never been studied by any methods including the numerical renormalization-group method. We predict that the Kondo resonance peaks are spin split due to the spin dependence of the chemical potentials. Finally, it should be especially em-

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phasized that our improved EOM scheme is not only able to obtain the similar results with the NRG method but also it can be naturally used to study the finite temperature effect. Since the finite temperature NRG approach has been implemented very recently to study equilibrium problems and is much more numerically involved. To our best knowledge, it has not yet been applied to study the nonequilibrium problems. As a result, our improved EOM scheme can be used as a complementary method to address the Kondo impurity problems.

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