Front. Phys. China (2007) 1: 41−43
DOI 10.1007/s11467-007-0011-x

RAPID COMMUNICATLON

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Influence of local spin polarization to the Kondo effect

Abstract We use the spin non-degenerate single impurity Anderson model to investigate the influence of the local spin polarization to the Kondo effect. By using the Schrieffer-Wolff transformation, we obtain a generalized s-d exchange Hamiltonian, which describes the interaction between a polarized local spin and conduction electrons. In this case, the singlet is no longer an eigenstate as shown by variational calculations where the splitting of the local energy $\Delta = \varepsilon_{d\uparrow} - \varepsilon_{d\downarrow}$ can be arbitrarily small. The local spin polarization generates the instability of the singlet ground state of the S = 1/2 s-d exchange model.

Keywords the Kondo effect, spin polarization, quantum dot

PACS numbers 71.27.+a, 75.20.Hr, 73.21.La

1 Introduction

The Kondo effect is a many-body phenomenon of strongly correlated electrons, which is the screening of a localized spin by surrounding conduction electrons as described by the spin S = 1/2 s-d exchange model where the local spin is bound to the conduction electron in a singlet state. A narrow many-body resonance, so called "Kondo resonance", is induced through magnetic scattering in the density of states at the Fermi level. In the past decade, the observation of this effect in quantum dot systems revived experimental and theoretical interest [1–4]. The quantum dot provides a tool in probing the microscopic interactions between local spins and conduction electrons. The ground state of the S = 1/2 Kondo system is a resonating singlet state, which is sensitive to the local spin polarization. One of the theoretical interests arising from experiments is that how does the local spin polarization induced by the internal field compete with the Kondo effect? In an experiment, a quantum dot system with dissolved magnetic impurities in the leads of an all-metal device, the Kondo resonance is suppressed at zero bias due to interactions between the net spin in the quantum dot and the magnetic impurity in the leads [5]. The suppression of the Kondo effect indicates that the singlet ground state of the Kondo system is unstable when the local spin is placed in a magnetic environment. The interacting quantum dot system is properly described by the Anderson model [1]. For simplicity, here we give a theoretical analysis of the effect of local spin polarization in a bulk material based on the spin-non-degenerate Anderson model. From which, we can derive a generalized s-d exchange model to specify the nature of the ground state of the S = 1/2 Kondo system in the presence of an internal field by a variational approach. The first order mean field calculation shows that the weak local spin polarization, in spite of its strength, decouples the Kondo singlet.

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Received November 24, 2006

2 Canonical transformation

The spin non-degenerate single impurity Anderson model describes the interaction between a polarized local spin and conduction electrons in bulk materials, which is

$$H = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} + \sum_{s} \varepsilon_{ds} d_s^{\dagger} d_s + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \sum_{ks} V_k \left(d_s c_{ks}^{\dagger} + d_s^{\dagger} c_{ks} \right) \quad (1)$$

where $c_{k\sigma}^{\dagger}$ is the creation operator of the conduction electrons, $d_s^{\dagger}$ the local electron. ε_k and $\varepsilon_{d\sigma}$ are the energies of conduction and localized orbital. V_k is the hybridization interaction. U is the Coulomb interaction between the localized electrons. The spin degeneracy of the local states is lifted by

$$\Delta = \varepsilon_{d\uparrow} - \varepsilon_{d\downarrow} \quad (2)$$

In this case, we can derive a generalized s-d exchange model by using a canonical transformation [6]:

$$\tilde{H} = e^{\mathcal{S}} H e^{-\mathcal{S}} \quad (3)$$

by taking

$$\mathcal{S} = \sum_{ks} \frac{V_k}{\varepsilon_k - \varepsilon_{ds}} \left(1 - \frac{U\hat{n}_{-s}}{\varepsilon_{ds} + U - \varepsilon_k}\right)\left(c_{ks}^{\dagger} c_s - c_s^{\dagger} c_{ks}\right) \quad (4)$$

we note the first three terms in Eq. (1) by H_0, and the term involving V_k by H', then by choosing $\mathcal{S}$ to be first order in V_k, to second order in V, $\tilde{H}$ can be expressed by

$$\tilde{H} = H_0 + \frac{1}{2}[\mathcal{S}, H'] \quad (5)$$

with the restriction of $n_d = 1$. From Eq. (5) we obtain

$$\tilde{H} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} - \frac{J}{2N} \sum_{kk'} \Big[\left(c_{k'\uparrow}^{\dagger} c_{k\uparrow} - c_{k'\downarrow}^{\dagger} c_{k\downarrow} \right) S_z + c_{\vec{k}'\uparrow}^{\dagger} c_{\vec{k}\downarrow} S^{-} + c_{\vec{k}'\downarrow}^{\dagger} c_{\vec{k}\uparrow} S^{+} \Big] + \Delta S_z \quad (6)$$

Eq. (6) is derived in the limit of $|\mathit{\Delta}/\varepsilon_d| \ll 1$, which is a generalized s-d exchange model with an additional Zeeman term giving rise to local spin polarization and the starting point to study the competition between spin fluctuation and spin polarization. We can show in the following by adopting the Yosida variational approach that Eq. (6) has a different ground state from the s-d exchange model, where the singlet is no longer an eigenstate.

3 Effect of local spin polarization on the singlet ground state of S=1/2 Kondo system

By taking the first order approximation, we can use Yosida's variational approach to calculate the ground state energy of Eq. (6); the trial wavefunction takes the form

$$|\psi\rangle = \sum_{k>k_{\mathrm{F}}} \Big[\left(\Gamma_{\vec{k}\uparrow}^{\alpha} c_{\vec{k}\uparrow}^{\dagger} + \Gamma_{\vec{k}\downarrow}^{\alpha} c_{\vec{k}\downarrow}^{\dagger} \right) \chi_{\alpha} |F\rangle + \left(\Gamma_{\vec{k}\uparrow}^{\beta} c_{\vec{k}\uparrow}^{\dagger} + \Gamma_{\vec{k}\downarrow}^{\beta} c_{\vec{k}\downarrow}^{\dagger} \right) \chi_{\beta} |F\rangle \Big] \quad (7)$$

where χ_α and χ_β are the wavefunctions of spin up and spin down states of the local spins, $|F\rangle$ is the ground state of non-interacting electrons. $|\psi\rangle$ is a solution of the Schrödinger equation

$$\tilde{H}|\psi\rangle = E|\psi\rangle \quad (8)$$

If $\mathit{\Delta} = 0$, the ground state of the Schrödinger equation is a singlet composed by the local spin and the conduction electron spin [7]:

$$\Gamma_{k\downarrow}^{\alpha} = -\Gamma_{k\uparrow}^{\beta}; \quad \Gamma_{k\uparrow}^{\alpha} = \Gamma_{k\downarrow}^{\beta} = 0 \quad (9)$$

with the binding energy

$$E = -D \exp\left(-\frac{4}{3\rho |J|} \right) \quad (10)$$

where ρ is the density of states. In the case of $\mathit{\Delta} \neq 0$, we repeat Yosida's calculation to see the effect of spin polarization on the singlet ground state, which yields four equations for parameters $\Gamma_{k\uparrow}^{\alpha}$, $\Gamma_{k\downarrow}^{\alpha}$, $\Gamma_{k\uparrow}^{\beta}$, and $\Gamma_{k\downarrow}^{\beta}$:

$$\left(\varepsilon_k - E + \frac{1}{2}\mathit{\Delta} \right) \Gamma_{k\uparrow}^{\alpha} - \frac{J}{4N} \sum_{k'>k_{\mathrm{F}}} \Gamma_{k'\uparrow}^{\alpha} = 0 \quad (11)$$

$$\left(\varepsilon_k - E + \frac{1}{2}\mathit{\Delta} \right) \Gamma_{k\downarrow}^{\alpha} - \frac{J}{2N} \sum_{k'>k_{\mathrm{F}}} \Gamma_{k'\uparrow}^{\beta} + \frac{J}{4N} \sum_{k'>k_{\mathrm{F}}} \Gamma_{k'\downarrow}^{\beta} = 0 \quad (12)$$

$$\left(\varepsilon_k - E - \frac{1}{2}\mathit{\Delta} \right) \Gamma_{k\uparrow}^{\beta} - \frac{J}{2N} \sum_{k'>k_{\mathrm{F}}} \Gamma_{k'\downarrow}^{\alpha} + \frac{J}{4N} \sum_{k'>k_{\mathrm{F}}} \Gamma_{k'\uparrow}^{\beta} = 0 \quad (13)$$

$$\left(\varepsilon_k - E - \frac{1}{2}\mathit{\Delta} \right) \Gamma_{k\downarrow}^{\beta} - \frac{J}{4N} \sum_{k'>k_{\mathrm{F}}} \Gamma_{k'\downarrow}^{\beta} = 0 \quad (14)$$

If the trial wavefunction is a singlet, we have the equation

$$\mathit{\Delta} \cdot \Gamma_{\vec{k}\downarrow}^{\alpha} = 0 \quad (15)$$

It shows clearly that if $\mathit{\Delta}$ is not equal to zero, $\Gamma_{\vec{k}\downarrow}^{\alpha}$ and $\Gamma_{\vec{k}\uparrow}^{\beta}$ must be zero; the local spin polarization overwhelms the Kondo effect. Accordingly, the suppression of the Kondo effect observed in a quantum dot system can also be attributed to the disintegration of the Kondo singlet. Since $\mathit{\Delta}$ can be arbitrarily small, the Kondo singlet is unstable in the presence of the internal field.

4 Summary and discussion

If we apply an external field $\boldsymbol{B}$ on the $S = 1/2$ Kondo system, which is along the z axis and we assume the internal field is absent, the s-d model Hamiltonian becomes

$$H = \sum_{k\sigma} \varepsilon_{k\sigma} c_{k\sigma}^{\dagger} c_{k\sigma} - \frac{J}{2N} \sum_{kk'} \Big[\left(c_{k'\uparrow}^{\dagger} c_{k\uparrow} - c_{k'\downarrow}^{\dagger} c_{k\downarrow} \right) S_z + c_{\vec{k}'\uparrow}^{\dagger} c_{\vec{k}\downarrow} S^{-} + c_{\vec{k}'\downarrow}^{\dagger} c_{k\uparrow} S^{+} \Big] + \Delta S_z \quad (16)$$

where $\mathit{\Delta} = 2\mu_{\mathrm{B}}B$, $\varepsilon_{k\sigma} = \varepsilon_k + \Delta\sigma/2$, where $\sigma = +1$ for the spin up state, −1 for the spin down state. By solving Schrö dinger's equation, we have equations for the coefficients of the Yosida wavefunction, which is

$$\left(\varepsilon_{k\downarrow} - E + \frac{1}{2}\mathit{\Delta} \right) \Gamma_{k\downarrow}^{\alpha} - \frac{J}{2N} \sum_{k'>k_{\mathrm{F}}} \Gamma_{k'\uparrow}^{\alpha} + \frac{J}{4N} \sum_{k'>k_{\mathrm{F}}} \Gamma_{k'\downarrow}^{\alpha} = 0 \quad (17)$$

$$\left(\varepsilon_{k\uparrow} - E - \frac{1}{2}\mathit{\Delta} \right) \Gamma_{k\uparrow}^{\beta} - \frac{J}{2N} \sum_{k'>k_{\mathrm{F}}} \Gamma_{k'\downarrow}^{\alpha} + \frac{J}{4N} \sum_{k'>k_{\mathrm{F}}} \Gamma_{k'\uparrow}^{\alpha} = 0 \quad (18)$$

From the above equations we can see that the energy shifts of the conduction electrons in the presence of the external field compensate the spin polarization energy of the local spin giving a bound singlet state solution:

$$(\varepsilon_k - E)\Gamma_{k\downarrow}^{\alpha} + \frac{3J}{4N} \sum_{k'>k_{\mathrm{F}}} \Gamma_{k'\downarrow}^{\alpha} = 0 \quad (19)$$

The external field does not affect the Kondo resonance in a bulk material. In the quantum dot experiment by Heersch *et al*., the measurement on the conductivity showed that the Kondo resonance is restored at a certain bias voltage in the order of mV. A possible explanation is that the effect of the internal field is cancelled by bias voltage as we showed for the $S = 1/2$ Kondo system in the external field. We will give the result of the detailed calculations elsewhere.

In summary, we have shown that the singlet ground state of the $S = 1/2$ Kondo system is unstable in the presence of a weak internal field. In fact, it provides an example that the ground state of the interacting system can be changed in nature by an infinitesimal perturbation. It could happen if the ground state of the interacting system is a resonating state. The ground state of the Kondo system is a non-magnetic Fermi-liquid type. As we have shown, the screening of the local spin can be eliminated by the polarization of the local spin, which is important to understanding the microscopic origin of non-Fermi liquid behavior of the oxide compounds, especially the high T_c cuprates [8].

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