Can the spin-orbit interaction break the channel degeneracy of the two-channel orbital Kondo problem?

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Abstract. – Two-level systems (TLS) interacting with conduction electrons are possibly described by the two-channel Kondo Hamiltonian. In this case the channel degeneracy is due to the real spin of the electrons. The possibility of breaking that degeneracy has interest on his own. In fact, we show that the interaction of the conduction electrons with a spin-orbit scatterer nearby the TLS leads to the breaking of the channel degeneracy only in the case of electron-hole symmetry breaking. The generated channel symmetry breaking TLS-electron couplings are, however, too weak to result in any observable effects. Our analysis is also relevant for heavy fermion systems.

In the general form of the orbital Kondo model a single particle is moving between two localized orbitals and is interacting with the conduction electrons in a metal. This orbital Kondo model has been justified by a detailed scaling analysis, though it is presently unclear if the two-channel Kondo fixed point can be experimentally reached in the case of TLS’s. The particle can be an atom or a group of atoms. Similar orbital models emerge in the context of 4f heavy fermion impurities. In these models the real electronic spin variable does not occur in the coupling constants, thus there is a spin degeneracy in the variables of the particles and all interaction terms are diagonal in the conduction electron spin. In realistic materials, however, spin-orbit interaction is always present, and it always induces cross-scattering between different spin orientations. It is, therefore, a fundamental question, whether spin-orbit interaction can break this channel symmetry and invalidate the 2CK description or not.

In this paper we examine the possibility of breaking the channel degeneracy of the orbital Kondo problem due to the interaction of the conduction electrons with a spin-orbit scatterer nearby the TLS, using the renormalization group method in leading logarithmic order. It turns out, that in case of electron-hole symmetry the spin-orbit interaction has no effect on the two-channel Kondo behavior. In contrary, in case of electron-hole symmetry breaking, new, relevant channel symmetry breaking couplings are generated between the TLS and the...
conduction electrons, which are driven by the rather small ratio of the TLS level splitting and the electronic bandwidth. As a consequence, despite of its relevance in the RG sense, this term cannot influence the two-channel behavior in an observable range of temperature, since the scaling is stopped by the infrared cutoff (TLS level splitting) long before the corresponding crossover is reached.

We consider a TLS interacting with conduction electrons which are also interacting with a spin-orbit scatterer at a position with respect to the TLS (see fig. 1). The TLS-conduction electron system is described by the usual Hamilton operator

\[ H_{\text{TLS-cl}} = \sum_{k,l,m,\sigma} \varepsilon_k a^\dagger_{k,l,m,\sigma} a_{k,l,m,\sigma} + \Delta_0 \sigma_\uparrow^{TLS} + \Delta \sigma_\downarrow^{TLS} + \sum_{i=x,y,z} V_i \sigma_i^{TLS} a^\dagger_{k,l} (\sigma_i^{cl}) \nu a_{k,l,\sigma} \]  

where \( a^\dagger_{k,l,m,\sigma} \) creates an electron with momentum \( k \), angular momentum \( l, m \) and spin \( \sigma \). \( \sigma^i \) stand for the Pauli matrices, \( \Delta_0 \) and \( \Delta \) are the spontaneous transition and the energy splitting between the two TLS states, respectively. Choosing the \( z \) axis in an appropriate way and assuming axial symmetry, the TLS is strongly coupled only to a reduced number of channels e.g. to those with azimuthal quantum number \( m = 0 \) of the conduction electrons, thus the \( m \) indices are dropped and only two angular momenta \( l = 0,1 \) are kept.

We describe the spin-orbit scatterer by an Anderson-like (\( l = 2 \)) model with parameters \( \varepsilon_0 \) and \( V_{kml'm'}(R) \) as

\[ H_{\text{s-o}} = \varepsilon_0 \sum_{m,\sigma} b^\dagger_{m,\sigma} b_{m,\sigma} + \sum_{kl',mm',\sigma} \left( V_{kml'm'}(R) b^\dagger_{m,\sigma} a_{kl',m',\sigma} + \text{h.c.} \right) + \lambda \sum_{mm',\sigma\sigma'} \langle m|L|m'\rangle \langle \sigma|\sigma'\rangle b^\dagger_{m,\sigma} b_{m',\sigma'} \]  

where \( b^\dagger_{m,\sigma} \) creates an electron on the spin-orbit scatterer orbital labeled by the quantum numbers \( m, \sigma \) and \( \lambda \) is the strength of the spin-orbit interaction. The hybridization matrix element, \( V_{kml'm'}(R) \) depends on the relative position of the two coordinate systems with origin at the TLS and the spin-orbit scatterer, respectively.

The calculation of the correction to the electron Green’s function due to spin-orbit interaction was performed in a similar way as in Section III of ref. The first order correction \( \delta G^{(1)} \) in the spin-orbit coupling is given by

\[ \delta G^{(1)}_{\sigma\sigma'}(0,0,i\omega_n) = G^{(0)}(0,R,i\omega_n) g_{\sigma'\nu} \sigma^{\nu}_{\sigma'} G^{(0)}(R,0,i\omega_n) \]  

where \( g \) depends on the parameters of the spin-orbit scatterer’s d-level, the strength of the spin-orbit interaction, the angle \( \theta \) between the TLS axis and \( R \), and on the distance \( R \) between

Fig. 1 – The TLS and the spin-orbit scatterer in a distance \( R \).
the TLS and the spin-orbit scatterer, like $\sim \frac{1}{(k_F R)^3}$ in leading order. In eq. (3) the orbital momentum variables of the electron are in the "TLS frame" (x,y,z) (z $\parallel$ TLS axis), whereas the spin variables are in a "local frame" (x',y',z') (z' $\parallel$ R) (see fig. 2).

After simultaneous rotation of both coordinate systems to a new TLS (x $\parallel$ TLS axis) and a new local (x' $\parallel$ R) frame (see fig. 2) the scattering amplitude contained by $\delta G(1)$ can be summed up to infinite order (i.e. infinite number of scatterings on the same spin-orbit scatterer is considered), resulting in

$$\delta G_{\sigma\sigma'}^{(1)}(0,0,i\omega_n) = \frac{g\sigma^x_{\hat{t}l}\sigma^x_{\hat{t}l'}}{1 - g_l \sigma^{(0)}(R,R,i\omega_n)} G^{(0)}(R,0,i\omega_n).$$

(4)

Calculating the corresponding change in the conduction electron density of states in first order in $g$ and using the linearized dispersion $k = k_F + \frac{\mathbf{v}}{v_F}$ near the Fermi level, we get for the spin-dependent part

$$\frac{\delta \rho_R(\omega \approx 0)}{\rho_0} = \Lambda \sigma^x_{\hat{t}l}\sigma^x_{\hat{t}l'}$$

(5)

where $\Lambda$ depends on $g$, the conduction electron density of states at Fermi level for one spin direction $\rho_0$, and in leading order it is $\sim \frac{1}{(k_F R)^3}$, therefore only the first neighboring atoms around the TLS give non-negligible contribution.

We used the above result to examine the TLS-conduction electron system in case of finite $\Lambda$. The new TLS-electron couplings, obtained by introducing the dimensionless TLS-electron couplings and taking into account the above changes in the conduction electron density of states, are

$$v^x = \rho_0 V^x \longrightarrow \tilde{v}^x = v^x \sqrt{1 + \Lambda \sqrt{1 - \Lambda}}$$

$$v^y = \rho_0 V^y \longrightarrow \tilde{v}^y = v^y \sqrt{1 + \Lambda \sqrt{1 - \Lambda}}$$

(6)

where the different signs in front of $\Lambda$’s are due to the off-diagonal behavior in $l$ and $l'$. Then the term with coupling $\sim v^z$ in the Hamiltonian (3) is replaced by the spin dependent term

$$v^z \sigma^z_{\hat{t}l}\sigma^z_{\hat{t}l'} \delta_{\sigma\sigma'} \longrightarrow \tilde{\sigma}^z_{\sigma\sigma'}(\sigma^z_{\hat{t}l}\delta_{\sigma\sigma'} + \Lambda \delta_{l'\sigma}\sigma^z_{\sigma'})$$

(7)

where $v_z = \rho_0 V_z$, and $l, l', \sigma, \sigma'$ correspond to the orbital momentum and the real spin of the conduction electrons, respectively, and $\sigma, \sigma'$ label the TLS states.

To investigate the possibility of breaking the channel degeneracy by the spin-orbit interaction, we performed a scaling analysis in leading logarithmic approximation for general, $v^x_{\mu\rho}\sigma^x_{\sigma\sigma'}\delta_{\sigma\sigma'}$, couplings where $\mu, \nu, \rho = 0, x, y, z$, and $\sigma^0$ is the unity matrix. In the calculation we used $\rho(\varepsilon) = \rho_0(1 + \frac{\varepsilon}{\delta_0})$ for the conduction electron density of states in order to
account for the electron-hole symmetry breaking in a simple way [8, 11], (where $D_0$ is in the range of the electronic bandwidth which is not subject of scaling and $|\alpha| < 1$).

The generating diagrams of the leading logarithmic scaling equations are shown in fig. 3 and the corresponding scaling equations read as

$$\frac{\partial v^\mu}{\partial x} = -\sum_{\mu_1, \mu_2 = 0, x, y, z, \nu_1, \nu_2 = 0, x, y, z, \rho_1, \rho_2 = 0, x, y, z} \left\{ i \varepsilon^{\mu_1 \nu_1 \rho_1} v^\mu_{\nu_1 \rho_1} \varepsilon^{\mu_2 \nu_2 \rho_2} v^\mu_{\nu_2 \rho_2} \left( \varepsilon^{\nu_1 \nu_2 \nu} \varepsilon^{\rho_1 \rho_2, \rho} - \varepsilon^{\nu_2 \nu_1 \nu} \varepsilon^{\rho_1 \rho_2, \rho} \right) \right\} + \sum_{i = x, y, z} \Delta_i \frac{\alpha}{D_0} \varepsilon^{\mu_1 i \mu_2} \varepsilon^{\mu_2 i \mu_1} \left( \varepsilon^{\nu_1 \nu_2 \nu} \varepsilon^{\rho_1 \rho_2, \rho} + \varepsilon^{\nu_2 \nu_1 \nu} \varepsilon^{\rho_1 \rho_2, \rho} \right)$$

where $\varepsilon^{\mu_1 \mu_2 \mu_3}$ is the usual Levi-Civita symbol for $\mu_1, \mu_2, \mu_3 = x, y, z$, $\varepsilon^{0 \mu_1 \mu_2} = \varepsilon^{\mu_1 0 \mu_2} = \varepsilon^{\mu_1 \mu_2 0} = -i \delta_{\mu_1 \mu_2}$, and $x = \ln \frac{D_0}{D}$. We can see immediately that in the presence of electron-hole symmetry (i.e. $\alpha = 0$) we reproduce the usual TLS-electron scaling equations, thus the spin-orbit interaction cannot influence the behavior of the TLS-electron system in this case.

Together with the initial conditions ($v^\mu_{sp}(0) = \delta_{sp} \tilde{v}_s$ for $s, p = x, y, z$, $v^z_{0z}(0) = \Lambda v^z$ and the other $v$’s are zero), the above scaling equation system is closed for the subspace $\rho = 0, z$, thus we can restrict the general equations to those values and then we divide the relevant couplings to spin independent and spin dependent parts as

$$v^\mu_{\nu} := \frac{v^\mu_{\nu \uparrow} + v^\mu_{\nu \downarrow}}{2} = v^\mu_{\nu 0}$$
$$\delta v^\mu_{\nu} := \frac{v^\mu_{\nu \uparrow} - v^\mu_{\nu \downarrow}}{2} = v^\mu_{\nu z}$$

where $v^\mu_{\nu \uparrow}$ and $v^\mu_{\nu \downarrow}$ are the couplings for up and down electron spins, respectively. The scaling equations for the spin independent and spin dependent couplings then read for $s, p = x, y, z$

$$\frac{\partial v^0_{0s}}{\partial x} = -4 \sum_{i = x, y, z} \Delta_i \frac{\alpha}{D_0} (v^0_{0i \nu} v^0_{0i \nu} + v^0_{z} v^0_{z})$$
\[
\frac{\partial v_x^s}{\partial x} = -4 \sum_{i=x,y,z} \Delta^i \frac{\alpha}{D_0} (v_{0,x}^i v_{0,y}^i + v_{0,z}^i v_x^i) + 2\Delta^s \frac{\alpha}{D_0} (\sum_{q=x,y,z} (v_{0,q}^0 v_{0,z}^0 + v_{0,y}^0 v_x^0) - v_{0,y}^0 v_{0,z}^0 - v_{0,z}^0 v_x^0)
\]

\[
\frac{\partial v_p^0}{\partial x} = -4 \sum_{i=x,y,z} \Delta^i \frac{\alpha}{D_0} (v_{0,i}^0 v_{0,y}^i + v_{0,y}^0 v_{0,i}^y)
\]

\[
\frac{\partial v_x^s}{\partial x} = 2 \sum_{i,x,y,z} \delta v_{x,i}^x \delta v_{y,s}^y \delta v_{z,p}^p - 4 \sum_{i,x,y,z} \Delta^i \frac{\alpha}{D_0} (v_{0,i}^0 v_{0,y}^i + v_{0,y}^0 v_{0,i}^y)
\] + \[4\Delta^s \frac{\alpha}{D_0} (\sum_{q=x,y,z} v_{0,q}^0 v_{0,q}^0 - v_{0,y}^0 v_{0,z}^0)
\] (10)

and

\[
\frac{\partial (\delta v_0^0)}{\partial x} = -4 \sum_{i=x,y,z} \Delta^i \frac{\alpha}{D_0} (v_{0,i}^0 \delta v_{0}^0 + v_{0,y}^0 \delta v_{0}^0 + \delta v_{0}^0 v_{0}^0)
\]

\[
\frac{\partial (\delta v_y^0)}{\partial x} = -4 \sum_{i=x,y,z} \Delta^i \frac{\alpha}{D_0} (v_{0,i}^0 \delta v_{0}^0 + v_{0,y}^0 \delta v_{0}^0 + \delta v_{0}^0 v_{0}^0)
\] + \[4\Delta^s \frac{\alpha}{D_0} (\sum_{q=x,y,z} (v_{0,q}^0 \delta v_{0}^0 + v_{0,q}^0 \delta v_{0}^0) - v_{0,y}^0 \delta v_{0}^0 - v_{0,z}^0 \delta v_{0}^0)
\] (11)

where the initial values are \[v_x^0(0) = \delta s, v_p^0(0) = 0, v_y^0(0) = 0, v_0^0(0) = 0, \delta v_0^0(0) = \Delta v^z,\] and the other spin dependent couplings are zero.

After linearization in the spin dependent couplings, the scaling equations for the spin independent couplings decouple from the others. In leading order in \[\frac{\alpha}{D_0}, \frac{\alpha}{D_0} (\Delta^x = \Delta, \Delta^y = \Delta_0, \Delta z = 0\text{ according to the coordinate system used})),\] the equations and, thus, the solutions for the spin independent couplings are the usual ones

\[
v_0^0(x) = v_x^0(x) = v_y^0(x) = v_0^0(x) = 0
\]

\[
v_p^0(x) = \delta s \delta x^p(x) \text{ for } s, p = x, y, z
\] (12)

except that couplings \[v_0^0 \sim \frac{\alpha}{D_0}, v_p^0 \sim \frac{\alpha}{D_0}\] are generated.

Assuming that these solutions are isotropic \(v^x(x) = v^y(x) = v^z(x) = \Psi(x)\) as is the case around \[x = \ln \frac{\alpha}{D_0}\text{, the equations for the spin dependent couplings in leading order in }\frac{\alpha}{D_0}, \frac{\alpha}{D_0}\text{, form a differential equation system with constant coefficients which can be solved by first order perturbation theory. Although the solutions for most of the spin dependent couplings remain zero } (\delta v_0^0, \delta v_0^0, \delta v_0^0, \delta v_0^0, \delta v_0^0, \delta v_0^0, \delta v_0^0, \delta v_0^0) \text{ or unrenormalized } (\delta v_0^0), \text{ new types of couplings } \delta v_0^0, \delta v_0^0, \delta v_0^0, \delta v_0^0, \delta v_0^0, \delta v_0^0 \text{ are also generated which are spin-dependent and relevant} (\text{growing like } \Psi(x) \frac{\alpha}{D_0}, \Psi(x) \frac{\alpha}{D_0}), \text{ thus in principle they break the channel degeneracy of the two-channel orbital Kondo problem. It is important to emphasize again, that these new
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couplings are generated only if the electron-hole symmetry is broken. However, using $\frac{\alpha\Delta}{D_0}$, $\frac{\alpha\Delta_0}{D_0} \approx 10^{-5}$ in the scaling equations, they are too small to influence the two-channel behavior in an observable range of temperature.

To summarize, in this paper we examined the possibility of channel degeneracy breaking of the two-channel orbital Kondo problem by the spin-orbit interaction of the conduction electrons. The calculation was performed in the TLS model, but our analysis is also relevant for heavy fermion systems. It turned out that in case of electron-hole symmetry breaking, the interaction of the conduction electrons with a spin-orbit scatterer in a position $R$ according to the TLS, new, relevant, real spin dependent (thus channel degeneracy breaking) couplings between TLS and conduction electrons are generated. However, the corresponding crossover between the 2CK and 1CK behavior cannot be reached as the factor $\frac{\alpha\Delta}{D_0}$ or $\frac{\alpha\Delta_0}{D_0}$ is contained in the scaling equations of the channel degeneracy breaking terms, which is very small. Thus, the channel symmetry breaking is driven by $\Delta$ or $\Delta_0$, but the same quantities stop the scaling long before the crossover is reached. This situation is very similar to the commutative TLS model with impurity potential [12] where the commutative marginal line becomes unstable due to $\frac{\alpha\Delta_0}{D_0}$, but the scaling region is restricted also by the infrared cutoff $\Delta_0$ [11]. Thus, we can conclude, that although the spin-orbit interaction, in principle, can break the channel degeneracy of the two-channel orbital Kondo problem, that cannot be relevant in physical systems.

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