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Can the spin-orbit interaction break the channel degeneracy (conservation) 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 (conservation) 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 (conservation) 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.

PACS. 72.15.Cz Electrical and thermal conduction in amorphous and liquid metals and alloys – 72.10.Fk Scattering by point defects, dislocations, surfaces, and other imperfections (including Kondo effect) – 71.55.-i Impurity and defect levels

1 Introduction

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 [1–4], though it is presently unclear if the two-channel Kondo fixed point can be experimentally reached in the case of TLS's [5–7]. The particle can be an atom or a group of atoms. Similar orbital models emerge in the context of $4f$ heavy fermion impurities [2]. 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.

Similar influence of the crystalline field on the n-channel orbital Kondo problem has been investigated earlier by deriving and solving Bethe ansatz equations [8].

In this paper we examine the possibility of breaking the channel degeneracy (conservation) 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 [9], 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.

2 Model and calculation

We consider a TLS interacting with conduction electrons which are also interacting with a spin-orbit scatterer at a position $\mathbf{R}$ with respect to the TLS (see Fig. 1). The TLS-conduction electron system is described by the usual

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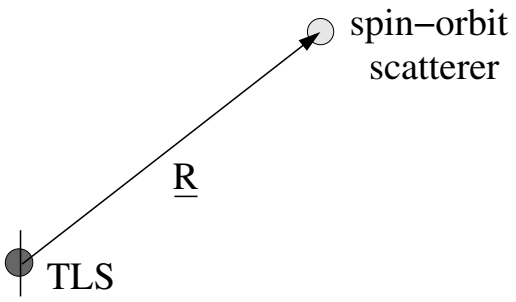

Fig. 1. The TLS and the spin-orbit scatterer in a distance **R**.

Hamilton operator [10]

$$H_{\mathrm{TLS-el}} = \sum_{k,l,m,\sigma} \varepsilon_k \, a^\dagger_{klm\sigma} a_{klm\sigma} + \Delta_0 \sigma^x_{\mathrm{TLS}} + \Delta \sigma^z_{\mathrm{TLS}} + \sum_{\substack{i=x,y,z \\ l,l' \\ k,k',\sigma}} V^i \sigma^i_{\mathrm{TLS}} a^\dagger_{kl\sigma} (\sigma^i_{el})_{ll'} a_{k'l'\sigma} \quad (1)$$

where $a^\dagger_{klm\sigma}$ creates an electron with momentum k, angular momentum l, m and spin σ, σ^i stand for the Pauli matrices, Δ_0 and Δ 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 [10].

The spin-orbit scattering is assumed to be due to spin-orbit scattering centers. In the following a single center at position **R** (see Figs. 1 and 2) is considered. In case of many scatterers the contributions are additive as the scattering strength is weak. The scattering Hamiltonian is given in two different coordinate systems, one is locked to the TLS (x, y, z) ($z \parallel$ TLS axis) and the other one to the spin-orbit center (x', y', z') ($z' \parallel \mathbf{R}$) as shown in Figure 2.

For the scattering a model Hamiltonian is used

$$H_{\mathrm{SO}} = g \sum_{\substack{k,k' \\ \sigma\sigma' \\ l,l'=0,1}} a^\dagger_{klm=0,\sigma} \sigma^y_{ll'} \sigma^y_{\sigma\sigma'} a_{k'l'm'=0,\sigma'} \quad (2)$$

where g is the coupling strength which depends on the position of the scatterer (R and angle θ in Fig. 2), the parameters of the spin-orbit scatterer's d-level, and on the strength of the spin-orbit interaction. Considering the azimuthal momentum only the channels coupled to the TLS is considered ($m = 0$), thus the angular and azimuthal momenta are defined in the coordinate system (x, y, z) locked to the TLS. For convenience the electron spin σ is defined in the system (x', y', z') at the center. The Hamiltonian H_{SO} couples the spin flip processes to the change of the angular momenta. If the center is rotated around the z axis by angle π then the direction y' is changing to the opposite. Thus in the simultaneous presence of a pair of the centers obtained by rotation the electron spin and orbital momentum are decoupled as the coupling to the two centers have opposite signs in the frame of TLS. That has an important consequence, namely only inhomogeneous distribution of the centers results in finite coupling by exhibiting certain spin direction.

The Hamiltonian given by equation (2) can be derived using specific models. Such a model was proposed in the study of magnetic spin anisotropy of a single Kondo impurity near the surface of the metal, where the spin-orbit scatterers responsible for the anisotropy are the host atoms of the metal showing an asymmetric distribution around the Kondo impurity due to the metallic surface [11]. The derivation of the Hamiltonian H_{SO} is sketched in the Appendix closely following Section 3 of reference [11].

The calculation of the correction to the electron Green's function due to spin-orbit interaction was performed using equation (2). The first order correction $\delta G^{(1)}$ in the spin-orbit coupling is given by

$$\delta G^{(1)}_{\substack{ll' \\ \sigma\sigma'}}(0, 0, i\omega_n) = G^{(0)}(0, \mathbf{R}, i\omega_n) g \sigma^y_{l'l} \sigma^y_{\sigma'\sigma} G^{(0)}(\mathbf{R}, 0, i\omega_n). \quad (3)$$

After simultaneous rotation of both coordinate systems to a new frame locked on the TLS ($x \parallel$TLS axis) and a new one at the center ($x' \parallel \mathbf{R}$) (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

$$\delta G_{\substack{ll' \\ \sigma\sigma'}}(0, 0, i\omega_n) = G^{(0)}(0, \mathbf{R}, i\omega_n) \frac{g \sigma^z_{l'l} \sigma^z_{\sigma'\sigma}}{1 - gl\sigma G^{(0)}(\mathbf{R}, \mathbf{R}, i\omega_n)} G^{(0)}(\mathbf{R}, 0, i\omega_n). \quad (4)$$

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

$$\frac{\delta \rho_R(\omega \approx 0)}{\rho_0} = \Lambda \sigma^z_{l'l} \sigma^z_{\sigma'\sigma} \quad (5)$$

where Λ depends on g, the conduction electron density of states at Fermi level for one spin direction ρ_0, and in leading order it is $\sim \frac{1}{(k_F R)^5}$, therefore only the first neighboring atoms around the TLS give non-negligible contribution.

We use the above result to examine the TLS-conduction electron system in case of finite Λ. 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

$$\begin{aligned} v^x = \rho_0 V^x \longrightarrow \tilde{v}^x = v^x \sqrt{1+\Lambda}\sqrt{1-\Lambda} \\ v^y = \rho_0 V^y \longrightarrow \tilde{v}^y = v^y \sqrt{1+\Lambda}\sqrt{1-\Lambda} \end{aligned} \quad (6)$$

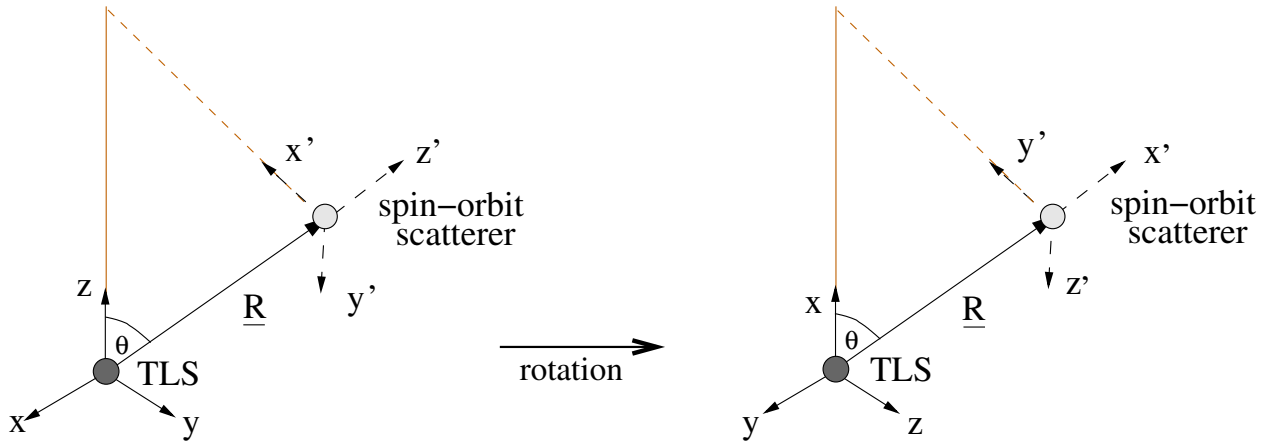

Fig. 2. The TLS (x, y, z) and the local (x', y', z') frame. The simultaneous rotations to the new TLS and the new local frame are also illustrated.

where the different signs in front of Λ's are due to the off-diagonal behavior in l and l'. Then the term with coupling $\sim v^z$ in the Hamiltonian (1) is replaced by the spin dependent term

$$v^z \sigma^z_{ll'} \sigma^z_{\alpha\alpha'} \delta_{\sigma\sigma'} \longrightarrow v^z \sigma^z_{\alpha\alpha'} (\sigma^z_{ll'} \delta_{\sigma\sigma'} + \Lambda \delta_{ll'} \sigma^z_{\sigma\sigma'}), \qquad (7)$$

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

To investigate the possibility of breaking the channel degeneracy (conservation) by the spin-orbit interaction, we performed a scaling analysis in leading logarithmic approximation for general, $v^\mu_{\nu\rho} \sigma^\mu_{\alpha'\alpha} \sigma^\nu_{l'l} \sigma^\rho_{\sigma'\sigma}$ couplings where $\mu, \nu, \rho = 0, x, y, z$, and σ^0 is the unity matrix. In the calculation we used $\rho(\varepsilon) = \rho_0(1 + \frac{\alpha\varepsilon}{D_0})$ for the conduction electron density of states in order to account for the electron-hole symmetry breaking in a simple way [9,12], (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 Figure 3 and the corresponding scaling equations read as

$$\begin{aligned} \frac{\partial v^\mu_{\nu\rho}}{\partial x} = - \sum_{\substack{\mu_1,\mu_2=0,x,y,z \\ \nu_1,\nu_2=0,x,y,z \\ \rho_1,\rho_2=0,x,y,z}} \Big\{ & i v^{\mu_1}_{\nu_1\rho_1} v^{\mu_2}_{\nu_2\rho_2} \varepsilon^{\mu_2\mu_1\mu} \\ & \times \left(\varepsilon^{\nu_1\nu_2\nu} \varepsilon^{\rho_1\rho_2\rho} - \varepsilon^{\nu_2\nu_1\nu} \varepsilon^{\rho_2\rho_1\rho} \right) \\ & + \sum_{\substack{i=x,y,z \\ \mu'=0,x,y,z}} \Delta^i \frac{\alpha}{D} v^{\mu_1}_{\nu_1\rho_1} v^{\mu_2}_{\nu_2\rho_2} \varepsilon^{\mu_2 i \mu'} \varepsilon^{\mu'\mu_1\mu} \\ & \times \left(\varepsilon^{\nu_1\nu_2\nu} \varepsilon^{\rho_1\rho_2\rho} + \varepsilon^{\nu_2\nu_1\nu} \varepsilon^{\rho_2\rho_1\rho} \right) \Big\} \end{aligned} \qquad (8)$$

where $\varepsilon^{\mu_1\mu_2\mu_3}$ is the usual Levi-Civita symbol for μ_1, μ_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.

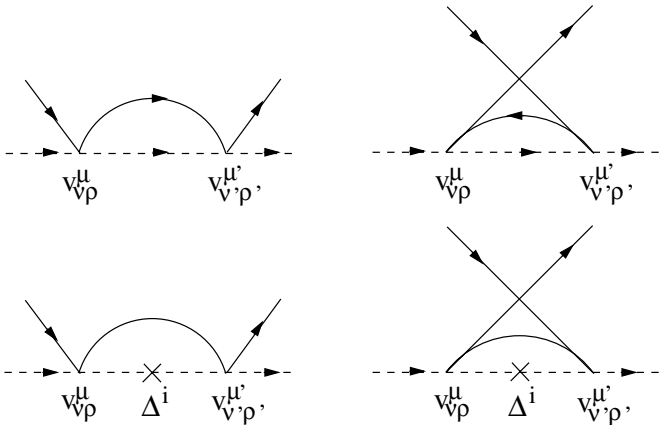

Fig. 3. The diagrams generating the leading logarithmic scaling equations. The solid and dotted lines represent the conduction electrons and the TLS, respectively, and the crosses indicate the TLS level splitting.

Together with the initial conditions ($v^s_{p0}(0) = \delta_{sp}\tilde{v}_s$ 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

$$\begin{aligned} v^\mu_\nu &:= \frac{v^\mu_{\nu\uparrow} + v^\mu_{\nu\downarrow}}{2} = v^\mu_{\nu 0} \\ \delta v^\mu_\nu &:= \frac{v^\mu_{\nu\uparrow} - v^\mu_{\nu\downarrow}}{2} = v^\mu_{\nu z} \end{aligned} \qquad (9)$$

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 $s,p=x,y,z$

$$\begin{aligned}
\frac{\partial v_0^0}{\partial x} &= -4\sum_{i=x,y,z}\Delta^i\frac{\alpha}{D_0}\left(v_0^0v_0^i+v_z^0v_z^i\right)\\
\frac{\partial v_0^s}{\partial x} &= -4\sum_{i=x,y,z}\Delta^i\frac{\alpha}{D_0}\left(v_0^sv_0^i+v_z^sv_z^i\right)\\
&\quad+2\Delta^s\frac{\alpha}{D_0}\left(\sum_{q=x,y,z}(v_0^qv_0^q+v_z^qv_z^q)-v_0^0v_0^0-v_z^0v_z^0\right)\\
\frac{\partial v_p^0}{\partial x} &= -4\sum_{i=x,y,z}\Delta^i\frac{\alpha}{D_0}\left(v_0^0v_p^i+v_p^0v_0^i\right)\\
\frac{\partial v_p^s}{\partial x} &= 2\sum_{\substack{i_1,i_2=x,y,z\\ j_1,j_2=x,y,z}}v_{j_1}^{i_1}v_{j_2}^{i_2}\varepsilon^{i_1i_2s}\varepsilon^{j_1j_2p}\\
&\quad-4\sum_{i=x,y,z}\Delta^i\frac{\alpha}{D_0}\left(v_0^sv_p^i+v_p^sv_0^i\right)\\
&\quad+4\Delta^s\frac{\alpha}{D_0}\left(\sum_{q=x,y,z}v_0^qv_p^q-v_0^0v_p^0\right)
\end{aligned}\tag{10}$$

and

$$\begin{aligned}
\frac{\partial\left(\delta v_0^0\right)}{\partial x} &= -4\sum_{i=x,y,z}\Delta^i\frac{\alpha}{D_0}\big(v_0^0\delta v_0^i+v_z^0\delta v_z^i\\
&\quad+\delta v_0^0v_0^i+\delta v_z^0v_z^i\big)\\
\frac{\partial\left(\delta v_0^s\right)}{\partial x} &= -4\sum_{i=x,y,z}\Delta^i\frac{\alpha}{D_0}\big(v_0^s\delta v_0^i+v_z^s\delta v_z^i\\
&\quad+\delta v_0^sv_0^i+\delta v_z^sv_z^i\big)\\
&\quad+4\Delta^s\frac{\alpha}{D_0}\Bigg(\sum_{q=x,y,z}(v_0^q\delta v_0^q+v_z^q\delta v_z^q)\\
&\quad-v_0^0\delta v_0^0-v_z^0\delta v_z^0\Bigg)\\
\frac{\partial\left(\delta v_p^0\right)}{\partial x} &= -4\sum_{i=x,y,z}\Delta^i\frac{\alpha}{D_0}\big(v_0^0\delta v_p^i+v_p^0\delta v_0^i\\
&\quad+\delta v_0^0v_p^i+\delta v_p^0v_0^i\big)\\
\frac{\partial\left(\delta v_p^s\right)}{\partial x} &= 4\sum_{\substack{i_1,i_2=x,y,z\\ j_1,j_2=x,y,z}}v_{j_1}^{i_1}\delta v_{j_2}^{i_2}\varepsilon^{i_1i_2s}\varepsilon^{j_1j_2p}\\
&\quad-4\sum_{i=x,y,z}\Delta^i\frac{\alpha}{D_0}\left(v_0^s\delta v_p^i+v_p^s\delta v_0^i+\delta v_0^sv_p^i+\delta v_p^sv_0^i\right)\\
&\quad+4\Delta^s\frac{\alpha}{D_0}\Bigg(\sum_{q=x,y,z}\left(v_0^q\delta v_p^q+v_p^q\delta v_0^q\right)\\
&\quad-v_0^0\delta v_p^0-v_p^0\delta v_0^0\Bigg)
\end{aligned}\tag{11}$$

where the initial values are $v_p^s(0)=\delta_{sp}\tilde{v}_s$, $v_0^s(0)=0$, $v_p^0(0)=0$, $v_0^0(0)=0$, $\delta v_0^z(0)=\Lambda v^z$, 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 $\frac{\alpha\Delta}{D_0}$, $\frac{\alpha\Delta_0}{D_0}$ ($\Delta^x=\Delta$, $\Delta^y=\Delta_0$, $\Delta_z=0$ according to the coordinate system used), the equations and, thus, the solutions for the spin independent couplings are the usual ones [2]

$$\begin{aligned}
&v_0^0(x)=v_x^0(x)=v_y^0(x)=v_z^0(x)=v_0^z(x)=0\\
&v_p^s(x)=\delta_{sp}v^p(x)\ \text{ for }\ s,p=x,y,z,
\end{aligned}\tag{12}$$

except that couplings $v_0^x\sim\frac{\alpha\Delta}{D_0}$, $v_0^y\sim\frac{\alpha\Delta_0}{D_0}$ are generated.

Assuming that these solutions are isotropic [2–4] ($v^x(x)=v^y(x)=v^z(x)=\Psi(x)$) as is the case around $x=\ln\frac{D_0}{T_K}$, the equations for the spin dependent couplings in leading order in $\frac{\alpha\Delta}{D_0}$, $\frac{\alpha\Delta_0}{D_0}$ 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 (δv_ν^0, δv_0^x, δv_0^y, δv_x^x, δv_y^x, δv_x^y, δv_y^y, δv_z^z) or unrenormalized (δv_0^z), new types of couplings δv_z^x, δv_z^y, δv_x^z, δv_y^z are also generated which are spin-dependent and relevant (growing like $\Psi(x)\frac{\alpha\Delta}{D_0}$, $\Psi(x)\frac{\alpha\Delta_0}{D_0}$), thus in principle they break the channel degeneracy (conservation) of the two-channel orbital Kondo problem. It is important to emphasize again, that these new couplings are generated only if the electron-hole symmetry is broken. However, using $\frac{\alpha\Delta}{D_0}$, $\frac{\alpha\Delta_0}{D_0}\approx10^{-5}$ in the scaling equations, they are too small to influence the two-channel behavior in an observable range of temperature.

3 Conclusions

To summarize, in this paper we examined the possibility of channel degeneracy (conservation) 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. 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 $\mathbf{R}$ according to the TLS, new, relevant, real spin dependent (thus channel degeneracy (conservation) 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 (conservation) breaking terms, which is very small. Thus, the channel symmetry breaking is driven by Δ or Δ_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 [13] 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 Δ_0 [12]. Thus, we can

conclude, that although the spin-orbit interaction, in principle, can break the channel degeneracy (conservation) of the two-channel orbital Kondo problem, that cannot be relevant in physical systems.

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Appendix

We describe the spin-orbit scatterer by an Anderson-like ($l = 2$) model with parameters ε_0 and $V_{kml'm'}(\mathbf{R})$ as [11]

$$H_{s-o} = \varepsilon_0 \sum_{m\sigma} b^\dagger_{m\sigma} b_{m\sigma} + \sum_{kl'mm'\sigma} \Big(V_{kml'm'}(\mathbf{R})\, b^\dagger_{m\sigma} a_{kl'm'\sigma} + \text{h.c.} \Big) + \lambda \sum_{\substack{mm'\\ \sigma\sigma'}} \langle m|\mathbf{L}|m'\rangle \langle \sigma|\boldsymbol{\sigma}|\sigma'\rangle b^\dagger_{m\sigma} b_{m'\sigma'} \qquad (13)$$

where $b^\dagger_{m\sigma}$ creates an electron on the spin-orbit scatterer orbital labeled by the quantum numbers m, σ and λ is the strength of the spin-orbit interaction. The hybridization matrix element, $V_{kml'm'}(\mathbf{R})$ depends on the relative position of the two coordinate systems with origin at the TLS and the spin-orbit scatterer, respectively [11] (see Fig. 2).

Considering the process in which a conduction electron with l', m', σ' jumps on the localized d-level of the atom, then the spin-orbit scattering is taken into account by the first order of the perturbation theory on the localized d-level and finally, the electron goes back to the conduction electron band with l, m, σ. That process is suitably described in the frame (x', y', z') of the center. The sum of the angular and spin momenta is conserved. As far as the conduction electron wave functions are spherical waves with center at $\mathbf{R}$, $l = l' = 2$, it is more suitable to use spherical waves centered at the TLS ($R = 0$). In this new sets $l, l' \neq 2$ occurs. In reference [11] the overlap integrals of these two sets of spherical waves are calculated. The final form of the transition amplitude is

$$W_{\substack{ll'\\ mm'\\ \sigma\sigma'}} = \frac{\lambda V^2}{\varepsilon_0^2} \big(B^+\sigma^- + B^-\sigma^+ + B^z\sigma^z \big)_{\substack{ll'\\ mm'\\ \sigma\sigma'}} \qquad (14)$$

where B^+, B^-, B^z matrices changing the azimuthal quantum numbers by $+1$, -1, 0, respectively. These quantities depend on R due to the two overlap integrals for the incoming and outgoing electrons. The overlap integrals for large distances behaves like $\sim \frac{\sin(k_F R)}{k_F R}$, $\frac{\sin(k_F R)}{(k_F R)^2}$ in channels $l = 0$, $l = 1$ (TLS frame) coupled to the TLS, respectively. Finally, the frame (x', y', z') of the spherical waves must be transformed to the TLS frame (x, y, z) (see e.g. similar Eq. (21) in Ref. [11]). In that TLS frame only the azimuthal momenta $m = m' = 0$ are coupled to the TLS. For convenience the spin variables σ, σ' are not transformed. At the end of a lengthy calculation due to the rotation, the truncated Hamiltonian (2) is obtained where only the channels coupled to the TLS are kept.

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