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Kondo effect in the presence of spin-orbit coupling

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We study the $T = 0$ Kondo physics of a spin-1/2 impurity in a non-centrosymmetric metal with spin-orbit interaction. Within a simple variational approach we compute ground state properties of the system for an *arbitrary* form of spin-orbit coupling consistent with the crystal symmetry. This coupling produces an unscreened impurity magnetic moment and can lead to a significant change of the Kondo energy. We discuss implications of this finding both for dilute impurities and for heavy-fermion materials without inversion symmetry.

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Introduction.– Kondo effect, i.e. screening of the impurity magnetic moment by the Fermi sea of itinerant electrons, is one of the best-known examples of correlations-driven phenomena in condensed matter physics[1]. A system involving a periodic array of such impurities interacting with conduction electrons (so-called Kondo lattice) is believed to provide a minimal model for heavy-fermion compounds[2]. Historically the Kondo screening was detected via resistivity measurements in dilute magnetic alloys, but recent advances in scanning tunneling spectroscopy allowed observation of this phenomenon on the atomic scale[3–5] and manipulation of individual Kondo resonances[6].

Details of the band structure of the host metal usually do not qualitatively influence the Kondo ground state, although they affect characteristic energy scales of the problem such as the Kondo temperature, T_K, below which the impurity spin is screened. Similarly, in the presence of spin-orbit scattering when spin is not a good quantum number, classification of the states by parity still allows mapping of the impurity problem onto a Kondo model with essentially same parameters but without the local SOI[7], in agreement with experiment[8,9].

In non-centrosymmetric materials a distinct non-local (dependent on the gradients of the crystal potential) spin-orbit interaction (SOI) appears. This interaction is odd in electron momentum and couples it to the electron spin[10]. The influence of this type of SOI on manifestations of the Kondo effect was discussed only recently[11–14] in quasi two-dimensional (2D) systems for specific cases of Rashba or Dresselhaus SOI, and in the context of topological insulators[15,16].

In Ref. 11 it was concluded that, to lowest order, the Rashba SOI only leads to a rescaling of the electron bandwidth and leaves the Kondo temperature essentially unchanged. A similar verdict was reached in Ref. 12 in the framework of the Anderson model for a half-filled f-band. However these results rely heavily on the specific form of the Rashba SOI term and 2D single-particle density of states. This particular combination allows reduction of the Kondo Hamiltonian with SOI (equivalent to a multichannel problem, see below) to a single-channel model without spin-orbit coupling. What happens with Kondo screening in more realistic and interesting cases, e.g. three-dimensional materials without inversion symmetry or systems with a non-Rashba SOI that do not allow the above simplification has not been explored.

In this Communication we consider a single spin-1/2 impurity interacting with a system of electrons in a non-centrosymmetric metal at zero temperature. Due to the explicit inversion symmetry breaking, the single-particle Hamiltonian that describes the conduction band contains an odd in momentum spin-orbit term compatible with the crystal symmetry[17]. We determine the ground state properties of the resulting Kondo Hamiltonian by generalizing Yosida's variational method[18] to take into account the spin-orbit splitting of the Fermi surface (FS), as well as all values of the total spin of the electrons and the impurity. In contrast with previous works[11–14] our analysis is valid for any form of SOI and the electron band structure, and incorporates the essentially multichannel nature of the problem. We give general expressions for the Kondo binding energy and show that the SOI may lead to an enhancement of the Kondo effect compared to that of a centrosymmetric material with the same parameters. Because the SOI breaks $SU(2)$ symmetry, the impurity spin no longer forms a singlet with the Fermi sea and is only partially screened. This conclusion is qualitatively similar to the situation in 2D helical metals[15]. Since our goal is to investigate only effects associated with SOI we ignore possible spin anisotropy terms analogous to those appearing in the study of impurities near sample surfaces[19].

In the next section we setup the variational framework used throughout the paper. Then we present results for the Kondo binding energy, total spin of the ground state and the impurity spin susceptibility. Our findings are put in perspective in the concluding section.

Variational formalism.– The Kondo model describes a localized magnetic impurity interacting with a single band of conduction electrons

$$H = \sum_{\boldsymbol{k}} \varepsilon_{\alpha\beta}(\boldsymbol{k}) c^\dagger_{\boldsymbol{k}\alpha} c_{\boldsymbol{k}\beta} + J_K \boldsymbol{S}\boldsymbol{\sigma}_{\alpha\beta} c^\dagger_{i_0\alpha} c_{i_0\beta}.$$

This Hamiltonian is defined on a lattice with N sites; $\boldsymbol{S}$ is the impurity spin ($S = 1/2$) located at site i_0, $\boldsymbol{\sigma}_{\alpha\beta}$

are Pauli matrices, $c^\dagger_{i\alpha}$ creates a fermion at site i with spin $\alpha=(\uparrow,\downarrow)$ ($c^\dagger_{\boldsymbol{k}\alpha}=\sqrt{1/N}\sum_i \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{x}_i}c^\dagger_{i\alpha}$ is its momentum space counterpart), and $\varepsilon_{\alpha\beta}(\boldsymbol{k})$ is the single-electron dispersion. We take $J_K>0$, assume summation over repeated indices, and set $\hbar\equiv 1$.

For a single band with SOI the matrix $\varepsilon_{\alpha\beta}(\boldsymbol{k})$ can be written[17] as:

$$\varepsilon_{\alpha\beta}(\boldsymbol{k})=\epsilon_{\boldsymbol{k}}\delta_{\alpha\beta}+\boldsymbol{\Gamma}_{\boldsymbol{k}}\boldsymbol{\sigma}_{\alpha\beta}.$$

The scalar $\epsilon_{\boldsymbol{k}}$ is the dipersion without SOI. The latter enters through the real pseudovector $\boldsymbol{\Gamma}_{\boldsymbol{k}}=-\boldsymbol{\Gamma}_{-\boldsymbol{k}}$ which is determined by the point group symmetry of the crystal. It is convenient to diagonalize $\varepsilon_{\alpha\beta}$ explicitly by introducing the helicity basis $c_{\boldsymbol{k}\alpha}=(U_{\boldsymbol{k}})_{\alpha\lambda}d_{\boldsymbol{k}\lambda}$ with $\lambda=\pm1$ and unitary matrix $U_{\boldsymbol{k}}$ such that $\boldsymbol{\Gamma}_{\boldsymbol{k}}U^\dagger_{\boldsymbol{k}}\boldsymbol{\sigma}U_{\boldsymbol{k}}=\sigma^z|\boldsymbol{\Gamma}_{\boldsymbol{k}}|$. In this representation the band energy is diagonal, $\varepsilon_{\boldsymbol{k}\lambda}=(U^\dagger_{\boldsymbol{k}})_{\lambda\alpha}\varepsilon_{\alpha\beta}(\boldsymbol{k})(U_{\boldsymbol{k}})_{\beta\lambda}=\epsilon_{\boldsymbol{k}}+\lambda|\boldsymbol{\Gamma}_{\boldsymbol{k}}|$. Note that $\boldsymbol{\Gamma}_{\boldsymbol{k}}$ breaks parity but preserves time-reversal, hence $\varepsilon_{\boldsymbol{k}\lambda}=\varepsilon_{-\boldsymbol{k},\lambda}$ because of the Kramers theorem. Now we can rewrite the Kondo Hamiltonian as:

$$H=\sum_{\boldsymbol{k},\lambda}\varepsilon_{\boldsymbol{k}\lambda}d^\dagger_{\boldsymbol{k}\lambda}d_{\boldsymbol{k}\lambda}+ \\ +\frac{J_K}{N}\sum_{\boldsymbol{k}',\boldsymbol{k}}\boldsymbol{S}\big(U^\dagger_{\boldsymbol{k}'}\boldsymbol{\sigma}U_{\boldsymbol{k}}\big)_{\lambda'\lambda}d^\dagger_{\boldsymbol{k}'\lambda'}d_{\boldsymbol{k}\lambda}. \tag{1}$$

To understand the influence of SOI on the Kondo screening, we use the Yosida-like[18] trial wavefunction

$$|\psi\rangle=\sum_{\boldsymbol{k},M,\lambda}A_{\boldsymbol{k}M\lambda}\theta(\varepsilon_{\boldsymbol{k}\lambda}-\varepsilon_F)|M\rangle d^\dagger_{\boldsymbol{k}\lambda}|\mathrm{FS}\rangle, \tag{2}$$

where $A_{\boldsymbol{k}M\lambda}$ are variational amplitudes, $M=(\uparrow,\downarrow)$ labels impurity states and $|\mathrm{FS}\rangle$ is the filled Fermi sea

$$|\mathrm{FS}\rangle=\prod_{\varepsilon_{\boldsymbol{k}+}<\varepsilon_F}d^\dagger_{\boldsymbol{k}+}\prod_{\varepsilon_{\boldsymbol{k}-}<\varepsilon_F}d^\dagger_{\boldsymbol{k}-}|0\rangle.$$

The Heaviside function $\theta(\varepsilon_{\boldsymbol{k}\lambda}-\varepsilon_F)$ limits summation to the energies above the Fermi level. The expectation value of the Hamiltonian Eq. (1) in the state $|\psi\rangle$ of Eq. (2) is

$$\langle\psi|H|\psi\rangle=\sum A^*_{\boldsymbol{k}'M'\lambda'}A_{\boldsymbol{k}M\lambda}\theta(\varepsilon_{\boldsymbol{k}'\lambda'}-\varepsilon_F)\theta(\varepsilon_{\boldsymbol{k}\lambda}-\varepsilon_F)\times \\ \times\left[\varepsilon_{\boldsymbol{k}\lambda}\delta_{\lambda'\lambda}\delta_{\boldsymbol{k}'\boldsymbol{k}}\delta_{M'M}+\frac{J_K}{N}\boldsymbol{S}_{M'M}\big(U^\dagger_{\boldsymbol{k}'}\boldsymbol{\sigma}U_{\boldsymbol{k}}\big)_{\lambda'\lambda}\right],$$

with the implicit summation over all indices in the r.h.s. In this expression we omitted the A-independent ground state energy of the Fermi sea, $E_0=\langle\mathrm{FS}|H|\mathrm{FS}\rangle$. Computing the expectation value of the Kondo interaction requires decoupling of the product

$$\langle\mathrm{FS}|d_{\boldsymbol{p}'\lambda'}d^\dagger_{\boldsymbol{k}'\alpha}d_{\boldsymbol{k}\beta}d^\dagger_{\boldsymbol{p}\lambda}|\mathrm{FS}\rangle=\theta(\varepsilon_{\boldsymbol{p}'\lambda'}-\varepsilon_F)\times \\ \times\big[\delta_{\alpha\beta}\delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\boldsymbol{p}\boldsymbol{p}'}\delta_{\lambda\lambda'}\theta(\varepsilon_F-\varepsilon_{\boldsymbol{k}\alpha})+ \\ +\delta_{\boldsymbol{k}\boldsymbol{p}}\delta_{\boldsymbol{k}'\boldsymbol{p}'}\delta_{\beta\lambda}\delta_{\alpha\lambda'}\theta(\varepsilon_{\boldsymbol{p}\lambda}-\varepsilon_F)\big].$$

In this equation the first term has the form $\sum_{\boldsymbol{k},\alpha}\theta(\varepsilon_F-\varepsilon_{\boldsymbol{k}\alpha})\big(U^\dagger_{\boldsymbol{k}}\boldsymbol{\sigma}U_{\boldsymbol{k}}\big)_{\alpha\alpha}=2\langle\mathrm{FS}|\boldsymbol{S}_e|\mathrm{FS}\rangle$, where $\boldsymbol{S}_e=(1/2)\sum_{\boldsymbol{k}}\boldsymbol{\sigma}_{\alpha\beta}c^\dagger_{\boldsymbol{k}\alpha}c_{\boldsymbol{k}\beta}$ is the total electron spin; $\langle\mathrm{FS}|\boldsymbol{S}_e|\mathrm{FS}\rangle=0$ due to the time-reversal symmetry.

Minimizing $\langle\psi|H|\psi\rangle$ w.r.t. $A_{\boldsymbol{k}M\lambda}$, one obtains an eigenvalue equation:

$$(\varepsilon_{k\lambda}-E)A_{\boldsymbol{k}M\lambda}\theta(\varepsilon_{\boldsymbol{k}\lambda}-\varepsilon_F)=-J_K\boldsymbol{S}_{MM'}\theta(\varepsilon_{\boldsymbol{k}\lambda}-\varepsilon_F)\times \\ \times\frac{1}{N}\sum_{\boldsymbol{p},\eta}\theta(\varepsilon_{\boldsymbol{p}\eta}-\varepsilon_F)\big(U^\dagger_{\boldsymbol{k}}\boldsymbol{\sigma}U_{\boldsymbol{p}}\big)_{\lambda\eta}A_{\boldsymbol{p}M'\eta}, \tag{3}$$

where again the summation over doubly repeated indices is assumed. To proceed further, we introduce

$$B_{\boldsymbol{k}M\lambda}=\sum_\eta\big(U_{\boldsymbol{k}}\big)_{\lambda\eta}\theta(\varepsilon_{\boldsymbol{k}\eta}-\varepsilon_F)A_{\boldsymbol{k}M\eta},$$

which allows us to rewrite Eq. (3) in the form

$$B_{\boldsymbol{k}M\alpha}=-J_K\boldsymbol{S}_{MR}\times \\ \times\left[\sum_\lambda\big(U_{\boldsymbol{k}}\big)_{\alpha\lambda}\frac{\theta(\varepsilon_{\boldsymbol{k}\lambda}-\varepsilon_F)}{\varepsilon_{\boldsymbol{k}\lambda}-E}\big(U^\dagger_{\boldsymbol{k}}\big)_{\lambda\beta}\right]\boldsymbol{\sigma}_{\beta\gamma}\left(\frac{1}{N}\sum_{\boldsymbol{p}}B_{\boldsymbol{p}R\gamma}\right). \tag{4}$$

This object plays the role of the ground state wavefunction for the system. Due to the θ-function in the definition of $B_{\boldsymbol{k}M\alpha}$ all $\boldsymbol{k}$-summations are over the entire Brillouin zone.

Results.– We shall now use Eqs. (2), (3), (4) to compute the Kondo energy, total spin of the system and impurity magnetic susceptibility. We apply the general expressions to several instructive examples: (i) quasi-2D systems with symmetry C_{4v} (with Rashba or Dresselhaus SOI), and (ii) cubic crystals with symmetry T or O.

Kondo energy.– The energy eigenvalue E in Eq. (3) is obtained by summing Eq. (4) over $\boldsymbol{k}$

$$X_{M\alpha}= \\ =-\frac{J_K}{N}\boldsymbol{S}_{MR}\sum_{\boldsymbol{k},\lambda}\left[\big(U_{\boldsymbol{k}}\big)_{\alpha\lambda}\frac{\theta(\varepsilon_{\boldsymbol{k}\lambda}-\varepsilon_F)}{\varepsilon_{\boldsymbol{k}\lambda}-E}\big(U^\dagger_{\boldsymbol{k}}\big)_{\lambda\beta}\right]\boldsymbol{\sigma}_{\beta\gamma}X_{R\gamma},$$

with $X_{M\alpha}=(1/N)\sum_{\boldsymbol{k}}B_{\boldsymbol{k}M\alpha}$. The λ-dependent terms between two U-matrices can be decomposed as

$$\theta(\varepsilon_{\boldsymbol{k}\lambda}-\varepsilon_F)\delta_{\lambda'\lambda}/(\varepsilon_{\boldsymbol{k}\lambda}-E)=\delta_{\lambda'\lambda}\kappa_++\sigma^z_{\lambda'\lambda}\kappa_-,$$

where

$$\kappa_\pm(\boldsymbol{k})=\frac{1}{2}\left(\frac{\theta(\varepsilon_{\boldsymbol{k}+}-\varepsilon_F)}{\varepsilon_{\boldsymbol{k}+}-E}\pm\frac{\theta(\varepsilon_{\boldsymbol{k}-}-\varepsilon_F)}{\varepsilon_{\boldsymbol{k}-}-E}\right). \tag{5}$$

Because $U_{\boldsymbol{k}}\sigma^zU^\dagger_{\boldsymbol{k}}=\boldsymbol{\Gamma}_{\boldsymbol{k}}\boldsymbol{\sigma}/|\boldsymbol{\Gamma}_{\boldsymbol{k}}|$ and $\boldsymbol{\Gamma}_{\boldsymbol{k}}$ ($\varepsilon_{\boldsymbol{k}\lambda}(\boldsymbol{k})$) is odd (even) in $\boldsymbol{k}$, the term containing $\sigma^z\kappa_-$ does not contribute to the sum and we find

$$X_{M\alpha}=-\frac{J_K}{N}\boldsymbol{S}_{MR}\boldsymbol{\sigma}_{\alpha\beta}\sum_{\boldsymbol{k}}\kappa_+X_{R\beta}. \tag{6}$$

Clearly, the lowest-energy solution has the "singlet" structure in the helicity space: $X_{M\alpha} = \big(\delta_{M\uparrow}\delta_{\alpha-} - \delta_{M\downarrow}\delta_{\alpha+}\big)/\sqrt{2}$. Then the sum is computed as

$$\frac{1}{N}\sum_{\boldsymbol{k}}\kappa_+ = \frac{1}{2}\sum_{\lambda}\int_{\varepsilon_F}^{\varepsilon_F+W}\frac{d\epsilon\, g_\lambda(\epsilon)}{\epsilon - E} \approx \frac{g_F^+ + g_F^-}{2}\ln\frac{W}{\delta E},$$

where W and $\varepsilon_F \sim W$ are the half-bandwidth and Fermi energy respectively, $\delta E = \varepsilon_F - E \ll W$, and g_F^λ is the density of states (DOS) in the λ-branch at the Fermi level. From this expression we finally obtain the energy of the Kondo bound state

$$\delta E = W\mathrm{e}^{-4/3J_K(g_F^+ + g_F^-)}. \tag{7}$$

When the SOI is absent $g_F^+ = g_F^- = g_F^{(0)}$ and Eq. (7) reduces to the well-known result for the usual Kondo effect[1]: $\delta E^{(0)} = W\exp[-2/3J_K g_F^{(0)}]$. If the characteristic SOI energy for electrons near the FS is $\Lambda_{SO} \ll \varepsilon_F$, we expand the DOS at the Fermi level up to the second order $g_F^\lambda \simeq g_F^{(0)} + \Lambda_{SO}\partial g_F^\lambda/\partial\Lambda_{SO} + \Lambda_{SO}^2\partial^2 g_F^\lambda/2\partial\Lambda_{SO}^2$, where the derivatives are evaluated at $\Lambda_{SO} = 0$. We estimate in a metal $\partial g_F^\lambda/\partial\Lambda_{SO} \sim -\lambda g_F^{(0)}/\varepsilon_F$, and $\partial^2 g_F^\lambda/\partial\Lambda_{SO}^2 \sim \pm g_F^{(0)}/\varepsilon_F^2$ with the sign depending on the curvature of the DOS around the FS. Therefore $(g_F^+ + g_F^-)/2 \sim g_F^{(0)}(1 \pm \Lambda_{SO}^2/\varepsilon_F^2)$. While in typical materials $\Lambda_{SO}/\varepsilon_F \sim 0.1$ and the above correction is only $\sim 1\%$, the exponential form of the Kondo energy, Eq. (7), makes the effect non-negligible

$$\delta E/\delta E^{(0)} = \mathrm{e}^{\pm\Lambda_{SO}^2/\varepsilon_F^2 J_K g_F^{(0)}} \simeq \mathrm{e}^{\pm\Lambda_{SO}^2/\varepsilon_F J_K}. \tag{8}$$

Assuming $\Lambda_{SO} \sim J_K$ this gives $\sim 10\%$ change in the Kondo energy relative to its value $\delta E^{(0)}$ without the SOI.

It is instructive to apply the general expressions (7) and (8) to two examples with parabolic bands (with an effective mass m) and a linear in $\boldsymbol{k}$ SOI: (i) quasi-2D tetragonal systems characterized by Rashba (Dresselhaus) spin-orbit coupling with $\boldsymbol{\Gamma}_{\boldsymbol{k}} = \Delta_{SO}[\boldsymbol{k}\times\boldsymbol{e}_z]$ ($\boldsymbol{\Gamma}_{\boldsymbol{k}} = \Delta_{SO}\boldsymbol{k}$) and tetragonal axis pointing in the z direction, and (ii) non-centrosymmetric cubic crystals[17] with $\boldsymbol{\Gamma}_{\boldsymbol{k}} = \Delta_{SO}\boldsymbol{k}$. The coupling constant Δ_{SO}, which has units of velocity, introduces a natural energy scale $\epsilon_{SO} = m\Delta_{SO}^2/2$, and is related to Λ_{SO} via $\Delta_{SO} \sim \Lambda_{SO}/k_F$ where k_F is the helicity-averaged Fermi momentum. Consequently, $\epsilon_{SO} \sim \Lambda_{SO}^2/\varepsilon_F$.

In case (i) the DOS per helicity λ and for positive energies is given by $g_\lambda(\epsilon > 0) = g_F^{(0)}[1 - \lambda\sqrt{\epsilon_{SO}/(\epsilon_{SO}+\epsilon)}]$ with $g_F^{(0)} = m/2\pi$. Consequently $g_F^+ + g_F^- = 2g_F^{(0)}$ and Eq. (7) yields no correction to the Kondo energy[11,12]: $\delta E = \delta E^{(0)}$. This conclusion is specific *solely* to 2D systems with parabolic bands and linear SOI. Of course, cubic in momentum SOI terms will introduce corrections of the form (8). In contrast, for case (ii) we have

$$g_\lambda(\epsilon > 0) = \frac{m^2\Delta_{SO}}{\pi^2}\left(\frac{1+\epsilon/2\epsilon_{SO}}{\sqrt{1+\epsilon/\epsilon_{SO}}} - \lambda\right).$$

When $\epsilon_{SO} \ll \varepsilon_F$ this DOS leads to an enhancement of the Kondo energy $\delta E/\delta E^{(0)} = \mathrm{e}^{\epsilon_{SO}/\varepsilon_F J_K g_F^{(0)}}$, in agreement with Eq. (8).

It is important to emphasize that Eqs. (7) and (8) correspond to a generally infinite channel Kondo problem even in the parabolic band approximation. Indeed, without SOI the Kondo Hamiltonian (1) can be reduced to a one-dimensional form which simply reflects the fact that only electrons with zero orbital angular momentum couple to the impurity[20]. When the SOI is taken into account, such reduction is not always possible because of the $U_{\boldsymbol{k}}$-matrices in Eq. (1) which entangle different orbital harmonics. While in systems with Rashba SOI one can still decouple orbital channels by introducing suitable linear combinations of c-operators and show that only one of them enters the Kondo term[11], other forms of SOI, e.g. case (ii) considered above, do not allow such simplification. Thus the validity of Eq. (7) is only restricted by the variational Ansatz (2).

Total spin in the ground state.– In the standard Kondo problem[1] at zero temperature the impurity is fully screened by the Fermi sea and the net spin of the system vanishes. This is not the case in the presence of a SOI. Because of the latter, even without the impurity the electron system has a non-zero spin, $\langle \mathrm{FS}|\boldsymbol{S}_e^2|\mathrm{FS}\rangle = (1/4)\sum|(U_{\boldsymbol{k}}^\dagger\boldsymbol{\sigma}U_{\boldsymbol{k}})_{\mu\nu}|^2\theta(\varepsilon_F - \varepsilon_{\boldsymbol{k}\mu})\theta(\varepsilon_{\boldsymbol{k}\nu} - \varepsilon_F)$. This expression is finite due to the mismatch between Fermi surfaces for different helicities. Therefore, our goal in this part is to compute the difference between net spins in the Kondo and normal metal phases, $\langle\psi|(\boldsymbol{S}+\boldsymbol{S}_e)^2|\psi\rangle/\langle\psi|\psi\rangle - \langle\mathrm{FS}|\boldsymbol{S}_e^2|\mathrm{FS}\rangle$. Note that due to time-reversal symmetry of the problem, the total spin polarization along any direction still vanishes.

Using Eq. (5) and the singlet structure of $X_{M\alpha}$ [see discussion after Eq. (6)], we can rewrite Eq. (4) as

$$B_{\boldsymbol{k}M\alpha} = \frac{3}{2}J_K\kappa_+ X_{M\alpha} - J_K\kappa_-\boldsymbol{S}_{MR}\big[U_{\boldsymbol{k}}\sigma^z U_{\boldsymbol{k}}^\dagger\boldsymbol{\sigma}\big]_{\alpha\gamma}X_{R\gamma},$$

so that the norm of the state (2) becomes

$$\langle\psi|\psi\rangle = \sum_{\boldsymbol{k}M\alpha}\big|A_{\boldsymbol{k}M\alpha}\big|^2\theta(\varepsilon_{\boldsymbol{k}\lambda} - \varepsilon_F) = \sum_{\boldsymbol{k}M\alpha}\big|B_{\boldsymbol{k}M\alpha}\big|^2 = \left(\frac{3J_K}{2}\right)^2\sum_{\boldsymbol{k}}\big(\kappa_+^2 + \kappa_-^2\big).$$

The cross-terms $\sim\kappa_+\kappa_-$ vanish due to the same argument as that used in deriving Eq. (6). Next, we consider the expectation value of $\boldsymbol{S}\boldsymbol{S}_e$

$$\langle\psi|\boldsymbol{S}\boldsymbol{S}_e|\psi\rangle = \frac{1}{2}\sum_{\boldsymbol{k}}B_{\boldsymbol{k}M'\alpha'}^*\boldsymbol{S}_{M'M}\boldsymbol{\sigma}_{\alpha'\alpha}B_{\boldsymbol{k}M\alpha} \equiv \equiv -\frac{3}{4}\left(\frac{3J_K}{2}\right)^2\sum_{\boldsymbol{k}}\kappa_+^2 + \frac{J_K^2}{2}\sum_{\boldsymbol{k}}\kappa_-^2 X_{R'\gamma'}^* T_{R\gamma}^{R'\gamma'}X_{R\gamma},$$

where again there are no cross-terms and $T_{R\gamma}^{R'\gamma'} = (S^iS^lS^j)_{R'R}(\sigma^iU_{\boldsymbol{k}}\sigma^zU_{\boldsymbol{k}}^\dagger\sigma^lU_{\boldsymbol{k}}\sigma^zU_{\boldsymbol{k}}^\dagger\sigma^j)_{\gamma'\gamma}$. Since $\boldsymbol{S}$ is a

spin-1/2 operator, we can evaluate T using the relations $X^*_{R'\gamma'}\sigma^a_{R'R}\sigma^b_{\gamma'\gamma}X_{R\gamma} = -\delta_{ab}$ and $\sigma^i\sigma^l\sigma^j = i\varepsilon_{ilj} + (\delta_{il}\delta_{sj} + \delta_{jl}\delta_{is} - \delta_{ls}\delta_{ij})\sigma^s$ where ε_{ilj} is the fully antisymmetric tensor:

$$T^{R'\gamma'}_{R\gamma} = \frac{1}{8}\left[(2\delta_{R'R}\delta_{\gamma'\gamma} - 3\boldsymbol{\sigma}_{R'R}\boldsymbol{\sigma}_{\gamma'\gamma}) + 2\sigma^a_{R'R}\frac{\Gamma^a_{\boldsymbol{k}}\Gamma^b_{\boldsymbol{k}}}{|\boldsymbol{\Gamma}_{\boldsymbol{k}}|^2}\sigma^b_{\gamma'\gamma}\right].$$

Collecting the above expressions we have

$$\langle\psi|\boldsymbol{S}\boldsymbol{S}_e|\psi\rangle = \frac{-3/4\sum_{\boldsymbol{k}}\kappa_+^2 + 1/4\sum_{\boldsymbol{k}}\kappa_-^2}{\sum_{\boldsymbol{k}}(\kappa_+^2+\kappa_-^2)},$$

and

$$\langle\psi|(\boldsymbol{S}+\boldsymbol{S}_e)^2|\psi\rangle - \langle \mathrm{FS}|\boldsymbol{S}_e^2|\mathrm{FS}\rangle = \frac{2\sum_{\boldsymbol{k}}\kappa_-^2}{\sum_{\boldsymbol{k}}(\kappa_+^2+\kappa_-^2)} - \\ - \frac{\sum_{\boldsymbol{k},\lambda}\theta(\varepsilon_F-\varepsilon_{\boldsymbol{k}\lambda})(\kappa_+^2+\kappa_-^2-6\lambda\kappa_+\kappa_-)}{4\sum_{\boldsymbol{k}}(\kappa_+^2+\kappa_-^2)},$$

with the second term in the r.h.s. coming from $\langle\psi|\boldsymbol{S}_e^2|\psi\rangle$. In the absence of spin-orbit band splitting $\kappa_- \equiv 0$ and the above expression implies complete screening. In the presence of SOI the change in the total spin is also finite and for cases (i) and (ii) considered above $\langle\psi|(\boldsymbol{S}+\boldsymbol{S}_e)^2|\psi\rangle - \langle \mathrm{FS}|\boldsymbol{S}_e^2|\mathrm{FS}\rangle \sim \Delta_{SO}^2$. In principle this change can be determined from local magnetic measurements, but more precise methods than the one used here may be needed to determine spatial dependence of the spin-spin correlations.

Impurity spin susceptibility.– Finally, we consider the linear susceptibility of the system. Since our focus is on the effect of SOI, we shall make a simplifying assumption that the system is either cubic or tetragonal with magnetic field pointing along the c-axis, and that the dominant effect of the field is on the impurity spin. In both cases the Hamiltonian, Eq. (1), acquires a perturbation $\delta H = -\mu B S_z$, where $\mu = g\mu_B$, μ_B is the Bohr magneton and g is the appropriate Lande factor.

In order to account for δH we need to change $E \to E + hM$ in Eqs. (4) and (6) with $h \equiv \mu B/2$ and $M = \pm 1$. A solution is sought in the form: $X_{M\alpha} = x_s Y^s_{M\alpha} + x_t Y^t_{M\alpha}$ with Y^s (Y^t) the normalized singlet (triplet with zero total spin z-projection) basis states.

$$\begin{pmatrix} 1-3P & Q \\ -3Q & 1+P \end{pmatrix}\begin{pmatrix} x_s \\ x_t \end{pmatrix} = 0,$$

where $P = (J_K/4N)\sum_{\boldsymbol{k},M}\kappa_+(E+hM)$ and $Q = (J_K/4N)\sum_{\boldsymbol{k},M}M\kappa_+(E+hM)$. To lowest order in $\mu B/\delta E$, the ground state energy becomes $E = \varepsilon_F - \delta E - \mu^2B^2/8\delta E$. Therefore changes in the Kondo energy (7) are straightforwardly reflected in the spin susceptibility

$$\chi = -\partial^2 E/2\partial B^2 = \mu^2/8\delta E.$$

Discussion.– Stimulated by the interest in non-centrosymmetric f-electron materials[2,21], we investigated the influence of the lack of inversion symmetry on interaction between conduction and localized electrons by studying a single impurity Kondo model with a SOI in the conduction band. Using a simple variational framework[1,18] we presented results for the ground-state properties of the system, valid for *any* form of SOI and band structure of the host metal, even in cases when one cannot reduce the problem to a single-channel Kondo Hamiltonian. It is the variational nature of our approach, what allows us to deal with a multichannel model. In particular, we demonstrated that: (1) the SOI can lead to an *exponential* change of the Kondo temperature; (2) as the SOI explicitly breaks $SU(2)$ symmetry the Fermi sea does not completely screen the impurity spin, allowing an extra magnetic degree of freedom in the Kondo phase.

Although a similar exponential enhancement of the Kondo temperature was found in Ref. 12, we note that their result is physically different from ours. The reason for this distinction is the fact that in Ref. 12 the authors started from an Anderson model and used a Schrieffer-Wolff transformation[22]. Although this is the usual way to "freeze" charge fluctuations at the impurity, in the presence of SOI it can lead to unexpected results, such as the Dzyaloshinky-Moriya coupling between impurity and conduction electrons spins, which appears because of virtual transitions of localized electrons into the conduction band where they accumulate a phase due to SOI. On the contrary we started with a Kondo model that includes only spin fluctuations. Thus modifications to the Kondo energy, Eq. (7), compared to its value in a centrosymmetric material originates *purely* from SOI.

Our findings lead to an intriguing question regarding the influence of SOI on the physics of the spin-1/2 Kondo lattice model. It is known[2,23] that the heavy-fermion (Kondo screened) state competes with magnetic phases. In the presence of a SOI impurity spins are not completely screened[24] and may order, thus leading to a coexistence of the heavy fermion state and magnetism. We leave investigation of this problem for a future work.

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