Anderson impurity in the bulk of topological insulators

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When an Anderson impurity is immersed in the bulk of a topological insulator that has an “inverted-Mexican-hat” band dispersion, a Kondo resonant peak appears simultaneously with an in-gap bound state. The latter generates another spin state thereby screening the Kondo effect. Using a weak-coupling RG scheme, it is shown that the system exhibits complex crossover behavior between different symmetry configurations and may evolve into a self-screened Kondo or an $SO(n)$ ($n = 3, 4$) low-energy fixed point. Experimental consequences of these scenarios are pointed out.

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I. INTRODUCTION

The significance of topological insulators (TIs) as a new state of matter has been stressed in numerous publications [1–7]. So far, the main attention has been focused on the surface states [8–24]. It was pointed out recently that impurity scattering may have nontrivial effects in the *bulk* of TIs due to its peculiar band structure [25–28]. More concretely, in topological insulators with “inverted-Mexican-hat” band dispersion around the Γ point, in-gap bound states occur due to impurities from which band electrons are scattered (even with arbitrary weak scattering rate) [25]. In the case of magnetic (Anderson) impurities (forming localized moments) the associated Kondo physics in bulk TIs is profoundly distinct from its metallic analog. Using a slave-boson mean-field theory [26], it was shown that an antiferromagnetic exchange interaction $\sim J_{df} \mathbf{S}_d \cdot \mathbf{S}_f$ (with $J_{df} > 0$) between the spins of the Anderson impurity d and the induced midgap bound state f leads to a self-screened Kondo effect (KE) [26]. In fact, the physics described above is not limited to TIs but is a general consequence of insulators (and semiconductors) with a large electronic density of states at the band edge such that in-gap bound states are easily induced by an Anderson impurity.

The goal of this work is to perform a detailed analysis of the interplay between the Anderson impurity and its induced in-gap bound state in bulk TIs, and, in particular, elucidate the observable quantities (such as conductivity and magnetic susceptibility) related to the underlying Kondo physics. Employing a weak-coupling renormalization group (RG) analysis, we show that the system exhibits complex crossover behavior between different symmetry sectors and that the exchange interaction J_{df} between the d and f spins may be renormalized dynamically to a negative value at suitable parameter regime. In this case the KE is not screened and the low-energy physics of the system is described by an $SU(2)$, $SO(4)$, or $SO(3)$ Kondo fixed point. The temperature dependence of the impurity-induced resistance and magnetic susceptibility is studied at various regimes.

The article is organized as follows. In Sec. II, we introduce the model considered starting from a bare Anderson-type Hamiltonian. It is shown that the presence of an Anderson impurity d leads to potential scattering of the conduction band electrons, that, in turn, brings about the formation of an in-gap localized quantum state f . We introduce the singlet and triplet

states of the composite ($d + f$) impurity. At the end of Sec. II we arrive at an effective Anderson Hamiltonian that will be analyzed further in the next sections. The local density of states (DOS) is calculated in Sec. III for the TI with the potential scattering term. Renormalization group analysis is carried out in Sec. IV. Depending on various energy domains, the RG analysis ends up with various Kondo Hamiltonians that possess different (dynamical) symmetries, $SU(2)$, $SO(3)$, or $SO(4)$. Section V is devoted to the calculations of electric resistivity and magnetic susceptibility in the relevant energy domains. One of the central results of our work is the occurrence of temperature-driven crossovers of the KE between different symmetry classes. The results are then summarized in Sec. VI. Some details of the calculation technique are presented in the appendices. These include physical origin of the potential scattering induced by an Anderson impurity (Appendix A), discussion of local density of states (Appendix B), the $SO(4)$ Kondo Hamiltonian (Appendix C), and finally, calculations of electric resistivity (Appendix D) and magnetic susceptibility (Appendix E) for different temperature intervals.

II. MODEL HAMILTONIAN

Our aim in this section is to derive an effective Hamiltonian that, in addition to the Anderson impurity d , contains also the midgap state f as discussed in Ref. [26]. Starting from a Hamiltonian describing an Anderson impurity d in the bulk of a TI, a few manipulations are required to transform it into its workable form, Eq. (15a) below. The bare Hamiltonian is

$$H = H_0 + H_d + H_t^{(0)} + V. \quad (1)$$

Here the first term, H_0 , describes electrons in the bulk of the TI,

$$\begin{aligned} H_0 &= \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger h_0(\mathbf{k}) \Psi_{\mathbf{k}}, \\ h_0(\mathbf{k}) &= \hbar v_F (\mathbf{k} \cdot \boldsymbol{\alpha}) + \beta M_k, \\ \Psi_{\mathbf{k}}^\dagger &= (a_{\mathbf{k}\uparrow}^\dagger, a_{\mathbf{k}\downarrow}^\dagger, b_{\mathbf{k}\uparrow}^\dagger, b_{\mathbf{k}\downarrow}^\dagger), \end{aligned} \quad (2)$$

where $M_k = m v_F^2 - B \hbar^2 k^2$, and $a_{\mathbf{k}\sigma}^\dagger$, $b_{\mathbf{k}\sigma}^\dagger$ are creation operators for electron of momentum $\mathbf{k}$ and spin projection σ . $h_0(\mathbf{k})$ is written in particle-hole $\otimes$ spin space, with $\boldsymbol{\alpha} = t_x \otimes \mathbf{s}$ and $\beta = t_z \otimes s_0$, where $\mathbf{t} = (t_x, t_y, t_z)$ or $\mathbf{s} = (s_x, s_y, s_z)$ are vectors

of the Pauli matrices acting in the space of isospins or spins; s_0 is the 2×2 identity matrix. H_d is the Hamiltonian for the Anderson impurity,

$$H_d = \epsilon_d \sum_{\sigma} n_{d\sigma} + U_d n_{d\uparrow} n_{d\downarrow}, \quad (3)$$

where ϵ_d is the impurity energy level and U_d is the interaction between electrons on the impurity. $n_{d\sigma} = d_{\sigma}^{\dagger} d_{\sigma}$; $d_{\sigma}^{\dagger}$ or d_{σ} is the creation or annihilation operator of the electron on the d level. The hybridization between the Anderson impurity d and the band electrons is described by

$$H_t^{(0)} = V_d \sum_{\mathbf{k}, \sigma} (a_{\mathbf{k}\sigma}^{\dagger} d_{\sigma} - i b_{\mathbf{k}\sigma}^{\dagger} d_{\sigma} + \text{H.c.}). \quad (4)$$

The last term appearing in the Hamiltonian (1) is an effective potential scattering between band electrons induced by the impurity,

$$V = V_0 \sum_{\mathbf{k}, \mathbf{k}'} (a_{\mathbf{k}\sigma}^{\dagger} - i b_{\mathbf{k}\sigma}^{\dagger})(a_{\mathbf{k}'\sigma} + i b_{\mathbf{k}'\sigma}). \quad (5)$$

A few words on the origin of the potential scattering term V are in order. When an Anderson impurity is immersed in a metal it leads to an s - d Hamiltonian and to a potential scattering. In the standard analysis of the Anderson impurity, the induced potential scattering term is neglected because it is irrelevant as far as Kondo physics is concerned. The situation is different when the impurity is immersed in an insulator. Here, as we shall see in the following, the potential scattering leads to a midgap bound state that profoundly affects the underlying physics. The detailed discussions about the physical origin of the strength V_0 and the derivation of the localized in-gap f level are given in Appendix A.

Diagonalization of H_0 . The eigenstate of H_0 alone is given by

$$H_0 = \sum_{\nu \sigma \mathbf{k}} \nu \epsilon_k \gamma_{\nu \mathbf{k}\sigma}^{\dagger} \gamma_{\nu \mathbf{k}\sigma}, \quad (6a)$$

where $\nu = \pm 1$ or c/v denotes the conduction and valence band.

$$\epsilon_k = \sqrt{M_k^2 + (\hbar v_F k)^2}, \quad M_k = m v_F^2 - B \hbar^2 k^2, \quad (6b)$$

is the band dispersion. $\gamma_{\nu \mathbf{k}\sigma}^{\dagger}$ and $\gamma_{\nu \mathbf{k}\sigma}$ are creation and annihilation operators of quasiparticle defined through the transformation

$$\begin{aligned} \tilde{\Psi}_{\mathbf{k}} &= \mathcal{S}_{\mathbf{k}} \mathcal{U}_{\mathbf{k}} \Psi_{\mathbf{k}}, \quad \tilde{\Psi}_{\mathbf{k}}^{\dagger} = (\gamma_{c\mathbf{k}\uparrow}, \gamma_{c\mathbf{k}\downarrow}, \gamma_{v\mathbf{k}\uparrow}, \gamma_{v\mathbf{k}\downarrow}), \\ \mathcal{U}_{\mathbf{k}} &= \cos \frac{\alpha_k}{2} + i \sin \frac{\alpha_k}{2} t_y \otimes (\mathbf{s} \cdot \mathbf{e}_k), \end{aligned} \quad (6c)$$

where $\mathbf{e}_k = \mathbf{k}/k$,

$$\tan \left(\frac{\alpha_k}{2} \right) = \sqrt{\frac{\epsilon_k - M_k}{\epsilon_k + M_k}}.$$

$\mathcal{S}_{\mathbf{k}}$ is a unitary matrix which commutes with $h_0(\mathbf{k})$ and $\mathcal{U}_{\mathbf{k}}$. ϵ_k is gapped and the insulator is topological for $Bm > 0$. For $Bm > 1/2$ (assumed hereafter), the band dispersion has an “inverted-Mexican-hat” form (see Fig. 1) with dispersion minimum at a

FIG. 1. (Color online) Energy dispersion (6b) for $Bm = 20$. The dark (bright) regions denote the energy levels below (above) the Fermi energy ϵ_F . The band-edges occur at momentum q at energies $\pm \epsilon_q$. (Here it is assumed that $\epsilon_q < \epsilon_F < m v_F^2$.) k_1 and k_2 are two solutions of the equation $\epsilon_k = \epsilon_F$.

surface of nonzero wave-vector $\mathbf{q}$'s, with

$$\epsilon_q = \frac{v_F^2}{2B} \sqrt{4Bm - 1}, \quad q = \frac{v_F}{\hbar B} \sqrt{Bm - \frac{1}{2}}, \quad (7)$$

where $q = |\mathbf{q}|$.

Transformation of $H_t^{(0)}$ and V . Here we express the terms $H_t^{(0)}$ and V defined in Eqs. (4) and (5) in terms of the quasiparticle operators. Applying the unitary transformation (6c) to the tunnel Hamiltonian (4), we get

$$H_t = \sum_{\mathbf{k}} \left\{ \tilde{\Psi}_{\mathbf{k}}^{\dagger} \mathcal{S}_{\mathbf{k}} \begin{pmatrix} \mathcal{V}_{\mathbf{k}} \\ -i \mathcal{V}_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} d_{\uparrow} \\ d_{\downarrow} \end{pmatrix} + \text{H.c.} \right\},$$

where $\mathcal{V}_{\mathbf{k}}$ is a 2×2 unitary matrix,

$$\mathcal{V}_{\mathbf{k}} = \cos \alpha_k - i \sin \alpha_k (\mathbf{s} \cdot \mathbf{e}_k), \quad \mathcal{V}_{\mathbf{k}}^{\dagger} \mathcal{V}_{\mathbf{k}} = 1.$$

Choosing $\mathcal{S}_{\mathbf{k}}$ as

$$\mathcal{S}_{\mathbf{k}} = \begin{pmatrix} \mathcal{V}_{\mathbf{k}}^{\dagger} & 0 \\ 0 & i \mathcal{V}_{\mathbf{k}} \end{pmatrix}, \quad (8)$$

we get

$$H_t = V_d \sum_{\mathbf{k}, \nu, \sigma} (\gamma_{\nu \mathbf{k}\sigma}^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} \gamma_{\nu \mathbf{k}\sigma}). \quad (9)$$

Applying transformations (6c) and (8) to the potential scattering Hamiltonian (5), we get

$$V = V_0 \sum_{\nu \nu' \mathbf{k} \mathbf{k}'} \gamma_{\nu \mathbf{k}\sigma}^{\dagger} \gamma_{\nu' \mathbf{k}'\sigma}.$$

Diagonalization of $H_0 + V$: Midgap state. The next step is crucial, as it demonstrates the formation of a midgap state f due to the potential scattering term V . Because the potential V emerges due to the Anderson impurity, we say that the midgap state is induced by the impurity. In order to find the eigenstates of $H_0 + V$, we solve the Heisenberg equation of motion

$$i \hbar \dot{\gamma}_{\nu \mathbf{k}\sigma} = [H_0 + V, \gamma_{\nu \mathbf{k}\sigma}].$$

Taking $\gamma_{\nu \mathbf{k}\sigma}(t) = \gamma_{\nu \mathbf{k}\sigma} e^{-i \epsilon t / \hbar}$, we get

$$\epsilon \gamma_{\nu \mathbf{k}\sigma} = \nu \epsilon_k \gamma_{\nu \mathbf{k}\sigma} + V_0 \sum_{\nu' \mathbf{k}'} \gamma_{\nu' \mathbf{k}'\sigma}. \quad (10)$$

Equation (10) has a nontrivial solution when ϵ satisfies the secular equation,

$$\sum_{\mathbf{v}\mathbf{k}} \frac{V_0}{\epsilon - v\epsilon_k} = 1. \quad (11)$$

The solutions for $|\epsilon| \geq \epsilon_q$ describe the band electrons, whereas the solution for $|\epsilon| < \epsilon_q$ corresponds to the localized f level.

It is seen that when $|\epsilon| < \epsilon_q$, the expression on the left-hand side of the secular equation (11) is positive when ϵ is negative and negative when ϵ is positive (V_0 is assumed to be positive here). When $|\epsilon| \rightarrow \epsilon_q$, the sum diverges as $(\epsilon_q^2 - \epsilon^2)^{-1/2} \text{sign}(-\epsilon)$ for energy bands with the “inverted Mexican hat” structure [26]. As a result, the secular equation gives us a midgap energy level ϵ_f which lies within the interval $-\epsilon_q < \epsilon_f < 0$. When $\epsilon_f + \epsilon_q \ll \epsilon_q$, we can write

$$\epsilon_f \approx -\epsilon_q \sqrt{1 - \left(\frac{V_0 q}{2\pi \hbar^2 B} \right)^2}. \quad (12)$$

This procedure leads to a minor modification of the annihilation and creation operators for the band electrons. Strictly speaking they are respectively expressed as a linear combination of $\gamma_{\mathbf{v}\mathbf{k}\sigma}$ and $\gamma_{\mathbf{v}\mathbf{k}\sigma}^\dagger$ using perturbation theory with V_0 as a small parameter. However, since the potential pulls only one level (out of many) from the band into the gap, the other levels are virtually unaffected. In what follows, we assume that the operators for the modified levels inside the band just slightly differ from the $\gamma_{\mathbf{v}\mathbf{k}\sigma}$ and $\gamma_{\mathbf{v}\mathbf{k}\sigma}^\dagger$. Thus, the main outcome of the potential scattering is the creation of a midgap level f . The annihilation operator f_σ for this localized level is given by

$$f_\sigma = \sum_{\mathbf{v}\mathbf{k}} \frac{AV_0}{\epsilon_f - v\epsilon_k} \gamma_{\mathbf{v}\mathbf{k}\sigma}, \quad A = \left(\sum_{\mathbf{v}\mathbf{k}} \frac{V_0^2}{(\epsilon_f - v\epsilon_k)^2} \right)^{-1/2}. \quad (13)$$

Hybridization term H_{df} . The last ingredient in our quest for constructing an effective tunneling Hamiltonian with d and f impurities is to identify a hopping term H_{df} between the Anderson impurity and the midgap state. The hybridization term $H_t^{(0)}$ between the bulk TI electrons and the d -impurity level leads to an effective tunneling term H_{df} between the d impurity and the f in-gap bound state, and an effective tunneling term H_t between the d impurity and the band states. We assume that H_t is still given by Eq. (9), whereas H_{df} is

$$H_{df} = V_{df} \sum_{\sigma} (f_\sigma^\dagger d_\sigma + d_\sigma^\dagger f_\sigma), \quad (14)$$

where $V_{df} \sim V_d$.

The effective Hamiltonian. Finally, to arrive at the desired effective tunneling Hamiltonian we collect all pieces into a sum of three parts structured as “band + composite impurity + hybridization” Hamiltonians,

$$H = H_l + H_C + H_t. \quad (15a)$$

Here $H_l = H_0 + V$ is the Hamiltonian of the two band electrons that includes also the potential scattering term, and

$$H_C = H_d + H_f + H_{df} \quad (15b)$$

is the Hamiltonian of the composite impurity, including the d and f levels. H_d is given by Eq. (3), H_{df} is given by Eq. (14), and

$$H_f = \epsilon_f \sum_{\sigma} n_{f\sigma} + U_f n_{f\uparrow} n_{f\downarrow}, \quad (15c)$$

where ϵ_f is the single-electron energy (12) of the localized f level, U_f is the interaction between electrons on the f level, and $n_{f\sigma} = f_\sigma^\dagger f_\sigma$. The hybridization term H_t is given by Eq. (9).

Energy scales. A few words about energy scales are in order: Unless otherwise specified, we shall assume $U_d \rightarrow \infty$ and

$$\epsilon_F - D_0 < \epsilon_d \ll \epsilon_f < \epsilon_F < \epsilon_f + U_f \ll \epsilon_F + D_0, \quad (16)$$

where D_0 (the initial bandwidth) is the highest energy cutoff, and ϵ_F is the Fermi energy (see Fig. 1). We use $\epsilon_F = 2\epsilon_q$, $\epsilon_f \approx -\epsilon_q$, $U_f = 5\epsilon_q$, and $\epsilon_d = -80\epsilon_q$ in the following calculations.

The eigenstates of H_C . Equation (15b) are specified by the configuration numbers (N_d, N_f) representing the number of electrons on the levels d and f . With energy scales specified by (16) the ground state has $N_d = N_f = 1$ and there are four possible states, a spin-singlet state $|S\rangle$ and three spin-triplet states $|T_m\rangle$ ($m = 0, \pm 1$). The singlet energy is modified when $V_{df} \neq 0$ while the triplet energy is unaffected. Explicitly,

$$|S\rangle = \left\{ \frac{\alpha_S}{\sqrt{2}} (d_\uparrow^\dagger f_\downarrow^\dagger - d_\downarrow^\dagger f_\uparrow^\dagger) - \beta_f f_\uparrow^\dagger f_\downarrow^\dagger \right\} |0\rangle, \quad (17a)$$

$$|T_1\rangle = d_\uparrow^\dagger f_\uparrow^\dagger |0\rangle, \quad |T_{-1}\rangle = d_\downarrow^\dagger f_\downarrow^\dagger |0\rangle, \quad (17b)$$

$$|T_0\rangle = \frac{1}{\sqrt{2}} \{d_\uparrow^\dagger f_\downarrow^\dagger + d_\downarrow^\dagger f_\uparrow^\dagger\} |0\rangle,$$

where

$$\epsilon_S = \epsilon_d + \epsilon_f - \frac{2V_{df}^2}{\Delta_f}, \quad \epsilon_T = \epsilon_d + \epsilon_f,$$

$$\alpha_S = \sqrt{1 - \beta_f^2}, \quad \beta_f = \frac{\sqrt{2}V_{df}}{\Delta_f},$$

$$\Delta_f = \epsilon_f - \epsilon_d + U_f.$$

In the absence of hybridization of the d electron with the band electrons (i.e., when $V_d = 0$), $\epsilon_S < \epsilon_T$, and the spin singlet state has lower energy.

III. LOCAL DENSITY OF STATES

Because of the potential scattering, the local density of states (DOS) depends on the energy ϵ of an electron and on the distance r from the impurity,

$$\rho(\epsilon, r) = -\frac{1}{\pi} \text{Im} \sum_{\mathbf{v}\mathbf{k}, \mathbf{v}'\mathbf{k}'} G_{\mathbf{v}\mathbf{k}, \mathbf{v}'\mathbf{k}'}(\epsilon) e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}}, \quad (18)$$

$$G_{\mathbf{v}\mathbf{k}, \mathbf{v}'\mathbf{k}'}(\epsilon) = \int \tilde{G}_{\mathbf{v}\mathbf{k}, \mathbf{v}'\mathbf{k}'}(t) e^{\frac{i(\epsilon-\eta)t}{\hbar}} dt. \quad (19)$$

FIG. 2. (Color online) Local DOS (21) for $\epsilon_0 = 24\epsilon_q$, $V_0\rho_c = 0.06$, and different values of qr .

Here η is a positive infinitesimal parameter, $\tilde{G}_{\nu\mathbf{k},\nu'\mathbf{k}'}(t)$ is a retarded Green's function,

$$\tilde{G}_{\nu\mathbf{k},\nu'\mathbf{k}'}(t) = -\frac{i}{\hbar} \Theta(t) \langle \{ \gamma_{\nu\mathbf{k}\sigma}(t), \gamma_{\nu'\mathbf{k}'\sigma}^\dagger \} \rangle, \quad (20)$$

where $\langle \dots \rangle$ denotes the thermal average with respect to the Hamiltonian $H_0 + V$.

Applying the Heisenberg equation of motion (10), we get the following expression for the local DOS:

$$\rho(\epsilon, r) = \rho_0(\epsilon) \frac{1 + \pi^2 V_0^2 [\rho_0^2(\epsilon) - \rho_0^2(\epsilon, r)]}{1 + \pi^2 V_0^2 \rho_0^2(\epsilon)}, \quad (21)$$

where

$$\begin{aligned} \rho_0(\epsilon, r) &= \Theta(|\epsilon| - \epsilon_q) \frac{\rho_c |\epsilon|}{2\sqrt{\epsilon^2 - \epsilon_q^2}} \\ &\times \left\{ \Theta(\epsilon_0 - |\epsilon|) \frac{\sin(qr g_1(\epsilon))}{qr} + \frac{\sin(qr g_2(\epsilon))}{qr} \right\}, \\ \rho_0(\epsilon) &= \rho_0(\epsilon, 0). \end{aligned} \quad (22)$$

Detailed derivation of the local DOS is given in Appendix B.

The local DOS (21) is shown in Fig. 2 for different values of qr . It is seen that $\rho(\epsilon, 0)$ vanishes as $(\epsilon^2 - \epsilon_q^2)^{1/2}$ when $|\epsilon| \rightarrow \epsilon_q$. When $qr > 2$, $\rho(\epsilon, r)$ approaches $\rho_0(\epsilon)$, the bare DOS.

IV. RENORMALIZATION-GROUP (RG) ANALYSIS

Within RG analysis, high-energy charge fluctuations are integrated out and one reaches a low-energy spin (s - d) Hamiltonian. The latter is written in terms of the spin operator $\mathbf{s}$ of the band electrons and a collection of vector operators of the composite impurity. These vector operators generate a dynamical symmetry group that characterize the pertinent Kondo physics [34]. If the ground state of H_C contains a single electron the symmetry group is SU(2), while if the ground state of H_C contains two electrons the symmetry group can be SO(3) [see Eq. (37)] or SO(4) [see Eq. (32)]. Technically, the high-energy degrees of freedom are successively integrated out such that $D_0 \rightarrow D < D_0$ is reduced and energies are renormalized. For the Kondo effect in metals, where the DOS is virtually constant, this is a standard procedure. The fact that $\rho(\epsilon) \neq \text{constant}$ requires some modifications. We introduce

FIG. 3. (Color online) Parametric diagram $j - D$ for $\epsilon_d = -80\epsilon_q$, $\epsilon_0 = 24\epsilon_q$, and $\epsilon_F = 2\epsilon_q$. The curves separate the different temperature intervals: the red curve is $D_i = \epsilon_F - \epsilon_d$ separating the regimes (i) [mixed valence regime] and (ii) [SU(2) Kondo regime], the purple line is D_{ii} separating the regimes (ii) [SU(2) Kondo regime] and (iii) [SO(4) Kondo regime], the blue curve is $D_{iii} = |J_{df}|$ [$J_{df} < 0$] separating the regimes (iii) [SO(4) Kondo regime] and (iv) [SO(3) Kondo regime], whereas the green curve is $D_{iv} = |J_{df}|$ [$J_{df} > 0$] separating the regimes (iv) [SO(4) Kondo regime] and (v) [self-screened Kondo regime].

the following definitions:

$$\bar{\rho}(D) = \frac{1}{2} [\rho(\epsilon_F + D) + \rho(\epsilon_F - D)], \quad (23)$$

$$\mathcal{L}(D_1, D_2) = \int_{D_1}^{D_2} \frac{2\bar{\rho}(D)dD}{\rho_c D}. \quad (24)$$

The RG flow is divided into the following regimes (see Fig. 3):

- (i) $\epsilon_d > \epsilon_F - D > \epsilon_F - D_0$, in which charge fluctuations in both d and f states exist and there is no KE;
- (ii) $\epsilon_F - D > \epsilon_d$ but $\epsilon_f(\sim -\epsilon_q) > \epsilon_F - D$ or $\epsilon_F + D > 2\epsilon_f + U_f$, where charge fluctuations on the d orbital are quenched but still exist on the f orbital. The system is in the single impurity [SU(2)] Kondo impurity regime;
- (iii) $\epsilon_F - D > \epsilon_f$ and $\epsilon_F + D < 2\epsilon_f + U_f$, but $D > |J_{df}|$ where charge fluctuations in both d and f orbitals are quenched, but the singlet-triplet energy splitting can be neglected. The singlet and triplet states can be considered as degenerate and the system demonstrates the SO(4) Kondo regime.
- (iv, v) The system is at the SO(3) Kondo regime [if $J_{df} < 0$, interval (iv)] or the self-screened Kondo regime [if $J_{df} > 0$, interval (v)]. These regimes exist only if $U_f > \epsilon_F - 2\epsilon_f \sim$ a few ϵ_q .

The RG analysis for the various regimes now follows.

Regime (i). Charge fluctuations on the d orbital are integrated out as in Ref. [29], but here the spin-singlet and spin-triplet energies are, generically, renormalized distinctly. Renormalization of other quantities such as V , ϵ_f , and V_{df} are weak and can be ignored. The scaling procedure of $\epsilon_{S(T)}$ then yields [31,32]

$$\frac{d\epsilon_{S(T)}}{d \ln D} = V_{S(T)}^2 \rho(\epsilon_F + D), \quad (25)$$

where $V_S^2 = \alpha_S^2 V_d^2$ and $V_T^2 = V_d^2$. The difference between V_S^2 and V_T^2 originates from the appearance of the normalization factor α_S in the singlet state [see (17a)]. Notice that $V_S^2 < V_T^2$ and the triplet energy level renormalizes faster than the singlet level. This opens the possibility that as RG stops, the ground state of the system may become a triplet if the single-triplet level crossing occurs before quenching of charge fluctuations in the d and f levels. Solving Eq. (25), we find that the singlet-triplet energy spacing $J_{df}^{(i)}(D) = \varepsilon_T(D) - \varepsilon_S(D)$ is given by

$$J_{df}^{(i)}(D) \sim \beta_f^2 \Delta_f \left(1 - \frac{2V_d^2 \rho_0 \sqrt{D_0} - \sqrt{D}}{\Delta_f \sqrt{\varepsilon_0}} \right), \quad (26)$$

where $D = D_i \sim \epsilon_F - \epsilon_d$ at the end of scaling.

Regime (ii). Charge fluctuations of the d level are quenched at $D_i \sim \epsilon_F - \epsilon_d$. A Schrieffer-Wolf transformation for the d level yields an effective Hamiltonian

$$H_I^{(ii)} = H_0 + H_f + H_{df} + H_K^{(ii)},$$

where

$$H_K^{(ii)} = \frac{1}{2} \sum_{\alpha\sigma, \beta\sigma'=\gamma\sigma, f\sigma} J_{\alpha\beta} (\alpha_\sigma^\dagger \mathbf{s}_{\sigma\sigma'} \beta_{\sigma'}) \cdot \mathbf{S}_d, \quad (27)$$

where

$$\gamma_\sigma = \sum_{v, \mathbf{k}} \gamma_{v\mathbf{k}\sigma},$$

$\mathbf{s}$ is the vector of Pauli matrices, $\mathbf{S}_d$ is the localized spin of the d level, and

$$J_{\gamma\gamma} = \frac{2V_d^2}{\epsilon_F - \epsilon_d}, \quad J_{ff} = \frac{2V_{df}^2}{\epsilon_f - \epsilon_d},$$

$$J_{\gamma f} = J_{f\gamma} = \frac{V_d V_f}{\epsilon_f - \epsilon_d} + \frac{V_d V_f}{\epsilon_F - \epsilon_d}.$$

The Hamiltonian $H_K^{(ii)}$ describes coupling of the d spin to γ and f electrons. Notice that charge fluctuations in the f orbital are allowed in $H_K^{(ii)}$ through the mixed spin operators

$$\mathbf{S}_m = \frac{1}{2} (\gamma_\sigma^\dagger \mathbf{s}_{\sigma\sigma'} f_{\sigma'})$$

and $\mathbf{S}_m^\dagger$. Figure 4 clarifies the physics of the various interactions encoded in $H_K^{(ii)}$.

Using poor-man's scaling [30], charge fluctuations in the f orbital can now be integrated out. The dimensionless exchange coupling constants $j_{\alpha\beta} \equiv \rho_0 J_{\alpha\beta}$ are renormalized as

$$\frac{dj_{\alpha\beta}}{d \ln D} = -j_{\alpha\gamma} j_{\gamma\beta} \frac{\bar{\rho}}{\rho_0}, \quad (28)$$

with the solution [see Eq. (23) for $\mathcal{L}(D, D_i)$]

$$j_{\alpha\beta}(D) = j_{\alpha\beta}(D_i) + \frac{j_{\alpha\gamma}(D_i) j_{\gamma\beta}(D_i) \mathcal{L}(D, D_i)}{1 - j_{\gamma\gamma}(D_i) \mathcal{L}(D, D_i)}. \quad (29)$$

The scaling invariant, that is, the Kondo temperature $T_K^{(ii)}$, is got by solving the equation

$$j_{\gamma\gamma}(D_i) \mathcal{L}(T_K^{(ii)}, D_i) = 1, \quad (30)$$

FIG. 4. (Color online) Transitions induced by $H_K^{(ii)}$, Eq. (27), leading from an initial state on the left and ending at a final state on the right. The various processes are associated with exchange constants (a) $J_{\gamma\gamma}$, (b) J_{ff} , and (c) $J_{\gamma f}$ and $J_{f\gamma}$.

and scaling stops if

$$T_K^{(ii)} > D_{ii} = \min\{\epsilon_F - \epsilon_f, U_f - \epsilon_F + \epsilon_f\},$$

at which the d spin is quenched by the KE. This happens if $j_{\gamma\gamma}(D_i)$ is large enough. We note that $\mathcal{L}(D_{ii}, D_i)$ remains finite as long as $D_{ii} > T_K^{(ii)}$. For $T_K^{(ii)} < D_{ii}$, scaling stops at $D = D_{ii}$ and the d spin is not quenched. The effective coupling between f and d spins is the sum of contributions from H_{df} and $H_K^{(ii)}$; i.e., $J_{df} = J_{df}^{(i)}(D_i) + J_{ff}(D_{ii})$. It is ferromagnetic if $J_{df} < 0$. Assuming that $1 - j_{\gamma\gamma}(D_i) \mathcal{L}(D_{ii}, D_i)$ is of order $O(1)$, $\epsilon_F \sim \varepsilon_q < \varepsilon_0 \ll |\epsilon_d|$, and U_f is a few ε_q [$\varepsilon_q \ll |\epsilon_d|$], we find that $J_{ff}(D_{ii})$ is of the same order as $\beta_f^2 \Delta_f$ and $J_{df} < 0$ if

$$|V_d|^2 \geq \varepsilon_0^{\frac{3}{2}} \sqrt{|\epsilon_d|}.$$

Regimes (iii) and (iv). The scaling stops at regime (ii) with $D_{ii} \sim \epsilon_F + \varepsilon_q$ if the chemical potential is located inside the band gap which is the usual case for insulators. A more interesting scenario occurs if the chemical potential ϵ_F is located above the band gap which may happen if the insulator is doped by impurities. Scaling continues in this case where charge fluctuations in the f level are also quenched. In this case the mixed spin term $\mathbf{S}_m$ becomes ineffective and we are left with an effective Hamiltonian $H^{(2)} = H_0 + H_K^{(iii)}$, where

$$H_K^{(iii)} = J_K \mathbf{S}_\gamma \cdot \mathbf{S}_d + J_{df} \mathbf{S}_f \cdot \mathbf{S}_d, \quad (31)$$

where

$$\mathbf{S}_\gamma = \frac{1}{2} \sum_{\mathbf{k}\sigma, \mathbf{k}'\sigma', v} (\gamma_{v\mathbf{k}\sigma}^\dagger \mathbf{s}_{\sigma\sigma'} \gamma_{v\mathbf{k}'\sigma'})$$

and

$$J_K = J_{\gamma\gamma}(D_{ii}) = \frac{J_{\gamma\gamma}(D_i)}{1 - j_{\gamma\gamma}(D_i)\mathcal{L}(D_{ii}, D_i)}.$$

Notice that $|J_{df}|$ is in general smaller than J_K [26].

SO(3) and SO(4) fixed points. For $D_{ii} \gg |J_{df}|$, there exists a regime $D \gg |J_{df}|$ where the system is governed by a critical point between the SO(3) and the quenched Kondo regimes which has SO(4) symmetry [33]. In this regime the behavior of the system is governed by the SO(4) critical point. The system crosses over to the low-temperature SO(3) or self-screened Kondo regime at $D < |J_{df}|$. We first consider the SO(4) regime $D \gg |J_{df}|$.

SO(4) Kondo fixed point. In this case we may set $J_{df} = 0$ and apply the Schrieffer-Wolf transformation directly to the spin-singlet and spin-triplet states to get

$$H_K^{SO(4)} = J_T(\mathbf{S} \cdot \mathbf{S}_\gamma) + J_{ST}(\mathbf{R} \cdot \mathbf{S}_\gamma), \quad (32)$$

where $\mathbf{S}$ and $\mathbf{R}$ are the ($S = 1$) spin and the Runge-Lenz operators, respectively, that are expressible in terms of Hubbard operators for the composed impurity, and satisfy the SO(4) algebra [34]. The exchange constants $J_T = J_K/2$ and $J_{ST} = \alpha_S J_T$ scale as

$$\frac{dj_T}{d \ln D} = -(j_T^2 + j_{ST}^2) \frac{\bar{\rho}}{\rho_0}, \quad (33a)$$

$$\frac{dj_{ST}}{d \ln D} = -2j_T j_{ST} \frac{\bar{\rho}}{\rho_0}. \quad (33b)$$

The combinations $j_n = j_T - (-1)^n j_{ST}$ ($n = 1, 2$) satisfy

$$j_n(D) = \frac{j_n(D_{ii})}{1 - j_n(D_{ii})\mathcal{L}(D, D_{ii})}, \quad (34)$$

whence

$$j_T(D) = \frac{1}{2}[j_1(D) + j_2(D)], \quad (35a)$$

$$j_{ST}(D) = \frac{1}{2}[j_1(D) - j_2(D)]. \quad (35b)$$

The corresponding Kondo temperature T_{K_4} is determined from the equation

$$\{j_T(\bar{D}_{ii}) + j_{ST}(\bar{D}_{ii})\}\mathcal{L}(T_{K_4}, \bar{D}_{ii}) = 1 \quad (36)$$

provided $T_{K_4} \gg |J_{df}|$. For $0 < T_{K_4} < J_{df}$ the two spins form a spin singlet (self-screened KE) at $D \sim J_{df}$.

SO(3) Kondo fixed point. For $J_{df} < 0$ and $T_{K_4} < |J_{df}|$, renormalization of j_{ST} stops at $D = D_{iii} \sim |J_{df}|$. For $D < D_{iii}$, the Kondo Hamiltonian becomes

$$H_K^{SO(3)} = J_T \mathbf{S} \cdot \mathbf{S}_\gamma. \quad (37)$$

The scaling equation for $j_T = J_T \rho_0$ and its solution are

$$\frac{dj_T}{d \ln D} = -j_T^2 \frac{\bar{\rho}}{\rho_0}, \quad (38a)$$

$$j_T(D) = \frac{j_T(D_{iii})}{1 - j_T(D_{iii})\mathcal{L}(D, D_{iii})}. \quad (38b)$$

Scaling stops at T_{K_3} determined from the equation

$$j_T(D_{iii})\mathcal{L}(T_{K_3}, D_{iii}) = 1. \quad (39)$$

V. RESISTIVITY AND IMPURITY MAGNETIC SUSCEPTIBILITY

Having elaborated upon the theory in the weak-coupling regime $T \gg T_K$ we are now in a position to carry out perturbation calculations of experimental observables. In 3D, the most accessible ones are the impurity resistivity $R_{\text{imp}}(T)$ and the impurity magnetic susceptibility $\chi_{\text{imp}}(T)$. We shall be guided by the quest to find out how the special features of the TIs are reflected in these observables. These features are the occurrence of gap and the structure of the DOS especially near the band edges $\pm \varepsilon_q$. In addition, reducing the temperature results in the crossover between different scaling regimes of the couplings. Explicitly, there are three relevant temperature regimes denoted as (ii), (iii), (iv) in order to match the notation of the corresponding scaling regimes discussed previously. The first regime, denoted as (ii), is defined by $[D_i > T > D_{ii}]$ as given by Eq. (28) for the scaling interval (ii). Local moment behavior exists only at the d level in this regime and therefore there is Kondo scattering with SU(2) symmetry. The second regime, denoted as (iii), is defined by Eq. (33) for scaling interval (iii) $[D_{ii} > T > D_{iii}]$. Here one may neglect the difference in energies between the singlet and triplet states and the system is at the SO(4) Kondo regime. The third regime, denoted as (iv), is defined by Eq. (38a) for scaling interval (iv) $[D_{iii} > T > T_{K_3}]$. Here there is Kondo scattering with SO(3) symmetry (when $J_{df} < 0$) or a self-screened KE if $J_{df} > 0$. The temperature dependence of the resistivity and magnetic susceptibility in these three different scaling regimes is distinct.

In the calculation of resistivity, we assume $\epsilon_F > \varepsilon_q$ (the TI is doped) and the system has a Fermi surface. The impurity resistivity as calculated in the framework of the “poor-man’s scaling” formalism is given by

$$R_{\text{imp}} = \frac{N_\nu R_0}{\mathcal{L}^2(T_{K_\nu}, T)}, \quad (40)$$

where $\nu = (\text{ii}), (\text{iii}), (\text{iv})$ denotes the pertinent temperature regime as detailed above. The corresponding Kondo temperatures are $T_{K_{ii}}$, Eq. (30), $T_{K_{iii}} \equiv T_{K_4}$, Eq. (36), or $T_{K_{iv}} \equiv T_{K_3}$, Eq. (39). The numerical factors N_ν are $N_{ii} = N_{iii} = 3/4$ and

FIG. 5. (Color online) Resistivity (40) as a function of temperature for $\epsilon_d = -80\varepsilon_q$, $\varepsilon_0 = 24\varepsilon_q$, $\epsilon_F = 2\varepsilon_q$, and different values of j : $j = 0.1$ (bottom red curve), $j = 0.12$ (middle purple curve), and $j = 0.14$ (top blue curve). The dots denote $T = D_{ii}$ and $T = D_{iii}$ separating the temperature intervals (ii), (iii), and (iv). Inset: Behavior of R_{imp} for the temperature $T \sim \varepsilon_q$.

FIG. 6. (Color online) Magnetic susceptibility (41) as a function of temperature for $\epsilon_d = -80\epsilon_q$, $\epsilon_0 = 24\epsilon_q$, $\epsilon_F = 2\epsilon_q$, and different values of j : $j = 0.1$ (red curve), $j = 0.12$ (purple curve), and $j = 0.14$ (blue curve). The dots denote $T = D_{ii}$ and $T = D_{iii}$ separating the temperature intervals (ii), (iii), and (iv).

$N_{iv} = 2$. Here

$$R_0 = \frac{3\pi c_{\text{imp}}}{\hbar e^2 \rho_0^2} \frac{1}{v_1^2 + v_2^2}, \quad v_i \approx \frac{1}{\hbar} \left(\frac{\partial \epsilon_{k_i}}{\partial k_i} \right),$$

and k_1, k_2 are two solutions of $\epsilon_k = \epsilon_F$ (see Fig. 1).

The resistivity as a function of the temperature is shown in Fig. 5 assuming a low-temperature SO(3) fixed point. It is seen that R_{imp} has different temperature dependence within the temperature intervals (ii), (iii), and (iv), with crossover observed at $T = D_{ii}$ and $T = D_{iii}$ (the points D_{ii} and D_{iii} are denoted by dots). In addition, crossovers are observed at $T = \epsilon_q$ [interval (iii)]. These crossovers appear since the function $\mathcal{L}(T_{K_{iii}}, T)$ changes its behavior at $T = \epsilon_F - \epsilon_q = \epsilon_q$ (we take $\epsilon_F = 2\epsilon_q$ here).

The Kondo scattering manifests itself also in the magnetic susceptibility [31]. The impurity susceptibility calculated in the framework of the “poor-man’s scaling” is

$$\chi_{\text{imp}} = \frac{K_v \chi_0 T_{K_{ii}}}{T} \left\{ P_v - \frac{1}{\mathcal{L}(T_{K_v}, T)} \right\}, \quad (41)$$

where $v = (\text{ii}), (\text{iii}), (\text{iv})$; the Kondo temperatures are $T_{K_{ii}}$, Eq. (30), $T_{K_{iii}} \equiv T_{K_4}$, Eq. (36), and $T_{K_{iv}} \equiv T_{K_3}$, Eq. (39). The numerical factors are $K_{ii} = K_{iii} = 1/4$, $K_{iv} = 2/3$, $P_{ii} = P_{iv} = 1$, and $P_{iii} = 2$. The constant χ_0 is

$$\chi_0 = \frac{4c_{\text{imp}}\mu_B^2}{T_{K_{ii}}}.$$

The impurity magnetic susceptibility as a function of T is shown in Fig. 6. The different temperature dependencies of χ_{imp} at different temperature regimes (ii), (iii), and (iv) are obvious, with crossovers observed at $T = D_{ii}$ and $T = D_{iii}$ (the points D_{ii} and D_{iii} are denoted by dots).

VI. CONCLUSIONS

We have analyzed the interplay between the Anderson impurity and its induced in-gap bound state in a model of 2D topological insulator. Using a weak-coupling RG analysis, it is shown that the exchange interaction J_{df} between the d spin and the induced in-gap f spin may be renormalized dynamically to either positive or negative values. The parameters required to observe the above phenomena are not too restrictive

($|V_d|^2 \geq \epsilon_0^{\frac{3}{2}} \sqrt{|\epsilon_d|}$, $\epsilon_q < U_f \ll U_d$) and are realistic. The system exhibits complex crossover behaviors at different parameter regimes as a result which can be observed in the temperature dependence of the impurity-induced resistance and magnetic susceptibility. The crossover in the temperature dependence of both the resistivity and the impurity magnetic susceptibility at different regimes is a peculiar feature that can serve as an experimental confirmation of the above analysis. For both screened and underscreened Kondo effect in the weak-coupling regime, the effective coupling constant j renormalizes as $1/\mathcal{L}(T_K, T)$ (or, as $1/\ln(T/T_K)$, when the DOS is flat; see Ref. [31]). As a result, the impurity resistivity, R_{imp} , behaves as $1/\mathcal{L}^2(T_K, T)$ [see Eq. (40)], whereas the susceptibility, χ_{imp} , is given by Eq. (41).

The physics described above is not limited to TIs but is a general consequence of (doped) insulators (and semiconductors) with a large electronic density of states at the band edge such that in-gap bound states are easily induced by an Anderson impurity. Similar physics may be found in, for example, two-layer graphene systems. Our paper is just a first step towards understanding the rich physics associated with impurities in these systems.

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APPENDIX A: INTERPRETATION OF V_0 IN EQUATION (5)

Electrons in a lattice move in the periodic potential $w_l(\mathbf{r})$,

$$w_l(\mathbf{r}) = \sum_{\mathbf{n}} w_a(\mathbf{r} - \mathbf{n}), \quad (A1)$$

where $w_a(\mathbf{r})$ is the interaction energy of electrons with an lattice atom and $\mathbf{n} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$; $\mathbf{a}_{1,2,3}$ are the lattice vectors and $n_{1,2,3}$ are integers. In this case, electrons tunnel from one atom to another and the single-electron atomic levels ϵ_a reduce to the energy band shown in Fig. 7.

When the atom of the lattice at the point $\mathbf{r} = \mathbf{0}$ is replaced by an impurity atom, the potential energy $w_i(\mathbf{r})$ of interaction of electrons with the impurity differs from $w_a(\mathbf{r})$. As a result, the potential energy of electrons in the lattice with the impurity,

$$w(\mathbf{r}) = \sum_{\mathbf{n} \neq \mathbf{0}} w_a(\mathbf{r} - \mathbf{n}) + w_i(\mathbf{r}), \quad (A2)$$

is not periodic anymore (see the purple curve in Fig. 7).

Then the potential scattering can be estimated as

$$V_0 = \int d^3 \mathbf{r} \{w_i(\mathbf{r}) - w_a(\mathbf{r})\} \sim w_0 a_0^3, \quad (A3)$$

$$w_0 = w_i^{(0)} - w_a^{(0)},$$

where $w_i^{(0)}$ or $w_a^{(0)}$ is the peak of the potential energy of the impurity or the atom. Here we assume that the electric potential is screened at the interatomic distance a_0 .

FIG. 7. (Color online) Potential energy of electrons in the lattice with the impurity put at the point $\mathbf{r} = \mathbf{0}$. The solid purple curve is the potential energy (A2), whereas the dashed blue curve is the potential energy (A1) of electrons in the lattice without impurity. The filled areas denote the valence and conduction bands. The red line is the impurity level. It is assumed that $|\mathbf{a}_{1,2,3}| = a_0$ and $V_d \ll w_0$, where V_d is the hybridization rate between d impurity and the band electrons.

APPENDIX B: LOCAL DENSITY OF STATES

The potential scattering V , Eq. (5), results in modification of the density of states and formation of an in-gap energy level. In order to derive an explicit expression for the local DOS (18), we calculate the retarded Green's function (19). Applying the equation of motion (10), we get

$$G_{v\mathbf{k},v'\mathbf{k}'}(\varepsilon) = g_{v\mathbf{k}}(\varepsilon)\delta_{\mathbf{k}\mathbf{k}'}\delta_{vv'} + V_0 g_{v\mathbf{k}}(\varepsilon) \sum_{v''\mathbf{k}''} G_{v''\mathbf{k}'',v'\mathbf{k}'}(\varepsilon), \quad (\text{B1})$$

where

$$g_{v\mathbf{k}}(\varepsilon) = \frac{1}{\varepsilon - v\varepsilon_{\mathbf{k}} + i\eta}.$$

The solution of Eq. (B1) is

$$G_{v\mathbf{k},v'\mathbf{k}'}(\varepsilon) = g_{v\mathbf{k}}(\varepsilon)\delta_{\mathbf{k}\mathbf{k}'}\delta_{vv'} + \frac{V_0 g_{v\mathbf{k}}(\varepsilon)g_{v'\mathbf{k}'}(\varepsilon)}{1 - V_0 \sum_{v''\mathbf{k}''} g_{v''\mathbf{k}''}(\varepsilon)}. \quad (\text{B2})$$

Then the DOS (18) is

$$\rho(\varepsilon, r) = \rho_0(\varepsilon) - \text{Im} \frac{\pi V_0 \{\mathcal{R}^2(\varepsilon, r) + \pi^2 \rho_0^2(\varepsilon, r)\}}{1 + \pi V_0 \{\mathcal{R}(\varepsilon, 0) + i\rho_0(\varepsilon, 0)\}}, \quad (\text{B3})$$

where $\mathcal{R}(\varepsilon, r)$ and $\rho_0(\varepsilon, r)$ are real and imaginary parts of the Green's function,

$$\tilde{g}(\varepsilon, r) = -\frac{1}{\pi} \sum_{v\mathbf{k}} g_{v\mathbf{k}}(\varepsilon) e^{i\mathbf{k}\mathbf{r}}.$$

Explicitly, $\rho_0(\varepsilon, r)$ is given by Eq. (22) and

$$\mathcal{R}(\varepsilon, r) = -\frac{\Theta(\varepsilon_q - |\varepsilon|)}{\pi} \sum_{v\mathbf{k}} \frac{\sin(kr)}{kr(\varepsilon - v\varepsilon_{\mathbf{k}})}.$$

When $|\varepsilon| > \varepsilon_q$, $\mathcal{R}(\varepsilon, r)$ vanishes and Eq. (B3) reduces to Eq. (21). When $|\varepsilon| < \varepsilon_q$, the bare DOS vanishes, but the

DOS (B3) gets a delta peak due to the localized f level,

$$\rho(\varepsilon, r) = \pi^2 V_0 \mathcal{R}^2(\varepsilon_f, r) \delta(1 + \pi V_0 \mathcal{R}(\varepsilon, 0)), \quad (\text{B4})$$

where the condition of vanishing of the argument of the delta function gives us the secular equation (11) for ε_f . The amplitude $\mathcal{R}^2(\varepsilon_f, r)$ of the delta peak vanishes when $r \rightarrow \infty$, so that ε_f is a localized state.

APPENDIX C: THE SO(4) KONDO HAMILTONIAN, EQUATION (32)

The SO(4) Hamiltonian is derived in regime (iii) of the RG analysis when ε_F is located above the band gap. It has the form

$$H_K^{\text{SO}(4)} = J_T(\mathbf{S} \cdot \mathbf{S}_\gamma) + J_{ST}(\mathbf{R} \cdot \mathbf{S}_\gamma), \quad (\text{C1})$$

where $\mathbf{S}$ and $\mathbf{R}$ are the ($S = 1$) spin operator and the Runge-Lenz operator, respectively, with

$$\begin{aligned} S^+ &= \sqrt{2}(X^{10} + X^{0\bar{1}}), & S^- &= \sqrt{2}(X^{01} + X^{\bar{1}0}), \\ S^z &= X^{11} - X^{\bar{1}\bar{1}}, \end{aligned} \quad (\text{C2})$$

$$\begin{aligned} R^+ &= \sqrt{2}(X^{1S} - X^{S\bar{1}}), & R^- &= \sqrt{2}(X^{S1} - X^{\bar{S}\bar{1}}), \\ R^z &= -(X^{0S} + X^{S0}). \end{aligned} \quad (\text{C3})$$

Here $X^{\lambda\lambda'} = |\lambda\rangle\langle\lambda'|$, $|\lambda(\lambda')\rangle = |S\rangle, |T_m\rangle$ ($m = 0, \pm 1$) are the spin singlet and triplet states. The operators $\mathbf{S}$ and $\mathbf{R}$ are the generators of the group SO(4), as they satisfied the following commutation relations ($i, j, k = x, y, z$, summation convention implied):

$$[S_i, S_j] = i\varepsilon_{ijk} S_k, \quad [R_i, R_j] = i\varepsilon_{ijk} S_k, \quad [R_i, S_j] = i\varepsilon_{ijk} R_k. \quad (\text{C4})$$

APPENDIX D: RESISTIVITY

The resistivity for the SU(2) symmetry [regime (ii)] calculated within the third order of the perturbation theory is [31]

$$R_{\text{imp}}^{\text{SU}(2)} = \frac{3R_0}{4} j_D^2 + \frac{3R_0}{2} j_D^3 \mathcal{L}(T, \bar{D}), \quad (\text{D1})$$

where

$$R_0 = \frac{3\pi c_{\text{imp}}}{\hbar e^2 \rho_0^2} \frac{1}{v_1^2 + v_2^2}, \quad v_i \approx \frac{1}{\hbar} \left(\frac{\partial \varepsilon_{k_i}}{\partial k_i} \right);$$

k_1 and k_2 are two solutions of the equation $\varepsilon_k = \varepsilon_F$ (see Fig. 1 of the main text). The function $\mathcal{L}(T_1, T_2)$ is given by Eq. (7) of the main text.

Applying the condition of invariance of the resistivity under the “poor-man’s scaling,” we get

$$R_{\text{imp}}^{\text{SU}(2)}(T) = \frac{3R_0}{4\mathcal{L}^2(T_{K_2}, T)}. \quad (\text{D2})$$

Here the factor $N_v = 3/4$ comes from the factor $S(S+1)$ which is $3/4$ for $S = 1/2$.

The resistivity for the SO(4) symmetry [regime (iii)] calculated within the third order of the perturbation theory

is

$$R_{\text{imp}}^{\text{SO}(4)} = \frac{3R_0}{2}(j_T^2 + j_{ST}^2) + 3R_0[j_T(j_T^2 + j_{ST}^2) + 2j_T j_{ST}^2]\mathcal{L}(T, \bar{D}). \quad (\text{D3})$$

The couplings j_T and j_{ST} renormalize in such a way that the difference $j_T - j_{ST}$ is finite (and small) even when the temperature T approaches the Kondo temperature T_{K_4} , whereas $j_T + j_{ST} \rightarrow \infty$ when $T \rightarrow T_{K_4}$ [see Eqs. (16)–(18) in the main text]. As a result, the resistivity for the SO(4) symmetry in the low-temperature regime [$\bar{D} \gg T \gg T_{K_4}$] is described by Eq. (D2).

For the SO(3) symmetry [regime (iv)], the resistivity calculated within the third order of the perturbation theory is

$$R_{\text{imp}}^{\text{SO}(3)} = 2R_0 j_T^2 + 4R_0 j_T^3 \mathcal{L}(T, \bar{D}). \quad (\text{D4})$$

Applying the condition of invariance of the resistivity under the “poor-man’s scaling,” we get

$$R_{\text{imp}}^{\text{SO}(3)}(T) = \frac{2R_0}{\mathcal{L}^2(T_{K_3}, T)}. \quad (\text{D5})$$

The factor $N_\nu = 2$ comes from the factor $S(S+1)$ which is 2 for $S = 1$.

APPENDIX E: MAGNETIC SUSCEPTIBILITY

The susceptibility for the SU(2) symmetry calculated within the second order of the perturbation theory is [31]

$$\chi_{\text{imp}}^{\text{SU}_2}(T) = \frac{\chi_0 T_{K_2}}{4T} \{1 - 2J_D \rho_0 - 4J_D^2 \rho_0^2 \mathcal{L}(T, \bar{D})\}.$$

Applying the RG transformations, we get

$$\chi_{\text{imp}}^{\text{SU}_2}(T) = \frac{\chi_0 T_{K_2}}{4T} \left\{ 1 - \frac{1}{\mathcal{L}(T_{K_2}, T)} \right\}, \quad (\text{E1})$$

where the factor $K_{ii} = 1/4$ comes from $S(S+1)/3$ which is $1/4$ for $S = 1/2$.

For SO(4) symmetry, the impurity susceptibility calculated to the second order in J is

$$\chi_{\text{imp}}^{\text{SO}_4}(T) = \frac{\chi_0 T_{K_4}}{2T} \{1 - J_T \rho_0 - (J_T^2 \rho_0^2 + J_{ST}^2 \rho_0^2) \mathcal{L}(T, \bar{D})\}.$$

Applying the RG transformations, we get

$$\chi_{\text{imp}}^{\text{SO}_4}(T) = \frac{\chi_0 T_{K_4}}{4T} \left\{ 2 - \frac{1}{\mathcal{L}(T_{K_4}, T)} \right\}. \quad (\text{E2})$$

The factors $P_{iii} = 2$ and $K_{iii} = 1/4$ have the following origin: there are two spins $S = 1/2$ (so that $P_{iii} = 2$); every spin gives the factor $K_{iii} = S(S+1)/3 = 1/4$.

For SO(3) symmetry, the impurity susceptibility calculated to the second order in J is

$$\chi_{\text{imp}}^{\text{SO}_3}(T) = \frac{2\chi_0 T_{K_3}}{3T} \{1 - J_T \rho_0 - J_T^2 \rho_0^2 \mathcal{L}(T, \bar{D})\}.$$

Applying the RG transformations, we get

$$\chi_{\text{imp}}^{\text{SO}_3}(T) = \frac{2\chi_0 T_{K_3}}{3T} \left\{ 1 - \frac{1}{\mathcal{L}(T_{K_3}, T)} \right\}. \quad (\text{E3})$$

The factor $K_{iv} = 2/3$ comes from $S(S+1)/3$ for $S = 1$.

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