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Anderson Impurity in the Bulk of 3D Topological Insulators: II. The Strong Coupling Regime

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Electron scattering off an Anderson impurity immersed in the bulk of a 3D topological insulator is studied in the strong coupling regime, where the temperature T is lower than the Kondo temperature T_K. The system displays either a self-screened Kondo effect, or a Kondo effect with SO(3) or SO(4) dynamical symmetries. Low temperature Kondo scattering for systems with SO(3) symmetry displays the behavior of a singular Fermi liquid, an elusive property that so far has been observed only in tunneling experiments. This is demonstrated through the singular behavior as $T \to 0$ of the specific heat, magnetic susceptibility and impurity resistivity, that are calculated using well known (slightly adapted) conformal field theory techniques. Quite generally, the low temperature dependence of some of these observables displays a remarkable distinction between the SO(n=3,4) Kondo effect, compared with the standard SU(2) one.

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I. INTRODUCTION

In this work we continue our study of a system composed of an Anderson impurity d immersed in a 3D topological insulator (3DTI) with an "inverted-Mexican-hat" band dispersion around the Γ-point[1–6]. For the sake of self-consistency let us very briefly recapitulate the peculiar feature of the pertinent system: Due to the special band structure, the ensuing Kondo effect (KE) is profoundly distinct from its metallic analog in normal metals, because in addition to the original Anderson impurity d, there is an in-gap bound state (henceforth denoted as an f impurity), that is formed as a result of potential scattering[1,2]. The d and f impurities form a "composite quantum impurity" (CQI) that turns the pertinent Kondo physics much richer. The reason for that is as follows: When isolated, the CQI can host two electrons that are found in singlet or triplet states with corresponding energies E_S and E_T. Due to hybridization of the localized electrons in the CQI with the band electrons, the levels E_S and E_T are renormalized with decreasing bandwidth *albeit with different rates*[2]. As a result, there is either a self-screened KE, or a KE with SO(3) or SO(4) dynamical symmetry (depending on whether at the end of renormalization, E_T lies above, below or coincides with E_S[1,2].

In our previous work[2], we have analyzed the pertinent Kondo physics *in the weak coupling regime* using perturbative RG analysis techniques. The goal of the present work is to perform an analysis of the Kondo scattering with SO(3) and SO(4) dynamical symmetry in the *strong coupling regime* $T < T_K$. The main physical motivation is to elucidate the occurrence of singular Fermi liquid in the SO(3) symmetric sector, that is exposed *only in the strong coupling regime*. More than a decade ago it has been shown that the traditional classification of quantum impurity models into Fermi liquids and non Fermi liquids should be modified in such a way that one has to distinguish between regular Fermi liquids and singular Fermi liquids (SFL)[11–13]. The former case is exemplified by the standard SU(2) Kondo model where electrons are scattered from a magnetic impurity of spin $S = \frac{1}{2}$ and at zero temperature the impurity is *fully screened*. This makes it possible to describe the system in terms of Nozières Fermi-liquid picture. On the other hand, it was shown in Ref.[13] that when the impurity is *under-screened*, the corresponding Fermi liquid is singular. Practically, it implies that the density of states is (logarithmically) singular at the Fermi energy.

As is already stressed, this manifestation of SFL occurs only at low temperature $T < T_K$, and that requires the calculations to be carried out in the strong coupling regime, where perturbation theory is not applicable. One need to resort to other approaches, such as Bethe ansatz or conformal field theory (CFT, that is employed here). Calculated experimental observables for SO(3) and SO(4) symmetric Kondo effect include the impurity contribution to the temperature dependence of the specific heat, magnetic susceptibility and resistivity. Comparing these results with those of the standard SU(2) Kondo effect, we indeed elucidate the remarkable SFL nature of the KE for the SO(3) symmetric sector.

Experimentally, under-screened Kondo effect (USKE) has been observed in tunneling transport measurements through molecular transistors[14–16]. It is shown therein that the tunneling conductance G approaches the unitary limit when the temperature T tends to zero, but the derivative dG/dT is divergent. The possibility of detecting USKE in Kondo scattering in the bulk of metals is hampered by the fact that quantum impurities with high spin give rise to Coqblin-Schrieffer type of Kondo scattering which eventually flows to a regular Fermi liquid fixed point[18]. In this work we overcome this obstacle and demonstrate the feasibility of observing USKE in bulk materials employing the occurrence of composite impurities.

The organization of the paper is facilitated by the fact that the model and the relevant starting Kondo Hamiltonian as well as the Kondo temperature have already been derived in our previous work (starting from the single impurity Anderson Hamiltonian). Therefore, in Sec. II we start right away by writing down the Kondo Hamiltonian H_K describing low-energy exchange scattering of the band electrons by the d and f impurities as well as an exchange interactions between the d and f impurities. The Hamiltonian H_K possesses different dynamical symmetries, SO(3) or SO(4), within various energy domains. The local density of states (DOS) of the TI with magnetic impurity immersed in it is calculated in Sec. III. Kondo Interaction of the "dressed" Fermi liquid (formed by the band electrons and the d impurity) with the f-impurity is discussed in Sec. IV. In Sec. V we study and calculate the temperature dependence of the impurity contribution to the specific heat, while the magnetic susceptibility of the impurity is considered in Sec. VI. Sec. VII is devoted to the calculations of electric resistivity. The results are then summarized in Sec. VIII. Some technical details are relegated to the Appendices. In Appendix A 1 we describe the ground state of the isolated composite impurity. Weak coupling renormalization of the exchange interaction strength of the f-impurity with the band is considered in Appendix A 2.

II. KONDO HAMILTONIAN

As it is shown in our previous work[2], the lowest-energy states of the isolated CQI are the singlet and triplet states with one electron on the d-level and a second electron on the f-level. Electron tunneling between the d-level and the band modifies the number of electrons in the CQI. Integrating out high energy states from the band edges renormalizes the singlet and triplet levels until charge fluctuations are quenched and one arrives at the local moment regime. In this regime, the Schrieffer-Wolff transformation is used to map the Anderson Hamiltonian onto an effective Hamiltonian $H = H_0 + H_K$. Here the first term, H_0, describes electrons in the bulk of the TI,

$$H_0 \;=\; \sum_{\nu\sigma\mathbf{k}} \nu\varepsilon_k \gamma^\dagger_{\nu\mathbf{k}\sigma}\gamma_{\nu\mathbf{k}\sigma}, \tag{1a}$$

where $\nu = \pm 1$ denotes the conduction and valence band.

$$\varepsilon_k = \sqrt{M_k^2 + (\hbar v k)^2}, \quad M_k = mv^2 - B\hbar^2 k^2, \tag{1b}$$

is the band dispersion. Accordingly, 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 with dispersion minimum at a surface of nonzero wave-vector $\mathbf{q}$'s, with

$$\varepsilon_q \;=\; \frac{v^2}{B}\sqrt{Bm - \frac{1}{4}}, \quad q \;=\; \frac{v}{\hbar v}\sqrt{Bm - \frac{1}{2}}, \tag{2}$$

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

The Kondo Hamiltonian H_K assumes the following form[2]:

$$H_K = J_d\big(\mathbf{S}_d \cdot \mathbf{s}\big) + J_f\big(\mathbf{S}_f \cdot \mathbf{s}\big) + J_{df}\big(\mathbf{S}_d \cdot \mathbf{S}_f\big), \tag{3}$$

where $\mathbf{S}_d$ or $\mathbf{S}_f$ is the localized spin of the d- or f-impurity, $\mathbf{s}$ is the spin operator of the band electrons,

$$\mathbf{s} = \frac{1}{2}\sum_{\nu\mathbf{k}\sigma,\nu'\mathbf{k}'\sigma'}\Big(\gamma^\dagger_{\nu\mathbf{k}\sigma}\boldsymbol{\tau}_{\sigma\sigma'}\gamma_{\nu'\mathbf{k}'\sigma'}\Big),$$

$\hat{\boldsymbol{\tau}} = (\hat{\tau}^x, \hat{\tau}^y, \hat{\tau}^z)$ is the vector of the Pauli matrices. The couplings J_K, J_f and J_{df} are explicitly given as[2],

$$J_d \;\sim\; \frac{2V_d^2}{\epsilon_F - \epsilon_d}, \qquad J_f \;\sim\; \frac{J_d\beta_f^2}{4}, \tag{4a}$$

$$J_{df} \;\sim\; \beta_f^2\Delta_f\left(1 - \frac{2V_d^2\rho_c}{\Delta_f}\,\frac{\sqrt{D_0} - \sqrt{|\epsilon_f|}}{\sqrt{\varepsilon_0}}\right), \tag{4b}$$

where

$$\beta_f \;=\; \frac{\sqrt{2}\,V_{df}}{\Delta_f}, \qquad \Delta_f \;=\; \epsilon_f - \epsilon_d + U_f.$$

Here ϵ_d and ϵ_f are single electron energies of the d- and f-impurities, V_d is hybridization rate of the d-impurity and the band and V_{df} is the hybridization of the d- and f-impurities [see Fig. 6 below], and U_f is the Coulomb blockade parameter for the f-impurity. The Coulomb blockade U_d of the d-impurity is assume to be infinity[2]. Notice that, generally, $J_f \ll J_d$[2,3].

The low-energy physics of the model depends on J_{df}. More concretely, there are three different regimes for J_{df} determining the different ground states (GS)[2,10]:

- When $J_{df} = 0$, the impurities are decoupled, and Kondo scattering of the band electrons is determined mostly by the hybridization of the d-impurity with the band, whereas the f-impurity can be considered as an isolated magnetic moment (i.e., it is not coupled to the band or to the d-impurity). In this case, there is standard Kondo effect with full screening of the spin of the d-impurity. The exchange interaction of the f-impurity with the band manifests itself just at temperature below Kondo temperature. Therefore, J_f enters into consideration only for temperatures below the Kondo temperature.

- When $J_{df} < 0$ with $|J_{df}| \gg J_d$, the ground state of the CQI is a triplet and the singlet state is highly excited. In this case, band electrons are scattered from a CQI with spin $S = 1$, and there is an USKE of the magnetic impurity. Since the magnetic moments of the d- and f-impurities in the triplet ground state are parallel to one another, the exchange interaction strength J_f of the f-impurity with the lead gives rise to slight modification of $J_d{}^2$, (that is the exchange interaction strength of the d impurity with the band electrons). Therefore we assume $J_f = 0$ in this regime.

- When $J_{df} > 0$ with $J_{df} \gg J_d$, the ground state of the CQI is singlet and the triplet state has high excitation energy. In this case, there is no Kondo effect.

Before presenting our calculations pertaining to physical observables in our system, let us recapitulate the nature of the GS, specific heat and magnetic susceptibility for the ordinary case of a magnetic impurity immersed in an *ordinary metal* [7]. For the fully screened (FS) and the under screened (US) cases of the KE they are listed in the table below. Recall that the GS of the FSKE is a Fermi a liquid (FL) while that of the USKE turns out to be a SFL. Explicitly,

KE	GS	C_V	χ
FS	FL	$\sim T$	$\sim T_K^{-1}$
US	SFL	$\sim T\ln^4\left(\frac{T}{T_K}\right)$	$\sim T^{-1}\ln^{-2}\left(\frac{T}{T_K}\right)$

In the following, we will consider physical properties of the system in the strong coupling regime (when the temperature is below the Kondo temperature) for the cases $J_{df} < 0$ and $J_{df} = 0$, in turn.

III. DENSITY OF STATES

In this section we apply the already known Bethe ansatz expression for the scattering phase shift and write down the density of states (DOS) that is peculiar to the system of spin S CQI immersed in a material with inverse Mexican hat band structure. Specifically, we focus on the low-energy spectrum of the system where it is justified to approximate the dispersion (1b) by linear expressions in $k - k_i$ $(i = 1, 2)$, where k_1 and k_2 are two solutions of the equation $\varepsilon_k = \epsilon_F$ (see Fig. 1). The DOS $N_S(\omega)$ of the Fermi gas near the impurity position is expressed in terms of the phase shift $\delta_S(\omega)$ through the Friedel sum rule[13],

$$N_S(\omega) \;=\; \frac{1}{\pi}\,\frac{d\delta_S(\omega)}{d\omega}, \tag{5}$$

where $S = \frac{1}{2}$ or 1 is the impurity spin. Calculations based on the Bethe anzats[13] applied for the full screened $S = \frac{1}{2}$ and the under-screened $S = 1$ Kondo effect, yield

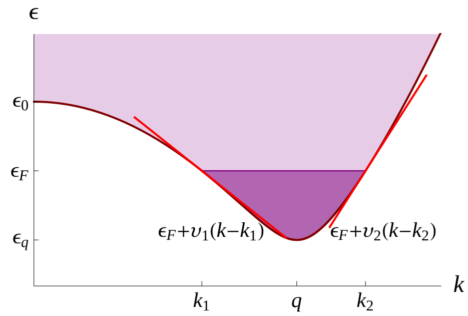

FIG. 1: (Color online) Dispersion ε_k, Eq. (1b). k_i $(i = 1, 2)$ are two solutions of the equation $\varepsilon_k = \epsilon_F$. $v_i = v_{k_i}$ are the Fermi velocities at the inner or outer Fermi surfaces ($k = k_1$ or k_2).

the following expression for the phase shift,

$$\begin{aligned}\delta_S(\omega) \;&=\; \frac{\pi}{2} + \frac{1}{2i}\,\ln\left(\frac{\Gamma\big(S+\frac{1}{2}+\frac{i}{\pi}\ln\big(\frac{\omega}{T_K}\big)\big)}{\Gamma\big(S+\frac{1}{2}-\frac{i}{\pi}\ln\big(\frac{\omega}{T_K}\big)\big)}\right) + \\ &\quad + \frac{1}{2i}\,\ln\left(\frac{\Gamma\big(S-\frac{i}{\pi}\ln\big(\frac{\omega}{T_K}\big)\big)}{\Gamma\big(S+\frac{i}{\pi}\ln\big(\frac{\omega}{T_K}\big)\big)}\right).\end{aligned} \tag{6}$$

For $S = \frac{1}{2}$, the above expression takes the form,

$$\delta_{\frac{1}{2}}(\omega) \;=\; \frac{\pi}{2} - \arctan\left(\frac{\omega}{T_K}\right), \tag{7}$$

whereas for $S = 1$ and $\omega \ll T_K$, $\delta_S(\omega)$ has the asymptotic expression,

$$\delta_1(\omega) \;=\; \frac{\pi}{2}\left\{1 + \frac{1}{2\ln\left(\frac{T_K}{\omega}\right)}\right\}. \tag{8}$$

Note that $\delta_1(\omega)$ demonstrates a singular behavior near the point $\omega = 0$, whereas $\delta_{\frac{1}{2}}(\omega)$ is regular. Differentiating δ_S (6) gives the following expression for the DOS[13]:

$$N_S(\omega) \;=\; \frac{1}{2\pi\omega}\,\mathrm{Re}\left[\beta\left(S + \frac{i}{\pi}\,\ln\frac{\omega}{T_K}\right)\right]. \tag{9}$$

Here $S = 1/2$ or 1 is the spin of the impurity, and the function $\beta(x)$ is defined as

$$\beta(x) \;=\; \frac{1}{2}\left\{\psi\left(\frac{x+1}{2}\right) - \psi\left(\frac{x}{2}\right)\right\}, \tag{10}$$

where $\psi(x)$ is the digamma function,

$$\psi(x) \;=\; \frac{d\ln\Gamma(x)}{dx} \;=\; \frac{\Gamma'(x)}{\Gamma(x)}.$$

The DOS Eq. (9) is shown in Fig. 2 for $S = \frac{1}{2}$ and $S = 1$. It is seen that the DOS for $S = 1$ is singular. As a result the conventional Fermi liquid expansion of the phase shift can not be carried out[13]. The origin of this singularity is the non-analytic behavior of the phase shift $\delta_1(\omega)$, eq. (6), near the point $\omega = 0$.

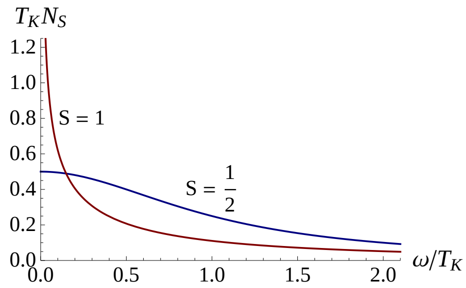

FIG. 2: (Color online) DOS Eq. (9) for the SO(4) KE (blue curve) and the SO(3) KE (red curve).

IV. KONDO INTERACTION OF THE FERMI LIQUID WITH THE f-IMPURITY

When $|J_{df}| \ll T_{K_4}$ [where T_{K_4} is the Kondo temperature for the SO(4) KE, see Ref. [2] and Eq. (A8) in Appendix A 2], the d-impurity and the conduction band electrons form a singlet state, and the system composed of the d-impurity *and the band electrons* forms a local Fermi liquid that can be described within Nozières Fermi liquid theory[17]. The f-impurity is coupled to this local Fermi liquid through an effective exchange Hamiltonian,

$$H_K^{(2)} \;=\; \tilde{J}_f(\mathbf{S}_f\cdot\mathbf{s}), \tag{11}$$

where

$$\tilde{J}_f \;=\; \frac{J_{df}(T_{K_4})}{\rho_0}. \tag{12}$$

The density of states of the local Fermi liquid is,

$$\tilde{\rho}(\epsilon) \;=\; \frac{T_{K_4}}{\left(\epsilon-\epsilon_F\right)^2+T_{K_4}^2}. \tag{13}$$

The dimensionless coupling $\tilde{j}_f$ is,

$$\tilde{j}_f \;=\; \tilde{J}_f\tilde{\rho}(\epsilon_F) \;\sim\; \frac{j_f\varepsilon_q}{T_{K_4}} \;\sim\; \sim\; j_f\,\frac{\varepsilon_q}{D_{ii}}\,\exp\left(\frac{1}{j_d}\right), \tag{14}$$

where we take into account that $\rho_c \sim 1/\varepsilon_q$. The scaling equation for $\tilde{j}_f$ is,

$$\frac{\partial\tilde{j}_f}{\partial\ln D} \;=\; -\tilde{j}_f^2. \tag{15}$$

The initial value $\tilde{j}_f(T_{K_4})$ of $\tilde{j}_f(D)$ is given by eq. (14). The solution of the scaling equation (15) is,

$$\tilde{j}_f(D) \;=\; \frac{1}{\ln\left(\dfrac{D}{T_K^{(2)}}\right)}, \tag{16}$$

where the scaling invariant, the second Kondo temperature, is

$$T_K^{(2)} = T_{K_4}\exp\left\{-\frac{1}{j_f}\,\frac{D_{ii}}{\varepsilon_q}\,\exp\left(-\frac{1}{j_d}\right)\right\}. \tag{17}$$

For $\epsilon_d = -80\epsilon_q$, $\varepsilon_0 = 24\varepsilon_q$, $\epsilon_F = 2\varepsilon_q$, $j = 0.08$ and $j_f = 0.025$, we get $T_{K_4} = 0.15\varepsilon_q$ and $T_K^{(2)} = 0.0021T_{K_4}$.

Having set up the calculation framework we turn now to elucidate numerous physical observable. These include specific heat, magnetic susceptibility and impurity resistivity. Since $T_K^{(2)}$ is very small, we shall restrict ourselves to the temperature regime $T \gg T_K^{(2)}$ in the following. For the SO(4) KE, the temperature is in the range $T_{K_4} > T \gg T_K^{(2)}$. For the SO(3) KE, we consider $T < T_{K_3}$, where T_{K_3} and T_{K_4} are the Kondo temperatures for the SO(3) and SO(4) KE, respectively[2]. For the SO(3) KE, we employ CFT techniques, whereas for the SO(4) KE, we will apply CFT techniques for the interaction between the d-impurity and the conduction band electrons, and then we employ poor man's scaling formalism to take into account the interaction between the local Fermi liquid and the f-impurity.

V. SPECIFIC HEAT

The first observable to be calculated is the specific heat of the TI within which the CQI is immersed. Its definition reads,

$$C_V^{(0)} \;=\; \frac{\partial}{\partial T}\int d\epsilon\;\epsilon f(\epsilon)N_S\big(|\epsilon-\epsilon_F|\big), \tag{18}$$

where $f(\epsilon)$ is the Fermi function. Noting that

$$\frac{\partial f(\epsilon)}{\partial T} \;=\; \frac{\epsilon-\epsilon_F}{4T^2\cosh^2\left(\frac{\epsilon-\epsilon_F}{2T}\right)},$$

we have

$$C_V^{(0)} \;=\; 4T\int_0^\infty \frac{N_S(2Tx)\;x^2\;dx}{\cosh^2(x)}. \tag{19}$$

For the SO(3) KE, the specific heat is $C_V = C_V^{(0)}$ [given by Eq. (19)]. For the SO(4) KE, there is contribution to the specific heat due to the f-impurity. This contribution can be written as,

$$\delta C_V \;=\; \frac{3\pi^2}{4}\,\tilde{j}_f^4(T), \tag{20}$$

where $\tilde{j}_f(T)$ is given by Eq. (16). The total specific heat for the SO(4) KE is $C_V = C_V^{(0)} + \delta C_V$.

The ratio C_V/T [where C_V is the specific heat (19)] is shown in Fig. 3 for the SO(4) and SO(3) KE. In this case, the Kondo temperature is T_{K_4}. For comparison, the

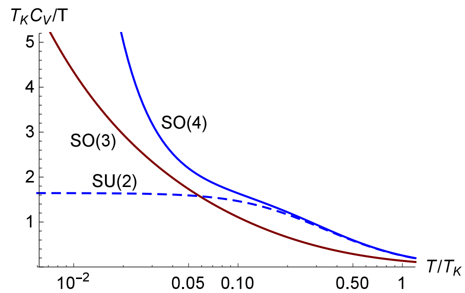

FIG. 3: (Color online) Ratio C_V/T [where C_V is the specific heat (19)] for the SO(4), SO(3) and SU(2) KE (solid blue, solid red and dashed blue curves). Here $T_K = T_{K_4}$ for the SO(4) and SU(2) KE or T_{K_3} for the SO(3) KE.

specific heat for the SU(2) KE (i.e., for the case when the f-impurity is absent), is shown as well. It is seen that for the SU(2) KE, C_V/T saturates to constant as $T \to 0$, in agreement with the prediction of Fermi liquid theory. The ratio C_V/T for the SO(4) KE is close to that for the SU(2) KE for T close to T_{K_4}. For low temperatures, C_V/T for the SO(4) and SU(2) KE deviate substantially from one another. This is result is due to the exchange interaction of the f-impurity with the local Fermi liquid. For the SO(3) KE, the ratio C_V/T diverges indicating the feature of a SFL behavior[13].

VI. MAGNETIC SUSCEPTIBILITY

When $J_{df} < 0$ and the ground state of the isolated CQI is $S = 1$, the magnetic susceptibility is,

$$\chi(T) = 2\mu_B^2 \int d\epsilon\ N_1\big(|\epsilon - \epsilon_F|\big) \left(-\frac{\partial f(\epsilon)}{\partial \epsilon}\right), \qquad (21)$$

where $N_1(\epsilon)$ is given by Eq. (9) with $S = 1$. Taking into account that

$$-\frac{\partial f(\epsilon)}{\partial \epsilon} = \frac{1}{4T\cosh^2\left(\frac{\epsilon-\epsilon_F}{2T}\right)}, \qquad (22)$$

we can write,

$$\chi(T) = \frac{2\chi_0 T_K}{T} \int \frac{N_1(|\epsilon - \epsilon_F|)\ d\epsilon}{\cosh^2\left(\frac{\epsilon-\epsilon_F}{2T}\right)}, \qquad (23)$$

where

$$\chi_0 = \frac{\mu_B^2}{T_K}. \qquad (24)$$

For the case $J_{df} = 0$ (see Eq. (4)), the susceptibility is calculated in the following way: First, we employ the CFT technique to calculate the susceptibility for $\tilde{j}_f = 0$ (see Eq. (16)). Within this approximation, the CQI splits into two noninteracting impurities, one of them is coupled to the band electrons, and the other is fully decoupled. In this case, the susceptibility is given by,

$$\chi^{(0)}(T) = 2\mu_B^2 \int d\epsilon\ N_{\frac{1}{2}}\big(|\epsilon - \epsilon_F|\big) \left(-\frac{\partial f(\epsilon)}{\partial \epsilon}\right) + \\ + \frac{\mu_B^2}{T}, \qquad (25)$$

where $N_{\frac{1}{2}}(\epsilon)$ is given by Eq. (9) with $S = \frac{1}{2}$. The second term, μ_B^2/T, is the susceptibility of the f-impurity. Taking into account Eq. (22), we can write,

$$\chi^{(0)}(T) = \frac{2\chi_0 T_K}{T} \int \frac{N_{\frac{1}{2}}\big(|\epsilon - \epsilon_F|\big)\ d\epsilon}{\cosh^2\left(\frac{\epsilon-\epsilon_F}{2T}\right)} + \frac{\mu_B^2}{T}, \qquad (26)$$

where χ_0 is given by Eq. (24). The contribution to the susceptibility due to the interaction of the local Fermi liquid with the f-impurity is,

$$\delta\chi(T) = -\frac{\chi_0 T_K}{T}\ \tilde{j}_f(T), \qquad (27)$$

where $\tilde{j}_f(T)$ is given by Eq. (16). The total susceptibility for the SO(4) KE is

$$\chi(T) = \chi^{(0)}(T) + \delta\chi(T). \qquad (28)$$

The functions $T\chi(T)$ for the SO(3), SU(2) and SO(4) KE are shown in Fig. 4. The SU(2) KE corresponds to the case when the f-impurity is absent. For this case, the Kondo temperature is T_{K_4}. It is seen that for the SU(2) or SO(4) KE, $T\chi(T) \to T_K\chi_0$ for $T \to 0$. For the SO(3) KE, $T\chi(T)$ vanishes as $\ln^{-2}(T/T_K)$ when $T \to 0$, which is a manifestation of a singular Fermi liquid fixed point.

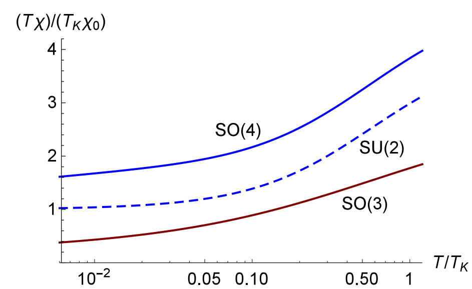

FIG. 4: (Color online) The quantity $T\chi(T)$ for the SO(3), SU(2) and the SO(4) KE is displayed as a function of temperature. The saturation as $T \to 0$ for the SU(2) and SO(4) KE is reminiscent of the Curie law. On the other hand, for the SO(3) KE, $T\chi(T) \to 0$.

VII. IMPURITY RESISTIVITY

In this section we will calculate the impurity contribution to the resistivity. Here, the peculiar band structure of the TI plays a central role. The calculation method of the impurity contribution to the resistivity depends on the underlying symmetry. The CFT technique used above to derive the specific heat and magnetic field will be employed to derive the resistivity of the KE with the SO(3) symmetry. On the other hand, for the KE with the SO(4) symmetry, we apply a somewhat different approach: First, we apply the CFT technique to derive the resistivity for the case $\tilde{j}_f = 0$ (see Eq. (16)). In the next step, we apply the perturbative RG (poor man's scaling approach) to get the correction to the resistivity due to the interaction of the f-impurity with the local Fermi liquid.

For $\tilde{j}_f = 0$, the impurity resistivity can be written as[18]

$$\rho^{(0)}(T) \;=\; \frac{1}{\sigma^{(0)}(T)}. \tag{29a}$$

Here the conductivity $\sigma^{(0)}(T)$ is

$$\sigma^{(0)}(T) = \frac{2e^2}{3}\int \frac{d^3\mathbf{k}}{(2\pi)^3}\Big[-\frac{\partial f(\epsilon_k)}{\partial \epsilon_k}\Big] v_k^2 \tau_{\rm tr}(k), \tag{29b}$$

where $f(\epsilon)$ is the Fermi-Dirac distribution, and $v_k = |\mathbf{v_k}|$ is the group velocity,

$$\mathbf{v_k} \;=\; \frac{1}{\hbar}\,\frac{\partial \epsilon_k}{\partial \mathbf{k}} = \frac{1}{\hbar}\,\hat{\mathbf{k}}\frac{\partial \varepsilon_k}{\partial k}.$$

For the dispersion (1b), $\mathbf{v_k}$ is given explicitly by,

$$\mathbf{v_k} \;=\; \frac{\varepsilon_0}{\varepsilon_k}\,\big(2Bm-1\big)\,\bigg(\frac{k^2}{q^2}-1\bigg)\,\frac{\hbar\mathbf{k}}{mv}, \tag{30}$$

where

$$\varepsilon_0 \;=\; mv^2.$$

The resistivity is directly related to the inverse of the transport relaxation time $\tau_{\rm tr}(k)$ that is expressible in terms of the phase shifts $\eta_l(k)$ (corresponding to angular moment l) appearing in the partial wave expansion of the electron scattering from the impurity [see Eq. (2.20) in Ref.[18]]. Explicitly,

$$\frac{1}{\tau_{\rm tr}(k)} = \frac{2c_{\rm imp}}{\pi\hbar\nu(k)}\sum_{l=1}^{\infty} l\sin^2\big[\eta_l(k)-\eta_{l-1}(k)\big], \tag{31}$$

where $\nu(k)$ is the bare density of states (DOS),

$$\nu(k) \;=\; \frac{1}{L^3}\sum_{\mathbf{k}'}\delta(\epsilon_k-\epsilon_{k'}), \tag{32}$$

$\delta(\epsilon)$ is the Dirac delta function and L is the linear size of the bulk. For the dispersion (1b), the DOS is

$$\nu(k) = \nu_1(\epsilon_k)+\nu_2(\epsilon_k), \tag{33a}$$

$$\nu_1(\epsilon) = \vartheta(|\epsilon|-\epsilon_q)\;\vartheta(\epsilon_0-|\epsilon|)\;\frac{\rho_c|\epsilon|g_1(\epsilon)}{2\sqrt{\epsilon^2-\epsilon_q^2}}, \tag{33b}$$

$$\nu_2(\epsilon) = \vartheta(|\epsilon|-\epsilon_q)\;\frac{\rho_c|\epsilon|g_2(\epsilon)}{2\sqrt{\epsilon^2-\epsilon_q^2}}, \tag{33c}$$

where

$$\rho_c = \frac{v}{4\pi^2B^2\hbar^3}\;\sqrt{Bm-\frac{1}{2}}, \tag{33d}$$

$$g_i(\epsilon) = \sqrt{1+\big(-1\big)^i\;\sqrt{\frac{\epsilon^2-\epsilon_q^2}{\epsilon_0^2-\epsilon_q^2}}}, \tag{33e}$$

$i=1,2$. Here $g_1(\epsilon)$ and $g_2(\epsilon)$ correspond to the two solutions of the equation $\epsilon_k=\epsilon$.

For pure s wave scattering, $\eta_0(k)=\delta_S(|\epsilon_k-\epsilon_F|)$ and $\eta_l=0$ for $l\neq 0$. Then Eq. (31) can be written as,

$$\frac{1}{\tau_{\rm tr}(k)} = \frac{2c_{\rm imp}}{\pi\hbar\nu(k)}\;\sin^2\delta_S(|\epsilon_k-\epsilon_F|). \tag{34}$$

The scattering phase $\delta_S(\omega)$ is given by Eq. (6). For $\omega=|\epsilon-\epsilon_F|\ll T_K$, $\delta_S(\omega)$ is given by eq. (7) for $S=\frac{1}{2}$ and by eq. (8) for $S=1$.

Zero temperature resistivity: As $T\to 0$ we can write

$$-\frac{\partial f(\epsilon)}{\partial \epsilon} \;=\; \delta(\epsilon-\epsilon_F). \tag{35}$$

Substituting Eq. (35) into Eq. (29b) and taking into account Eqs. (30), (6) and (33), we get

$$\sigma^{(0)}(0) \;=\; \frac{\pi e^2}{3n_{\rm imp}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\;\delta(\epsilon_k-\epsilon_F)\;v_k^2\;\nu(k).$$

When the Fermi energy is constrained according to

$$\varepsilon_q<\epsilon_F<\varepsilon_0,$$

the equation $\varepsilon_k=\epsilon_F$ has two solutions, $k=k_1$ and $k=k_2$, (see Fig. 1). The equation for the zero-temperature resistivity then takes the form,

$$\rho^{(0)}(0) = \frac{1}{\sigma^{(0)}(0)},\quad \sigma^{(0)}(0)=\sigma_1^{(0)}(0)+\sigma_2^{(0)}(0),$$
$$\sigma_i^{(0)}(0) = \frac{\pi e^2\nu_i^2(\epsilon_k)v_{k_i}^2}{3c_{\rm imp}},\quad i=1,2. \tag{36}$$

Finite temperature resistivity: When the temperature is below the Kondo temperature T_K, the conductivity (29b) can be written as,

$$\sigma^{(0)}(T) \;=\; \frac{e^2}{3\pi^2}\int_0^q \frac{k^2dk}{4T\cosh^2(\frac{\epsilon_k-\epsilon_F}{2T})}\;v_k^2\tau_{\rm tr}(k)\,+$$
$$+\;\frac{e^2}{3\pi^2}\int_q^\infty \frac{k^2dk}{4T\cosh^2(\frac{\epsilon_k-\epsilon_F}{2T})}\;v_k^2\tau_{\rm tr}(k).$$

Substitute into each of integrals a factor unity, $\int d\epsilon\;\delta(\epsilon-\varepsilon_k)$=1, and taking into account that for $k<q$ or $k>q$, the equation $\varepsilon_k=\epsilon$ has a single solution, $k_1(\epsilon)$

or $k_2(\epsilon)$ (see Fig. 1 for illustration), we can write

$$\sigma^{(0)}(T) = \frac{2e^2}{3}\int_{\epsilon_q}^{\epsilon_0}\frac{\nu_1(\epsilon)v_1^2(\epsilon)\tau_{\rm tr}(k_1(\epsilon))d\epsilon}{4T\cosh^2(\frac{\epsilon-\epsilon_F}{2T})} + \\ + \frac{2e^2}{3}\int_{\epsilon_q}^{\infty}\frac{\nu_2(\epsilon)v_2^2(\epsilon)\tau_{\rm tr}(k_2(\epsilon))d\epsilon}{4T\cosh^2(\frac{\epsilon_k-\epsilon_F}{2T})}, \quad (37)$$

where

$$v_i(\epsilon) \equiv v_{k_i(\epsilon)}, \qquad k_i(\epsilon) = qg_i(\epsilon), \qquad i = 1, 2,$$

and the functions $g_i(\epsilon)$ are given by Eq. (33e). Taking into account Eqs. (34) and (33a), we can write the conductivity (37) as,

$$\sigma^{(0)}(T) = \frac{\pi\hbar e^2}{3c_{\rm imp}}\int_{\epsilon_q}^{\epsilon_0}\frac{\nu_1^2(\epsilon)v_1^2(\epsilon)\sin^{-2}\left(\delta_S(|\epsilon-\epsilon_F|)\right)d\epsilon}{4T\cosh^2(\frac{\epsilon-\epsilon_F}{2T})} + \\ + \frac{\pi\hbar e^2}{3c_{\rm imp}}\int_{\epsilon_q}^{\infty}\frac{\nu_2^2(\epsilon)v_2^2(\epsilon)\sin^{-2}\left(\delta_S(|\epsilon-\epsilon_F|)\right)d\epsilon}{4T\cosh^2(\frac{\epsilon-\epsilon_F}{2T})}. \quad (38)$$

The integrands on the right hand side of Eq. (38) have a factor $\cosh^{-2}(\frac{\epsilon-\epsilon_F}{2T})$ which is equal to 1 for $\epsilon = \epsilon_F$ and rapidly vanishes for $\epsilon - \epsilon_F \gg T$. The behaviour of the other factors, $\nu_i^2(\epsilon)$ and $v_i^2(\epsilon)$ $(i = 1, 2)$, depends on the ratio $(\epsilon_F - \varepsilon_q)/T$. When $T \ll \epsilon_F - \varepsilon_q$, then $\nu_i^2(\epsilon)$ and $v_i^2(\epsilon)$ change slowly within the interval $|\epsilon - \epsilon_F| \lesssim T$ and can be safely replaced by $\nu_i^2(\epsilon_F)$ and $v_i^2(\epsilon_F)$. In what follows, we will assume the inequality $T_K \ll \epsilon_F - \varepsilon_q$.[2] Then for $T < T_K$ the conductivity (38) takes the form,

$$\sigma^{(0)}(T) = \sigma^{(0)}(0)\int_{-\infty}^{\infty}\frac{\sin^{-2}\left[\delta_S(|\epsilon|)\right]d\epsilon}{4T\cosh^2(\frac{\epsilon}{2T})}. \quad (39)$$

(The limits of the integration can safely be changed to $\mp\infty$). Finally, the impurity resistivity is,

$$\rho^{(0)}(T) = \rho^{(0)}(0)\left\{\int_{-\infty}^{\infty}\frac{\sin^{-2}\left(\delta_S(|\epsilon|)\right)d\epsilon}{4T\cosh^2(\frac{\epsilon}{2T})}\right\}^{-1}, \quad (40)$$

where $\rho^{(0)}(0) = 1/\sigma^{(0)}(0)$ is the zero temperature impurity resistivity, see Eq. (36).

Contribution of $\tilde{j}_f$ to the resistivity: The impurity resistivity for the KE with the SO(3) symmetry is given by Eq. (40). That for the KE with SO(4) symmetry is contributed also by the interaction of the f-impurity with the local Fermi liquid. In order to derive this contribution, we apply the perturbation poor man's scaling technique,

$$\delta\rho(T) = \frac{3R_0}{4}\,\tilde{j}_f^2(T), \quad (41)$$

where $\tilde{j}_f(T)$ is given by Eq. (16). The constant R_0 is,

$$R_0 = \frac{3\pi c_{\rm imp}}{\hbar e^2\rho_{\rm c}^2}\,\frac{1}{v_1^2+v_2^2}, \quad (42)$$

where

$$v_i = v_{k_i}, \qquad i = 1, 2,$$

k_i are two solutions of the equation $\varepsilon_k = \epsilon_F$, see Fig. 1. Hence, the resistivity for the SO(4) KE reads,

$$\rho(T) = \rho^{(0)}(T) + \delta\rho(T), \quad (43)$$

where $\rho^{(0)}(T)$ is given by Eq. (40). The resistivity (40)

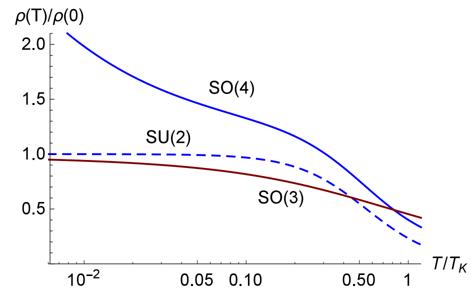

FIG. 5: (Color online) Resistivity (40) as a function of temperature for the SO(3) and SU(2) symmetries (solid red and dashed blue curves), and the resistivity (43) for the SO(4) KE (solid blue curve).

as a function of temperature is shown in Figure 5 for the SO(4), SO(3) and SU(2) symmetries. Recall that as $T \ll T_K$, the resistivity for the SU(2) symmetry is given by,

$$\rho^{(0)}(T) \approx \rho^{(0)}(0)\left\{1 - \frac{\pi^2T^2}{3T_K^2} + O\left(\frac{T^4}{T_K^4}\right)\right\}. \quad (44)$$

This behaviour is typical for the Fermi liquid zero temperature fixed point. Deviation from Eq. (44) in the curves for the SU(2) and SO(4) KE is due to the Kondo interaction between the f-impurity and the local Fermi liquid. The temperature dependence of the resistivity for the SO(3) symmetry is rather distinct. Indeed, for $T \ll T_K$, we can write

$$\rho^{(0)}(T) \approx \rho^{(0)}(0)\left\{1 - \frac{\pi^2}{16\ln^2\left(\frac{T_K}{2T}\right)} + \\ + O\left(\ln^{-3}\left(\frac{T_K}{T}\right)\right)\right\}. \quad (45)$$

The singular temperature dependence of the resistance is the result of the singular energy dependence of the scattering phase (6).

VIII. CONCLUSIONS

The present work is motivated by the quest to elucidate the elusive SFL behavior within bulk materials.

This property, associated with USKE, has so far been observed only in electron tunneling experiments through quantum dots[14–16], where it is demonstrated that the tunneling conductance G approaches the unitary limit as $T \to 0$, but the derivative dG/dT diverges logarithmically. Elucidating SFL in metals based on the USKE (e.g iron immersed in cupper) is not obvious because magnetic impurities with high spin give rise to Coqblin-Schrieffer type of scattering which falls on a regular Fermi liquid fixed point[18]. Here we achieved this goal by analyzing Kondo scattering of electrons off an Anderson impurity in a 3D topological insulator with an "inverted Mexican hat" band dispersion. We used the fact that the interplay between the Anderson impurity and its induced in-gap bound state results in self-screened Kondo effect or in the Kondo effect with SO(4) or SO(3) dynamical symmetries. Using the conformal field theory technique, we have calculated the low temperature ($T \ll T_K$) dependence of the specific heat, the magnetic susceptibility and the electric resistivity of the impurity for both screened and under-screened Kondo effect. Physical properties of the impurity for the under-screened case demonstrate zero temperature singularity which corresponds to a singular Fermi liquid phase. In addition to the SFL behavior exposed here, this system exposes an interesting screening mechanism where the impurity f is screened by the quasi-particles of the Fermi sea that is formed when the band electrons and the d impurity form a singlet state at $T < T_K$.

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Appendix A: Anderson Model and Scaling Equations

Part of the material presented in this appendix has already been developed in our previous paper[2] where we analyzed the same system in the weak coupling regime. It is included here for the sake of self-consistency. In the first part we write down the bare Anderson model and specify the peculiarities resulting from the special form of the band structure. In the second part we elaborate on the scaling equations and RG flow for the SO(4) dynamical symmetry.

1. Anderson Model

The system considered here is schematically displayed in Fig. 6a. It consists of a topological insulator whose energy band has the "inverted mexican hat" structure, and an Anderson impurity immersed in its bulk (denoted as d-impurity). Potential scattering of electrons on the impurity result in the formation a mid-gap localized energy level[2], denoted hereafter as an f-impurity. The effective Hamiltonian of the system is,

$$H \;=\; H_0 + H_c + H_t. \tag{A1}$$

Here the first term, H_0, is the Hamiltonian (1a) describing electrons in the bulk of the TI.

The second term on the right hand side of eq. (A1) is the Hamiltonian of the isolated CQI, composed of the d- and f-levels,

$$H_c \;=\; H_d + H_f + H_{df}. \tag{A2a}$$

Here H_d and H_f are the (atomic) Hamiltonians of the d- and f-impurities, and H_{df} describes the hybridization between them,

$$H_d \;=\; \epsilon_d \sum_\sigma n_{d\sigma} + U_d n_{d\uparrow} n_{d\downarrow}, \tag{A2b}$$

$$H_f \;=\; \epsilon_f \sum_\sigma n_{f\sigma} + U_f n_{f\uparrow} n_{f\downarrow}, \tag{A2c}$$

$$H_{df} \;=\; V_{df} \sum_\sigma \left(f^\dagger_\sigma d_\sigma + d^\dagger_\sigma f_\sigma \right), \tag{A2d}$$

where ϵ_d or ϵ_f is the d- or f-impurity energy level and U_d or U_f is the interaction between electrons on the impurity. Here $n_{d\sigma} = d^\dagger_\sigma d_\sigma$, $n_{f\sigma} = f^\dagger_\sigma f_\sigma$, $d^\dagger_\sigma$ or d_σ is the creation or annihilation operator of electron on the d-level, $f^\dagger_\sigma$ or f_σ is the creation or annihilation operator of electron on the f-level.

The last term on the right hand side of eq. (A1), H_t, is the hybridization between the Anderson impurity d and the band electrons,

$$H^{(0)}_t = V_d \sum_{\mathbf{k},\nu,\sigma} \left(\gamma^\dagger_{\nu\mathbf{k}\sigma} d_\sigma + d^\dagger_\sigma \gamma_{\nu\mathbf{k}\sigma} \right). \tag{A3}$$

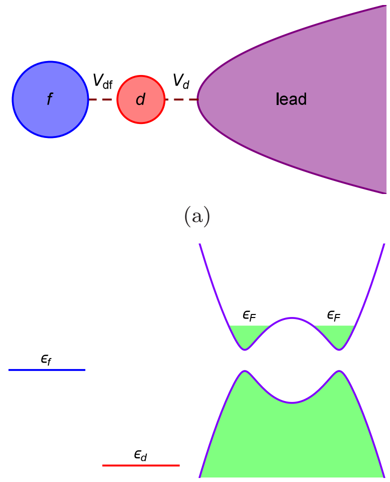
Note that hybridization prevails only between the band electrons and the d impurity. The f-level is formed as a result of the potential scatering of the conduction band electron on the d-impurity[2]. Therefore, hybridization of f-impurity and the band electrons is absent.

Energy scales: Few words about energy scales are in order: Unless otherwise specified, we shall assume that $U_d \to \infty$ and

$$\epsilon_F - D_0 < \epsilon_d \ll \epsilon_f < \epsilon_F < \epsilon_f + U_f \ll \epsilon_F + D_0, \tag{A4}$$

where D_0 (the initial bandwidth) is the highest energy cutoff, and ϵ_F is the Fermi energy (see Figure 6). In the calculations below we use $\epsilon_F = 2\varepsilon_q$, $\epsilon_f \approx -\varepsilon_q$, $U_f = 5\varepsilon_q$ and $\epsilon_d = -80\varepsilon_q$.

The eigenstates of H_c, equation (A2a), are specified by the configuration numbers (N_d, N_f) indicating the number of electrons on the levels d and f. With energy scales specified in Eq. (A4), the ground state (GS) 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 $V_{df} \neq 0$



(a)

(b)

FIG. 6: (Color online) **Panel (a)**: Illustration of the Anderson model consisting of a band, d- and f-impurities. The hybridization rates of the d-impurity with the band and the f-impurity are V_d and V_{df}, respectively. **Panel (b)** Energy dispersion (1b), and energy levels ϵ_d and ϵ_f. Here ϵ_F denotes the Fermi energy. All the energy levels of the band below the Fermi energy are occupied (green area), whereas the white area above ϵ_F denotes unoccupied levels.

while the triplet energy is unaffected. Explicitly,

$$|S\rangle = \left\{\frac{\alpha_S}{\sqrt{2}}\Big(d^\dagger_\uparrow f^\dagger_\downarrow - d^\dagger_\downarrow f^\dagger_\uparrow\Big) - \beta_f f^\dagger_\uparrow f^\dagger_\downarrow\right\}|0\rangle, \quad \text{(A5a)}$$

$$|T_1\rangle = d^\dagger_\uparrow f^\dagger_\uparrow|0\rangle, \qquad |T_{-1}\rangle = d^\dagger_\downarrow f^\dagger_\downarrow|0\rangle,$$
$$|T_0\rangle = \frac{1}{\sqrt{2}}\Big\{d^\dagger_\uparrow f^\dagger_\downarrow + d^\dagger_\downarrow f^\dagger_\uparrow\Big\}|0\rangle, \quad \text{(A5b)}$$

where

$$\varepsilon_S = \epsilon_d + \epsilon_f - \frac{2V_{df}^2}{\Delta_f}, \qquad \varepsilon_T = \epsilon_d + \epsilon_f,$$
$$\alpha_S = \sqrt{1-\beta_f^2}, \qquad \beta_f = \frac{\sqrt{2}V_{df}}{\Delta_f},$$
$$\Delta_f = \epsilon_f - \epsilon_d + U_f.$$

In the absence of hybridization of d-electron with the band electrons (i.e., when $V_d = 0$), $\varepsilon_S < \varepsilon_T$: As expected, the singlet state has lower energy than the triplet state.

2. Scaling Equations for the SO(4) Dynamical Symmetry

In order to perform the RG analysis considered in Sec. IV [see Eq. (15)], we need the effective coupling $j_f(T_{K_4})$ at the effective bandwidth equal to T_{K_4}. To derive $j_f(T_{K_4})$, we apply the weak coupling RG analysis for the SO(4) KE. In the the weak coupling regime, the scaling equations for the dimensionless couplings $j_d = J_d\rho_0$ and $j_f = J_f\rho_0$ must proceed to third order in these parameters[18], that is,

$$\frac{\partial j_d}{\partial \ln D} = -j_d^2 + j_d\big(j_d^2 + j_f^2\big), \quad \text{(A6a)}$$
$$\frac{\partial j_f}{\partial \ln D} = -j_f^2 + j_f\big(j_d^2 + j_f^2\big). \quad \text{(A6b)}$$

The initial values of j_d and j_f at $D - D_{ii}$ are $J_d\rho_c$ and $J_f\rho_c$, where J_d and J_f are given by Eq. (4a). Scaling of

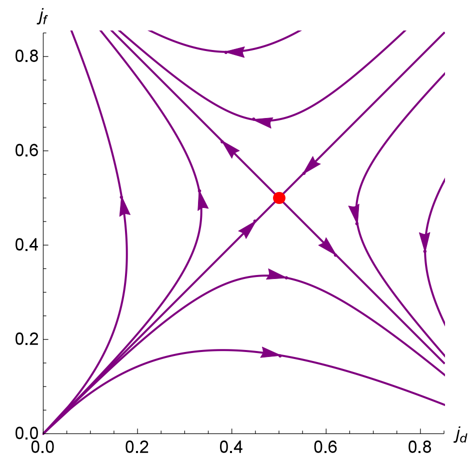


FIG. 7: (Color online) Scaling of j_d and j_f.

j_d and j_f is shown in the flow diagram, Fig. 7. The red dot denotes the two-channel fixed point $j_d^* = j_f^* = 1/2$. We are interested in the solution of these equations under the following inequalities:

$$j_f(D_{ii}) \ll j_d(D_{ii}) \ll 1,$$

so that we are far away from the two-channel fixed point. In this case $j_d(D)$ increases when D decreases, whereas $j_f(D)$ decreases and goes to zero when D vanishes. The solution of the scaling equation (A6a) can be approximated as,

$$j_d(D) = \frac{1}{\ln\left(\dfrac{D}{T_{K_4}}\right)}, \quad \text{(A7)}$$

where the scaling invariant, the Kondo temperature T_{K_4}, is

$$T_{K_4} = D_{ii}\ \exp\left\{-\frac{1}{J_d\rho_c}\right\}. \quad \text{(A8)}$$

The solution (A7) is valid just for $D \gg T_{K_4}$. A more satisfactory approximation is given in Ref.[18],

$$j_d(D) = \sqrt{\frac{8}{3\pi^2}}\sqrt{1 - \frac{\ln\left(\dfrac{D}{T_{K_4}}\right)}{\sqrt{\ln^2\left(\dfrac{D}{T_{K_4}}\right) + \dfrac{3\pi^2}{4}}}}. \quad \text{(A9)}$$

The solution of the scaling equation (A6b) is,

$$\frac{j_f(D)}{j_f(D_{ii})} \;=\; \exp\left\{-\int\limits_{D}^{D_{ii}}\frac{d\epsilon}{\epsilon}\;j_d^2(\epsilon)\right\}. \qquad \text{(A10)}$$

Taking into account eq. (A9), we get

$$\frac{j_f(D)}{j_f(D_{ii})} \;=\; \exp\left\{\frac{8}{3\pi^2}\Big(\mathcal{F}(D_{ii})-\mathcal{F}(D)\Big)\right\},$$

where

$$\mathcal{F}(D) \;=\; \sqrt{\ln^2\left(\frac{D}{T_{K_4}}\right)+\frac{3\pi^2}{4}}-\ln\left(\frac{D}{T_{K_4}}\right).$$

When D approaches T_{K_4}, $j_f(T_{K_4})$ can be approximated as

$$j_f(T_{K_4}) \;=\; j_f\big(D_{ii}\big)\;\exp\left\{-\frac{4}{\sqrt{3}\pi}\right\} \;\approx\; \approx\; 0.5 j_f\big(D_{ii}\big), \qquad \text{(A11)}$$

where we take into account that $D_{ii} \gg T_{K_4}$.

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