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Quantum impurity on the surface of a topological insulator

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It is shown that the Hamiltonian for a quantum magnetic impurity on the surface of a topological insulator can be mapped to the conventional pseudogap Anderson impurity model, albeit the combinations of the continuum states which hybridize with the impurity have more complex structure in the reciprocal and spin space. If the Fermi level is away from the Dirac point, the impurity is predicted to be fully screened at low-enough temperatures, i.e., there are no residual degrees of freedom.

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Due to the spin-orbit coupling, insulators in the class of "topological insulators" have nontrivial topological properties of the bulk band structure, which results in the presence of peculiar metallic states on their surfaces.[1–3] Recently studied materials such as Bi_2Se_3 and Bi_2Te_3 show topological-insulator behavior even at high temperatures and have the simplest allowed surface states: a single nondegenerate Dirac cone.[4–6] These surface states have a characteristic relation between the momentum and spin, which makes the surface electrons insensitive to scattering by impurities since a backscattering event would require the electron spin to be flipped, yet this is prohibited by the time-reversal symmetry.[7–11] Recent Fourier-transform scanning tunneling spectroscopy (FT-STS) experiments have confirmed this prediction.[7,9,10] Such topological-insulator materials may find applications in spintronics[5] and quantum computing.[12]

The surface-state electrons on topological insulators have definite chirality and for the nondegenerate states near the Dirac point one has $\langle \mathbf{s}(-\mathbf{k})\rangle = -\langle \mathbf{s}(\mathbf{k})\rangle$.[2,10,11] Such surface states are expected to be perturbed differently by nonmagnetic and magnetic impurities. The time-reversal symmetry-breaking perturbations allow scattering between the time-reversed states $|\mathbf{k},\uparrow\rangle$ and $|-\mathbf{k},\downarrow\rangle$.[11] The case of classical spins (which clearly break the time-reversal symmetry) has been explored in Ref. 13, where it was predicted that the impurity opens up a local gap and suppresses the local density of states. Scattering on static spin-dependent impurity potential was also addressed in Refs. 11 and 14, where characteristic interference features were predicted to be observable by spin-polarized FT-STS. The description of a magnetic impurity in terms of classical/static spin is, however, a rather crude approximation; magnetic impurities are dynamic objects and should be described using quantum impurity models.[15] For impurities described, for example, by the Anderson impurity model,[16] the local moment of a quantum impurity may be compensated at low temperatures by the Kondo effect.[15,17–20] Kondo screened impurities are effectively nonmagnetic, thus the extent of backscattering on magnetic adsorbates will critically depend on the degree of screening of the local moment by the surface-state electrons.[10] Due to the spin-orbit coupling, there is no SU(2) symmetry in the spin sector alone,[8] therefore it is not immediately clear how effectively the impurity spin can be screened by the chiral (or helical) surface-state electrons. In Ref. 21, this problem has been approached using the Varma-Yafet variational Ansatz. Only partial screening (one third) of the local moment was found and $1/T$ Curie-type magnetic-susceptibility behavior was predicted at low temperatures. In variational methods, there are no *a priori* guarantees that the correlation functions are correct. In addition, the variational Ansatz which projects out the double occupancy of the impurity might itself be problematic. For this reason, the deduction of the one-third screening from the spin-spin correlation functions is uncertain. In this work, this problem is reconsidered by a different approach, showing that the effective quantum impurity model actually takes a very simple form of the conventional single-channel Anderson impurity model, even though the nature of the hybridizing combinations of the conduction-band states is indeed nontrivial. For the generic situation with the Dirac point away from the Fermi level, the local moment will be screened below the Kondo temperature T_K, and the impurity would become effectively nonmagnetic. No anomalies are expected in the low-temperature thermodynamics in this case. Since the experimental studies of magnetically doped topological insulators are already under way,[22] it is important to arrive at better understanding of the Kondo effect in the case of chiral surface-state electrons.

In the simplest case, the surface-state electrons on the surface of a topological insulator may be described by the Hamiltonian[13]

$$H_0 = \sum_{\mathbf{k},\alpha,\beta} \psi^\dagger_{\mathbf{k}\alpha} h_{\alpha\beta}(\mathbf{k}) \psi_{\mathbf{k}\beta},$$

$$h_{\alpha\beta}(\mathbf{k}) = \hbar v_F (k_x \sigma^x_{\alpha\beta} + k_y \sigma^y_{\alpha\beta}), \tag{1}$$

where $\mathbf{k}=\{k_x,k_y\}$ is a two-dimensional (2D) vector in the reciprocal space of the surface-state band, α and β are spin indexes ($\uparrow$ or $\downarrow$), v_F is the Fermi velocity, and $\sigma^{x,y}$ are the Pauli matrices.[23] The σ matrix is proportional to real spin.[24] We write $\mathbf{k}=k\{\cos\phi,\sin\phi\}$, where $k=|\mathbf{k}|$, and we introduce the energy $\epsilon_k=\hbar v_F k$. We write

$$M_{\alpha\beta}(\phi) \equiv (\cos\phi\sigma^x + \sin\phi\sigma^y)_{\alpha\beta} = \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix} \tag{2}$$

and thus $h_{\alpha\beta}(\mathbf{k}) = \epsilon_k M_{\alpha\beta}(\phi)$. The hybridization term is

$$H_{\mathrm{hyb}} = \sum_{\mathbf{k},\alpha} V_{\mathbf{k}\alpha} d_\alpha^\dagger \psi_{\mathbf{k}\alpha} + V_{\mathbf{k}\alpha}^* \psi_{\mathbf{k}\alpha}^\dagger d_\alpha, \tag{3}$$

where $d^\dagger$ and d are the creation and annihilation operator for the impurity electron. In this work we take $V_{\mathbf{k}\alpha}=V_{\mathbf{k}}$; this is an approximation since the surface states labeled by the spin index σ are not eigenstates of S_z. The impurity Hamiltonian is simply

$$H_{\mathrm{imp}} = \sum_\alpha \epsilon n_\alpha + U n_\uparrow n_\downarrow, \tag{4}$$

where $n_\alpha = d_\alpha^\dagger d_\alpha$ is the occupancy of the spin α level, ϵ is the impurity energy level, and U the on-site electron-electron repulsion.

The reduction of the problem to an effective one-dimensional quantum impurity problem is analogous to the derivations in Ref. 25 but performed for the 2D case. We go from the discrete $\mathbf{k}$ to the continuous vectors $\mathbf{k}$ in the standard way, $\frac{1}{N}\Sigma_{\mathbf{k}} \to \frac{1}{(2\pi)^2}\int d^2\mathbf{k}$, where N is the number of the surface states, and the components of the wave vector on the right-hand side run from $-\pi$ to π. The continuum operators that correspond to $\psi_{\mathbf{k}\alpha}$ are $a_{\mathbf{k}\alpha}$ and they are normalized as $\{a_{\mathbf{k}\alpha}, a_{\mathbf{k}'\alpha'}^\dagger\} = \delta(\mathbf{k}-\mathbf{k}')\delta_{\alpha,\alpha'}$, thus the mapping of the operators is $\psi_{\mathbf{k}\alpha} \to (2\pi/\sqrt{N}) a_{\mathbf{k}\alpha}$. This leads to

$$H_0 = \sum_{\alpha,\beta} \int d^2\mathbf{k} a_{\mathbf{k}\alpha}^\dagger h_{\alpha\beta}(\mathbf{k}) a_{\mathbf{k}\beta},$$

$$H_{\mathrm{hyb}} = \sum_\alpha \frac{\sqrt{N}}{2\pi} \int d^2\mathbf{k} V_{\mathbf{k}} d_\alpha^\dagger a_{\mathbf{k}\alpha} + \mathrm{H.c.} \tag{5}$$

In the next step we expand the operators $a_{\mathbf{k}\alpha}$ in the azimuthal components. In fact, we allow for a slightly more general Ansatz

$$a_{\mathbf{k}\alpha} = \frac{1}{\sqrt{k}} \frac{1}{\sqrt{2\pi}} \sum_{m,\beta} e^{im\phi} U_{\alpha\beta}(\phi) c_{km\beta}, \tag{6}$$

where U is some unitary matrix which may depend on the azimuthal angle ϕ while $m \in \mathbb{Z}$. The operators $c_{km\beta}$ are normalized as

$$\{c_{km\beta}, c_{k'm'\beta'}^\dagger\} = \delta(k-k')\delta_{m,m'}\delta_{\beta,\beta'}. \tag{7}$$

The inverse transformation is

$$c_{km\beta} = \sqrt{k} \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} d\phi e^{-im\phi} \sum_\alpha U_{\alpha\beta}^\dagger(\phi) a_{\mathbf{k}\alpha}. \tag{8}$$

The matrix M in Eq. (2) may be diagonalized using the unitary matrix

$$W = \begin{pmatrix} 0 & e^{-i\phi/2} \\ e^{i\phi/2} & 0 \end{pmatrix} e^{-i\sigma^y \pi/4} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi/2} & e^{-i\phi/2} \\ e^{i\phi/2} & e^{i\phi/2} \end{pmatrix}, \tag{9}$$

which gives $W^\dagger M W = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right) = \sigma^z$. The transformation matrix W has period 4π, which reflects that a quantized Berry's phase of π is acquired by an electron circling the Fermi arc, as characteristic for a "topological metal" surface phase where the Fermi arc encloses a single Dirac point.[2,6]

Choosing $U=W$ in Eq. (6), we obtain a simple diagonal form for the band Hamiltonian

$$H_0 = \sum_{m,\sigma} \int dk \epsilon_{k\sigma} c_{km\sigma}^\dagger c_{km\sigma}, \tag{10}$$

with $\epsilon_{k\uparrow} = \epsilon_k$ and $\epsilon_{k\downarrow} = -\epsilon_k$. The density of states is

$$\rho_\sigma(\epsilon) = \frac{N}{(2\pi)^2} \int d^2\mathbf{k} \delta(\epsilon - \epsilon_{k\sigma}) = \frac{N}{2\pi} \frac{1}{(\hbar v_F)^2} |\epsilon| \theta_\sigma(\epsilon), \tag{11}$$

where $\theta_\uparrow(x) = \theta(x)$ and $\theta_\downarrow(x) = \theta(-x)$, with $\theta(x)$ the Heaviside step function. Thus $\sigma=\uparrow$ corresponds to the upper Dirac cone and $\sigma=\downarrow$ to the lower Dirac cone.

For simplicity, we will at first assume the hopping constants $V_{\mathbf{k}}$ to be isotropic in the 2D space, i.e., $V_{\mathbf{k}} = V_k$. Such $\mathbf{k}$ dependence corresponds, for example, to the $d_{3z^2-r^2}$ impurity orbital. The hybridization term then transforms as

$$H_{\mathrm{hyb}} = \frac{\sqrt{N}}{2\pi} \sum_{\alpha,\beta} \int \sqrt{k} dk V_k \times \left[\frac{1}{\sqrt{2\pi}} \int d\phi \sum_{m,\beta} e^{im\phi} W_{\alpha\beta}(\phi) \right] d_\alpha^\dagger c_{km\beta} + \mathrm{H.c.} \tag{12}$$

Noting that for integer m

$$\frac{1}{\sqrt{2}} \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{i(m\pm 1/2)\phi} = \frac{1}{\sqrt{2}} \frac{1}{2\pi} \frac{4i}{2m \pm 1} \equiv \gamma_m^\pm, \tag{13}$$

we obtain

$$H_{\mathrm{hyb}} = \frac{\sqrt{N}}{\sqrt{2\pi}} \sum_{m,\alpha,\beta} \int \sqrt{k} dk V_k \times \begin{pmatrix} \gamma_m^- & \gamma_m^- \\ \gamma_m^+ & \gamma_m^+ \end{pmatrix}_{\alpha\beta} d_\alpha^\dagger c_{km\beta} + \mathrm{H.c.} \tag{14}$$

Finally, we introduce the energy representation by defining $c_{\epsilon m\sigma} = (d\epsilon_{k\sigma}/dk)^{-1/2} c_{km\sigma}$, with $\epsilon = \epsilon_{k\sigma}$. The normalization then becomes $\{c_{\epsilon m\sigma}, c_{\epsilon' m\sigma'}^\dagger\} = \delta(\epsilon-\epsilon')\delta_{m,m'}\delta_{\sigma,\sigma'}$. Note that $\epsilon \geq 0$ for $\sigma=\uparrow$ and $\epsilon \leq 0$ for $\sigma=\downarrow$. We introduce an upper energy cutoff for $\sigma=\uparrow$ at $+D$ (the lower limit is 0) and a lower energy cutoff for $\sigma=\downarrow$ at $-D$ (the upper limit is 0). We then obtain

$$H_0 = \sum_m \int_0^D d\epsilon \epsilon c_{\epsilon m\uparrow}^\dagger c_{\epsilon m\uparrow} + \sum_m \int_{-D}^0 d\epsilon \epsilon c_{\epsilon m\downarrow}^\dagger c_{\epsilon m\downarrow}. \tag{15}$$

For the hybridization term we have

$$\begin{aligned} \frac{\sqrt{N}}{\sqrt{2\pi}} \int \sqrt{k} dk V_k c_{km\beta} &= \frac{\sqrt{N}}{\sqrt{2\pi}} \int \sqrt{k} dk \left(\frac{d\epsilon_{k\beta}}{dk} \right)^{1/2} V_k c_{\epsilon m\beta} \\ &= \frac{\sqrt{N}}{\sqrt{2\pi}} \int \sqrt{k_\epsilon} d\epsilon \left(\frac{dk}{d\epsilon_{k\beta}} \right)^{1/2} V(\epsilon) c_{\epsilon m\beta} \\ &= \int d\epsilon [\rho_\beta(\epsilon)]^{1/2} V(\epsilon) c_{\epsilon m\beta} \end{aligned} \tag{16}$$

since the density of states is $\rho_\sigma(\epsilon)=(N/2\pi)k_\epsilon|dk/d\epsilon|$. We conclude that

$$H_{\rm hyb}=\sum_{m,\alpha,\beta}\int d\epsilon\sqrt{\rho_\beta(\epsilon)}V(\epsilon)\begin{pmatrix}\gamma_m^- & \gamma_m^-\\ \gamma_m^+ & \gamma_m^+\end{pmatrix}_{\alpha\beta} d_\alpha^\dagger c_{\epsilon m\beta}+\text{H.c.} \tag{17}$$

The hybridization function is defined as $\Gamma_\sigma(\epsilon)=\pi\rho_\sigma(\epsilon)|V(\epsilon)|^2$. Since the coupling to a continuum of states in a quantum impurity model is fully defined by its hybridization function $\Gamma(\epsilon)$, we replace $\sqrt{\rho_\beta(\epsilon)}V(\epsilon)$ by $\sqrt{\Gamma_\beta(\epsilon)/\pi}$ in the following.

We now introduce the combinations of states

$$g_{\epsilon\sigma}=\frac{1}{\tau}\sum_m \gamma_m^+ c_{\epsilon m\sigma},$$

$$h_{\epsilon\sigma}=\frac{1}{\tau}\sum_m \gamma_m^- c_{\epsilon m\sigma}, \tag{18}$$

where the normalization factor τ is defined as

$$\tau=\left[\sum_m(\gamma_m^\pm)^2\right]^{1/2}=\sqrt{2}. \tag{19}$$

The two sets g and h are (canonical) fermionic operators, $\{g_{\epsilon\sigma},g_{\epsilon'\sigma'}^\dagger\}=\delta(\epsilon-\epsilon')\delta_{\sigma\sigma'}$ and likewise for h, and they are orthogonal to each other: $\{g_{\epsilon\sigma},h_{\epsilon'\sigma'}^\dagger\}=0$.

We obtain

$$H_0=\int_0^D d\epsilon\epsilon g_{\epsilon\uparrow}^\dagger g_{\epsilon\uparrow}+\int_{-D}^0 d\epsilon\epsilon g_{\epsilon\downarrow}^\dagger g_{\epsilon\downarrow}+\int_0^D d\epsilon\epsilon h_{\epsilon\uparrow}^\dagger h_{\epsilon\uparrow}+\int_{-D}^0 d\epsilon\epsilon h_{\epsilon\downarrow}^\dagger h_{\epsilon\downarrow},$$

$$H_{\rm hyb}=\int d\epsilon\sqrt{\Gamma(\epsilon)/\pi}\tau(\theta_\uparrow(\epsilon)d_\uparrow^\dagger h_{\epsilon\uparrow}+\theta_\downarrow(\epsilon)d_\uparrow^\dagger h_{\epsilon\downarrow}+\theta_\uparrow(\epsilon)d_\downarrow^\dagger g_{\epsilon\uparrow}+\theta_\downarrow(\epsilon)d_\downarrow^\dagger g_{\epsilon\downarrow})+\text{H.c.} \tag{20}$$

We introduced $\Gamma(\epsilon)=\Gamma_\uparrow(\epsilon)+\Gamma_\downarrow(\epsilon)$, which is nonzero for all ϵ except at $\epsilon=0$, where there is a linear pseudogap in the density of states. In H_0 we omitted writing those combinations of the conduction-band states which do not couple to the impurity, as they play no role in the following.

We note that the impurity spin-up orbital only couples to the h states, and the impurity spin-down orbital only to the g states. Since the g and h states are only defined for the combinations $\epsilon\geq 0$, $\sigma=\uparrow$ and $\epsilon\leq 0$, $\sigma=\downarrow$, we may actually drop the spin label and write

$$g_\epsilon=\theta_\uparrow(\epsilon)g_{\epsilon\uparrow}+\theta_\downarrow(\epsilon)g_{\epsilon\downarrow},$$

$$h_\epsilon=\theta_\uparrow(\epsilon)h_{\epsilon\uparrow}+\theta_\downarrow(\epsilon)h_{\epsilon\downarrow}. \tag{21}$$

Thus we are dealing with two channels of spinless electrons (defined for all ϵ) with a pseudogap density of states. The Hamiltonian is then

$$H_0=\int_{-D}^D d\epsilon\epsilon(g_\epsilon^\dagger g_\epsilon+h_\epsilon^\dagger h_\epsilon),$$

$$H_{\rm hyb}=\int_{-D}^D d\epsilon\sqrt{\Gamma(\epsilon)/\pi}\tau(d_\uparrow^\dagger h_\epsilon+d_\downarrow^\dagger g_\epsilon)+\text{H.c.} \tag{22}$$

As a final step, the particle-type label h and g can be replaced by a (pseudo)spin label, i.e., $b_{\epsilon\uparrow}=h_\epsilon$ and $b_{\epsilon\downarrow}=g_\epsilon$. The operators $b_{\epsilon\sigma}$ are canonical fermionic operators. The final Hamiltonian takes the form of the regular single-impurity Anderson model (compare with Ref. 25)

$$H_0=\sum_\sigma\int_{-D}^D d\epsilon\epsilon b_{\epsilon\sigma}^\dagger b_{\epsilon\sigma},$$

$$H_{\rm hyb}=\sum_\sigma\int_{-D}^D d\epsilon\sqrt{\Gamma(\epsilon)/\pi}\tau d_\sigma^\dagger b_{\epsilon\sigma}+\text{H.c.} \tag{23}$$

The end result of the derivation is thus trivial in its form, as the low-energy effective model corresponds to the conventional Anderson impurity model (with a pseudogap in the hybridization function). Nevertheless, it should be noted that the operators $b_{\epsilon\sigma}$ correspond to a rather complicated combination of the original conduction-band electron states. Recently, formally the same effective model has been studied in the context of Anderson impurities adsorbed on a graphene layer.[26] It is interesting to note that despite the differences between the physical content of the Hamiltonian in these two different cases (as already observed in Refs. 13 and 21) the effective impurity model in a suitably transformed basis is the same. It should also be noted that this reduction is only possible starting from an Anderson-type impurity model. Starting from a Kondo-type impurity model, $H_K=J\mathbf{S}\cdot(\Sigma_{kk'\alpha\beta}\psi_{k\alpha}^\dagger\boldsymbol{\sigma}_{\alpha\beta}\psi_{k'\beta})$, we would end up with an effective model with an infinite number of channels (index m) because there is no equivalent of Eq. (18) to perform a separation of the linear combinations of states. If a spin-only model is desired, the Schrieffer-Wolff transformation has to be performed as the last step of the derivation.

For orbitals which couple with the continuum via $V_{\mathbf{k}}$ which depends on the azimuthal angle, a similar result would ensue. For example, for d_{xz} and d_{yz} we have $V_{\mathbf{k}}=V_k\cos\phi$ and $V_{\mathbf{k}}=V_k\sin\phi$, respectively, while for $d_{x^2-y^2}$ and d_{xy} we have $V_{\mathbf{k}}=V_k\cos 2\phi$ and $V_{\mathbf{k}}=V_k\sin 2\phi$, respectively. It easy to see, however, that the angular additional factors corresponds to a mere shift of m by 1 or 2 in Eq. (13), thus we end up with the same effective model, although with different combinations of continuum states coupling to the impurity. Of course, the Fermi surface/line is not axially symmetric either but rather reflects the symmetry of the lattice (for example, due to warping effects resulting from the higher-order spin-orbit coupling terms, the Fermi surface in the case of Bi_2Te_3 has a hexagram/hexagon shape and becomes circular only in the vicinity of the Dirac point[5,8]). Again, this only affects the combinations of states which couple with the impurity orbital, however, it does not change the results in a qualitative way.

The properties of the Anderson impurity in pseudogap

Fermi baths are well known:[27,28] for a linear pseudogap, $\rho \propto |\omega|$, the system flows to a local-moment (LM) fixed point where the impurity is effectively decoupled from the conduction states and remains unscreened at low temperatures, unless the hybridization Γ is strong enough. The LM fixed point for $\epsilon_F=0$ is very resilient to various perturbation; in particular, it persists for a large range of parameters away from the particle-hole symmetric point.[28] With ϵ_F away from the Dirac point, however, the density of states is finite and the impurity is screened in the conventional Kondo effect, thus the system flows to the strong-coupling fixed point. In topological insulators, unlike in graphene, there is no *a priori* reason for the Fermi level to sit at the Dirac point, thus the impurity will typically undergo Kondo screening at some low-enough temperature T_K. The impurity contribution to the total entropy S_{imp} is 0 much below T_K,[15,19,25] which implies that despite a complex structure in the spin/reciprocal space, no anomalies are expected in the low-temperature thermodynamics (including the magnetic susceptibility): the impurity spin is fully screened (not one-third screened[21]). This does not preclude a complex structure of the Kondo cloud, which might indeed exhibit nontrivial spatial and spin dependence. It is, however, unclear whether these features could ever be directly observed since the Kondo cloud is rather elusive.

An Anderson-model-type magnetic impurity on the surface of a topological insulator may be fully Kondo screened. For temperature much below the Kondo temperature T_K, the backscattering of the surface-state electrons will be prohibited, as in the case of nonmagnetic adsorbates. No opening of the gap in the surface-state band is expected in this regime. At temperatures above T_K, however, the spin-flip scattering events will connect the points on the opposite sides of the Fermi surfaces. The possible opening of the gap might be, however, masked be thermal smearing effects. On the other hand, for ferromagnetically Kondo coupled impurities or for large-spin impurities with easy-axis magnetic anisotropy, Kondo screening is noneffective and strong scattering effects may indeed be expected. Further work should explore the behavior of multiorbital impurity models and take into account the full spin and orbital structure of the hybridization parameters $V_{k\alpha,m\beta}$, where m is the impurity orbital index while α and β are the spin indexes of surface and impurity states, respectively.

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