Tunable Dirac-point resonance induced by a STM-coupled Anderson impurity on a topological insulator surface

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Abstract

The interaction effect between the surface states of a topological insulator (TI) and a STM-coupled Anderson impurity is studied by using equations of motion of the Green’s functions. Remarkably, we show that when a coupling between the Anderson impurity and the STM tip is included, the tunneling resonance and the Kondo peak can be tuned to be exactly at the Dirac point, by adjusting the impurity level and Fermi energy, such that the local density of states at the Dirac point is significantly enhanced. This is in contrast to the case of a STM-decoupled Anderson impurity, where both resonances are always fully suppressed at the Dirac point. Our finding suggests a pathway to experimentally control the fundamental properties of the electrons on a TI surface.

1. Introduction

Topological insulators (TIs), characterized by robust linearly dispersing spin-split surface states, is a new class of topologically nontrivial materials discovered recently in condensed matter physics \([1–3]\). Due to the time-reversal (TR) symmetry and spin–orbit-coupling interaction, TIs have a bulk band gap and gapless edge states in two dimensions or metallic surface states in three dimensions. The topological surface states (TSSs) in three-dimensional TIs bear an odd number of massless Dirac cones with the spin of an electron locked to its momentum in a chiral spinstructure, where electrons with opposite momenta have opposite spins \([4–8]\). As a direct consequence of the spin–momentum locking, electron backscattering from TR invariant perturbation is forbidden \([9–11]\). Owing to their fundamental physics and promising applications in spintronics and topological quantum computation, TI materials have received widespread experimental and theoretical attention \([1–13]\).

The spin–momentum inter-locked TSSs are promising for unique technological applications, involving the manipulation of the Dirac electronic properties or engineering the Dirac cones \([14–16]\). Recently, engineering the TSSs through magnetically doping the TI materials has triggered strong interest. It was found that magnetically doping the bulk of TI materials can gap the TSSs because of broken TR symmetry \([17, 18]\). The effect of impurity doping on the TI surface also has exhibited interesting phenomena \([8, 15, 19–25]\). For example, recent theoretical investigations of magnetic doping on the TI surface, based on the classic impurity model, showed that low-energy resonances are produced, which visibly modify the electronic spectrum near the Dirac point, and even split the Dirac point into two nodes \([15, 21, 26, 27]\). For quantum impurity, the internal excitations of the impurities can profoundly modify the low-energy TSSs either by exchanging spin angular momentum, energy, and particles during the electron scattering processes. Highly localized impurity resonances associated with quantum impurities were experimentally revealed by scanning tunneling microscope (STM) performed on the strong TI Bi\(_2\)Se\(_3\) \([28]\). Moreover, the internal excitations of the impurities can result in the interesting Kondo effect \([29–34]\) and tunable low-energy resonances \([35]\). However, the low-energy resonances will be totally suppressed at the Dirac point because of the vanishing local density of states (LDOS) of the TSSs,
and the Kondo effect can never occur if the Fermi level of the TSSs coincides with the Dirac point [29–34]. Recently, Wang et al showed that coupling of the surface electrons to a quantum nanomagnet via spin–spin interactions can cause resonance even at the Dirac point [16], depending on the magnetic anisotropic energy, a signature that the properties of the Dirac electrons are modified substantially. The Dirac point resonance (DPR) is essentially different from the low-energy bound states induced by a classic impurity [21, 26, 27], which cannot occur at the Dirac point for a finite coupling strength.

In this paper, we study the scattering of the Dirac electrons with a quantum Anderson impurity on a TI surface through the exchange interaction, taking into account of the Kondo effect. Remarkably, we show that introduction of a coupling between the Anderson impurity and the STM tip can also result in the DPR. In a STM experiment [28], the impurity-STM coupling can dramatically affect the measured result, and the same coupling has been extensively employed for impurities adsorbed on the surfaces of ordinary metals [36, 37]. The DPR is controllable for the STM-coupled Anderson impurity, through creating low-energy tunneling resonance and Kondo peaks in the LDOS. By adjusting the impurity level and the Fermi energy, the tunneling resonance and the Kondo peaks can be tuned to be exactly at the Dirac point, which significantly enhances the DPR. This is in contrast to the case of a STM-decoupled Anderson impurity, where the tunneling resonances and the Kondo effect are always fully suppressed at the Dirac point. Here, we present an effective method to deal with the interacting system of the TSSs, Anderson impurity and STM tip, based on the equations of motion of the Green’s functions, instead of the slave-boson mean-field method and one-dimensional pseudogap Anderson model with complex hybridization functions [29, 30, 33].

In the next section, we introduce the model Hamiltonian, and describe the method for dealing with this interacting system. The Green’s function of the Anderson impurity is obtained in section 3. The related self-energies are evaluated in section 4. In section 5, the calculated results are discussed. The final section contains a summary.

2. Model and Method

To demonstrate the method and better understand the DPR, we first consider the impurity to be decoupled from the STM, and start from the low-energy effective Hamiltonian \( H_{\text{TI}} = \sum_{k} \epsilon_{k} \sigma \times k - \mu_{0} \sigma \) for the TI surface, with \( \sigma \) being the pauli-matrix for electron spin, \( v_{F} \) the Fermi velocity and \( k \) being \((k_{x}, k_{y})\) the in-plane wave vector. Here, we denote the annihilation operator for the TI surface electrons as \( \hat{c}_{k} = (c_{k, \uparrow}, c_{k, \downarrow})^{T} \). The impurity on the TI surface is considered to be Anderson-type and its Hamiltonian is taken to be

\[
H_{\text{imp}} = \sum_{\sigma} \epsilon_{\sigma} \hat{d}_{\sigma}^{\dagger} \hat{d}_{\sigma} + U n_{\sigma},
\]

where \( \hat{d}_{\sigma}^{\dagger} \) is the annihilation (creation) operator, \( \epsilon_{\sigma} \) is the spin-dependent dispersion for \( \sigma \) electrons on the impurity site \( (r_{\text{imp}}, n_{\sigma} = d_{\sigma}^{\dagger} d_{\sigma} \) is the spin-dependent number operator, and \( U \) is the Coulomb repulsion potential. The total Hamiltonian of the system is \( H = H_{\text{TI}} + H_{\text{imp}} + H_{\text{hyb}}, \) where

\[
H_{\text{hyb}} = \sum_{k} V_{\text{ho}} \hat{d}_{k}^{\dagger} \hat{c}_{k} + V_{\text{ki}} \hat{c}_{k}^{\dagger} \hat{d}_{k}
\]

is the exchange interaction between the TSSs and the impurity with \( V_{\text{ho}} = V_{\text{ki}} e^{k_{\parallel}/\nu_{F}} \) being the hybridization strength.

From the general equations of motion of a retarded Green’s function

\[
\omega\left\{ \langle A|B \rangle \right\} = \langle \{ A, B \} \rangle + \langle \{ A, H_{\text{TI}}|B \rangle \rangle \omega \langle \{ A|B, H_{\text{TI}} \} \rangle, \]

we obtain for the total Green’s function \( G_{\text{TI}}(k, k', \omega) = \langle \{ c_{k}^{\dagger}, c_{k'} \} \rangle \) of the TSSs

\[
G_{\text{TI}}(k, k', \omega) = G^{(0)}_{\text{TI}}(k, \omega) \delta_{kk'} + G^{(0)}_{\text{TI}}(k, \omega) e^{-i k_{\parallel} r_{\text{imp}}} V_{\parallel} \times G_{\text{G}}(\omega) V e^{i k_{\parallel} r_{\text{imp}}} G^{(0)}_{\text{TI}}(k', \omega),
\]

where

\[
V = \begin{pmatrix} V_{\parallel} & 0 \\ 0 & V_{\parallel} \end{pmatrix}
\]

and \( G^{(0)}_{\text{TI}}(k, \omega) = 1/(\omega - H_{\text{TI}}) \) is the Green’s function without perturbation of the impurity. \( G_{\text{G}}(\omega) \) is the retarded Green’s function of the impurity, which will be given in the next section. The Green’s function in real space \( G_{\text{TI}}(r, r', \omega) \) is given by the Fourier transform of \( G_{\text{TI}}(k, k', \omega) \), i.e.,

\[
G_{\text{TI}}(r, r', \omega) = \frac{1}{4\pi} \frac{1}{(H_{\text{TI}})} \frac{1}{(\omega)} 
\]

The spin-resolved LDOSs of the conducting electrons on the TI surface defined as \( \rho_{\text{TI,\sigma}} = -\text{Tr}(1 + \tau_{\sigma} \sigma_{z}) \text{Im} G_{\text{TI}}(r, r, \omega)/2\pi \) includes a part without the perturbation \( G^{(0)}_{\text{TI,\sigma}} \) and a correction part \( \delta \rho_{\text{TI,\sigma}} \) due to the second term in equation (2). After the Fourier transform of \( G^{(0)}_{\text{TI}}(k, \omega) \), we arrive at

\[
G^{(0)}_{\text{TI}}(r, \omega) = -\frac{N(\omega + \mu)}{2\pi (H_{\text{TI}})^{2}} F_{0} + \frac{N(\omega + \mu)(\sigma \times r)^{2}}{2\pi (H_{\text{TI}})^{2}} F_{1},
\]

where \( F_{0} = \frac{i}{2} H_{0}^{(1)}(\frac{\omega + \mu}{\nu_{F}}|r|) \) and \( F_{1} = -\frac{1}{2} H_{1}^{(1)}(\frac{\omega + \mu}{\nu_{F}}|r|) \) with \( H_{0}^{(1)} \) (\( H_{1}^{(1)} \)) as the first kind Hankel function of order zero (one). Substituting equation (3) into equation (2), the correction part for the spin-resolved LDOS is
derived to be
\[
\delta \rho_{\uparrow\downarrow} = -\frac{N}{2\pi^2}\frac{(\omega + \mu)^2}{(\hbar v_F)^2}\text{Im} \left[ \eta_\sigma G_{\sigma\sigma}(\omega) F_0^\sigma - \eta_\sigma G_{\uparrow\uparrow}(\omega) F_1^\uparrow \right]
\]
(4)

with \( \eta_\sigma = N|V_{k\sigma}|^2/2\pi(\hbar v_F)^2 \).

3. The Green’s function of the impurity

The retarded Green’s function of the impurity is defined as \( G_{\omega,\sigma'}^{\sigma}(\omega) = \langle \langle d_\sigma | d_\sigma' \rangle \rangle' \), which is the Fourier transform of \( \langle \langle d_\sigma(\tau) | d_\sigma'(0) \rangle \rangle' = -i\theta(\tau) \left\langle \{ d_\sigma(\tau), d_\sigma'(0) \} \right\rangle \) with \( \theta(\tau) \) as the heaviside function. From the standard equation of motion \( \omega \left\langle \{ d_\sigma, d_\sigma' \} \right\rangle + \left\langle \left[ d_\sigma, H \right] d_\sigma' \right\rangle \), we obtain for the first-order Green’s function
\[
(\omega - E_\sigma) \langle \langle d_\sigma | d_\sigma' \rangle \rangle = 1 + \sum_\mathbf{k} V_{k\sigma} \langle \langle c_{k\sigma} | d_\sigma' \rangle \rangle + U \langle \langle d_\sigma d_\sigma' d_\sigma' d_\sigma' \rangle \rangle.
\]
(5)

In the same way, we can also derive the following equations
\[
(\omega + \mu) \langle \langle c_{k\sigma} | d_\sigma' \rangle \rangle = \hbar v_F (k_x + \tau \sigma i k_y) \langle \langle c_{k\sigma} | d_\sigma' \rangle \rangle + V_{k\sigma} \langle \langle d_\sigma | d_\sigma' \rangle \rangle \quad \text{and}
\]
\[
(\omega + \mu) \langle \langle c_{k\sigma} | d_\sigma' \rangle \rangle = \hbar v_F (k_y + \tau \sigma i k_x) \langle \langle c_{k\sigma} | d_\sigma' \rangle \rangle + V_{k\sigma} \langle \langle d_\sigma | d_\sigma' \rangle \rangle.
\]
(6)

From these two equations, it follows
\[
\langle \langle d_\sigma | d_\sigma' \rangle \rangle = \frac{\omega + \mu}{(\omega + \mu)^2 - \xi^2} V_{k\sigma}^* \langle \langle d_\sigma | d_\sigma' \rangle \rangle + \frac{\hbar v_F (k_x + \tau \sigma i k_y)}{(\omega + \mu)^2 - \xi^2} V_{k\sigma}^* \langle \langle d_\sigma | d_\sigma' \rangle \rangle
\]
with \( \tau_1 = \pm 1 \) and \( \xi = \hbar v_F |k| \). By substituting equation (6) into equation (5) and replacing the summation by an integral \( \frac{1}{N} \sum_\mathbf{k} \rightarrow \frac{1}{(2\pi)^3} \int d^3k \), it is easy to obtain
\[
(\omega - E_\sigma - \Sigma_0) \langle \langle d_\sigma | d_\sigma' \rangle \rangle = 1 + U \langle \langle d_\sigma d_\sigma' d_\sigma' d_\sigma' \rangle \rangle,
\]
(7)

where \( \Sigma_0 = \frac{N}{2\pi} \int_0^\Lambda dk \frac{\omega + \mu}{(\omega + \mu)^2 - \xi^2} \) is readily evaluated as
\[
\Sigma_0 = \Gamma_\sigma(\omega) \ln \left\{ \frac{(\omega + \mu)^2}{(\omega + \mu)^2 - \xi^2} - \frac{i\pi \text{sign}(\omega + \mu)\theta(|\omega + \mu|)\theta(\Lambda - |\omega + \mu|)} \right\}
\]
(8)

with \( \Gamma_\sigma(\omega) = N|V_{k\sigma}|^2(\omega + \mu)/2\pi(\hbar v_F)^2 \) and \( \Lambda \) being the high-energy cutoff. Here, we have assumed \( V_{k\sigma} \) and \( \langle \langle d_\sigma | d_\sigma' \rangle \rangle \) to be isotropic in the \( k \)-space, so that the integral of the second term in equation (6) vanishes. The higher-order Green’s function \( \langle \langle d_\sigma d_\sigma' d_\sigma' d_\sigma' \rangle \rangle \) is technically processed further in order to obtain the analytical expression for the Green’s function of the impurity.

Generally, \( \langle \langle d_\sigma d_\sigma' d_\sigma' d_\sigma' \rangle \rangle \) can be treated by the Hartree–Fock approximation for temperatures higher than the Kondo temperature [38]. However, the Kondo effect is under our consideration and further iterative calculations are needed. Similarly to the above calculation, the equation of motion for \( \langle \langle d_\sigma d_\sigma' d_\sigma' d_\sigma' \rangle \rangle \) is
\[
(\omega - E_\sigma - U) \langle \langle d_\sigma d_\sigma' d_\sigma' d_\sigma' \rangle \rangle = \langle \langle d_\sigma d_\sigma' \rangle \rangle + \sum_\mathbf{k} V_{k\sigma} \langle \langle d_\sigma' c_{k\sigma} | d_\sigma' \rangle \rangle + \sum_\mathbf{k} V_{k\sigma} \langle \langle d_\sigma d_\sigma' c_{k\sigma} | d_\sigma' \rangle \rangle + \sum_\mathbf{k} V_{k\sigma} \langle \langle d_\sigma d_\sigma' c_{k\sigma} | d_\sigma' \rangle \rangle \]
and the relating higher-order Green’s functions are
\[
\langle \langle d_\sigma d_\sigma' c_{k\sigma} | d_\sigma' \rangle \rangle = \frac{\omega + \mu}{(\omega + \mu)^2 - \xi^2} V_{k\sigma}^* \langle \langle d_\sigma d_\sigma' d_\sigma' c_{k\sigma} | d_\sigma' \rangle \rangle
\]
\[
+ \sum_\mathbf{k} V_{k\sigma} \langle \langle d_\sigma d_\sigma' c_{k\sigma} | d_\sigma' \rangle \rangle - \langle \langle d_\sigma c_{k\sigma} c_{k\sigma} | d_\sigma' \rangle \rangle\]
\[
- \frac{\hbar v_F (k_x + \tau \sigma i k_y)}{(\omega + \mu)^2 - \xi^2} \sum_\mathbf{k} V_{k\sigma} \langle \langle d_\sigma c_{k\sigma} c_{k\sigma} | d_\sigma' \rangle \rangle + \langle d_\sigma c_{k\sigma} c_{k\sigma} | d_\sigma' \rangle \rangle
\]
(9a)

\[
\langle \langle d_\sigma d_\sigma' d_\sigma' c_{k\sigma} | d_\sigma' \rangle \rangle = \frac{\omega + \mu}{(\omega + \mu)^2 - \xi^2} V_{k\sigma}^* \langle \langle d_\sigma d_\sigma' d_\sigma' d_\sigma' c_{k\sigma} | d_\sigma' \rangle \rangle
\]
\[
+ \sum_\mathbf{k} V_{k\sigma} \langle \langle d_\sigma c_{k\sigma} c_{k\sigma} | d_\sigma' \rangle \rangle - \langle \langle d_\sigma c_{k\sigma} c_{k\sigma} c_{k\sigma} | d_\sigma' \rangle \rangle\]
\[
+ \frac{\hbar v_F (k_x + \tau \sigma i k_y)}{(\omega + \mu)^2 - \xi^2} \sum_\mathbf{k} V_{k\sigma} \langle \langle d_\sigma c_{k\sigma} c_{k\sigma} c_{k\sigma} | d_\sigma' \rangle \rangle - \langle \langle d_\sigma c_{k\sigma} c_{k\sigma} c_{k\sigma} | d_\sigma' \rangle \rangle
\]
(9b)
\[
\langle d_\sigma d_\sigma c_{\kappa \sigma}^\dagger d_{\sigma'}^\dagger \rangle = \frac{\omega_\sigma - \mu}{(\omega_\sigma - \mu)^2 - \xi^2} \left[ V_{\kappa \sigma} \langle d_\sigma d_\sigma c_{\kappa \sigma}^\dagger \rangle \right] + \frac{\omega_\sigma - \mu}{(\omega_\sigma - \mu)^2 - \xi^2} \sum_{k'} V_{k' \sigma} \left( \langle d_\sigma d_\sigma c_{k' \sigma}^\dagger \rangle - \langle d_\sigma d_\sigma c_{\kappa \sigma}^\dagger d_{\sigma'}^\dagger \rangle \right) + \frac{\omega_\sigma - \mu}{(\omega_\sigma - \mu)^2 - \xi^2} \sum_{k'} V_{k' \sigma} \left( \langle d_\sigma d_\sigma c_{k' \sigma}^\dagger \rangle - \langle d_\sigma d_\sigma c_{\kappa \sigma}^\dagger d_{\sigma'}^\dagger \rangle \right)
\] (9c)

with \(\omega_\sigma = \omega - \mu + \xi\) and \(\omega_\sigma = \omega - \mu - \xi\). To close the iterative equations, we truncate the higher-order Green’s functions following the standard approximate method adopted in [39–41] by contracting the operator pairs. Generally, there are three kinds of contractions for each higher order Green’s function in equation (9). For example, the first term of the second line in equation (9c) can be contracted as

\[
\langle d_\sigma d_\sigma c_{\kappa \sigma}^\dagger d_{\sigma'}^\dagger \rangle = \langle d_\sigma d_\sigma c_{\kappa \sigma}^\dagger \rangle \langle c_{\kappa \sigma}^\dagger d_{\sigma'}^\dagger \rangle + \langle c_{\kappa \sigma}^\dagger c_{\kappa \sigma}^\dagger \rangle \langle d_{\sigma} d_{\sigma}^\dagger \rangle + \langle d_{\sigma} d_{\sigma}^\dagger \rangle \langle c_{\kappa \sigma} c_{\kappa \sigma}^\dagger \rangle\]

For a graphene or normal metal host, since there is no spin-flip when the electron hops from the impurity to the host or propagates in the host, the last two terms vanish. However, on a TI surface, due to the strong spin-orbit interaction, the electron spin can be flipped, and thus \(\langle c_{\kappa \sigma} d_{\sigma'}^\dagger \rangle \neq 0\). With these techniques, the equation of motion for the Green’s function of the impurity is closed, yielding

\[
G_{d,\sigma\sigma'}(\omega) = \left[ \frac{1}{\omega - \epsilon_\sigma - \Sigma_{\sigma}^{d}} + \frac{\epsilon_\sigma - \epsilon_{\sigma'}}{\omega - \epsilon_\sigma - \epsilon_{\sigma'} - U - \Sigma_{\sigma}^{d}} \right] \delta_{\sigma\sigma'}
\] (10)

where \(\Sigma_{\sigma}^{d} = \Sigma_{\sigma,0}^{0} - U(\Sigma_{\sigma,0}^{0} + \Sigma_{\sigma,0}^{-})\). The self-energies are given by

\[
\Sigma_{\sigma,0}^{0} = \sum_{k} |V_{k\sigma}|^{2} \left[ \frac{\omega_{\sigma} + \mu}{(\omega_{\sigma} + \mu)^2 - \xi^2} + \frac{\omega_{\sigma} - \mu}{(\omega_{\sigma} - \mu)^2 - \xi^2} \right]
\] (11a)

\[
\Sigma_{\sigma,0}^{-} = \sum_{k} |V_{k\sigma}|^{2} \left[ \frac{(\omega_{\sigma} + \mu)(\epsilon_{k\sigma} + \epsilon_{k\kappa})}{(\omega_{\sigma} + \mu)^2 - \xi^2} + \frac{i\xi e^{i\theta}}{(\omega_{\sigma} + \mu)^2 - \xi^2} \right] + \frac{(\omega_{\sigma} - \mu)(\epsilon_{k\sigma} c_{k\kappa})}{(\omega_{\sigma} - \mu)^2 - \xi^2},
\] (11b)

\[
\Sigma_{\sigma,\kappa}^{-} = \sum_{k} |V_{k\sigma}|^{2} \left[ \frac{\omega_{\sigma} + \mu}{(\omega_{\sigma} + \mu)^2 - \xi^2} + \frac{\omega_{\sigma} - \mu}{(\omega_{\sigma} - \mu)^2 - \xi^2} \right] \langle d_{\sigma} c_{\kappa} \rangle \Sigma_{\kappa}^{0}
\] (11c)

with \(\theta_{k} = \tan^{-1}(k_{y}/\tau_{k} k_{x})\). The occupation number \(\langle n_{\sigma} \rangle\) is determined self-consistently by the fluctuation-dissipation theorem

\[
\langle n_{\sigma} \rangle = -\frac{1}{\pi} \int_{-\infty}^{\infty} \text{Im}[G_{d,\sigma\sigma}(\omega)] f(\omega) d\omega.
\] (12)

### 4. The self-energies

We notice that the expression for \(\Sigma_{\sigma,0}^{0}\) resembles that for \(\Sigma_{\sigma,0}^{-}\). In fact, one can obtain the final analytical expression for \(\Sigma_{\sigma,0}^{0}\) from equation (8) through the relation \(\Sigma_{\sigma,0}^{0} = \Sigma_{\sigma,0,\omega + \omega - \mu} + \Sigma_{\sigma,\omega - \mu, -\omega}\). Unlike \(\Sigma_{\sigma,0}^{0}\), \(\Sigma_{\sigma,0}^{-}\) includes the higher-order effects, and contains several averages of the operators of the TSSs. These averages can be calculated by using the retarded Green’s function of the TSSs, given in equation (1), and applying the spectral theorem

\[
\langle BA \rangle = -\int_{-\infty}^{\infty} d\omega f(\omega) \text{Im}\langle A B \rangle_{\omega,\omega} \quad \text{with} \quad f(\omega) = (1 + e^{i\omega - E_{F}/(k_{B} T)})^{-1}\]

Since they are global averages, on which the effect of the impurity scattering is small, we can keep only the first term of equation (1). After some straightforward algebra, we obtain \(\langle c_{k\sigma}^\dagger c_{k\sigma}^\dagger \rangle = f(\xi - \mu) + f(-\xi - \mu)/2\), \(\langle c_{k\sigma}^\dagger c_{k\sigma}^\dagger \rangle = ie^{-i\theta} \left[ f(\xi - \mu) - f(-\xi - \mu)/2 \right]\), and \(\langle c_{k\sigma}^\dagger c_{k\sigma}^\dagger \rangle = ie^{-i\theta} \left[ f(\xi - \mu) - f(-\xi - \mu)/2 \right]\).

Substituting these relations to equation (11), we arrive at

\[
\Sigma_{\sigma,\kappa}^{-} = \frac{\Gamma_{\sigma}(\omega_{\sigma})}{2} \int_{0}^{\Lambda} d\xi \left[ \frac{f(\xi - \mu)}{\omega_{\sigma} + \mu - \xi} = \frac{f(-\xi - \mu)}{\omega_{\sigma} + \mu + \xi} \right] - \frac{\Gamma_{\sigma}(\omega_{\sigma} + 2\mu)}{2} \int_{0}^{\Lambda} d\xi \left[ \frac{f(\xi - \mu)}{\omega_{\sigma} + \mu - \xi} = \frac{f(-\xi - \mu)}{\omega_{\sigma} + \mu + \xi} \right]
\] (13)
Following the same procedure as shown in [41, 42], for low temperatures, $\Sigma_2^\nu$ is derived to be

$$
\Sigma_2^\nu = \frac{\Gamma_2(\omega_n)}{2} \left[ 2\theta(\mu + E_F)\ln \frac{\omega_n + \mu}{2\pi i T} + \text{sign}(\mu + E_F) \psi\left(\frac{1}{2} + \frac{\omega_n - E_F}{2\pi i T}\right) - \ln \frac{\omega_n + \mu + \Lambda}{2\pi i T} \right]
$$


$$
+ \frac{\Gamma_2(\omega_n - 2\mu)}{2} \left[ 2\theta(\mu + E_F)\ln \frac{\omega_n - \mu}{2\pi i T} + \text{sign}(\mu + E_F) \psi\left(\frac{1}{2} + \frac{\omega_n + E_F}{2\pi i T}\right) - \ln \frac{\omega_n - \mu + \Lambda}{2\pi i T} \right]
$$

with $\psi$ being the digamma function. At low temperatures, $\Sigma_2^\nu \approx \langle \langle d_\nu | d_\nu^\dagger \rangle \rangle \Sigma_2^\nu \propto |V_{\text{imp}}|^4$ is a higher order term compared with $\Sigma_2^0$, $\Sigma_2^\nu \propto |V_{\text{ass}}|^2$ for weak impurity-surface coupling, so that we will neglect $\Sigma_2^\nu$ hereafter, which does not influence the qualitative results.

5. Results and discussion

We first analyze the DOS of the impurity, which is helpful for us to understand the effect of the Anderson impurity on the properties of the Dirac electrons. Then we turn to discuss the characteristics of the modified LDOS of the TSSs.

5.1. DOS of the Anderson impurity

Before analyzing the numerical results, we can infer some properties of the DOS of the impurity, defined as $\rho_{\text{imp}} = -\text{Im} [G_{\text{imp}}^{\text{re}}(\omega)]/\pi$, from the expressions for the self-energies. In the deep Coulomb blockade regime, e.g., $U \rightarrow \infty$, the impurity Green’s function is reduced to $G_{\text{imp}}^{\text{re}}(\omega) = (1 - (n_\nu))/(\omega - \varepsilon_\nu - \Sigma_2^\nu)$ and $\Sigma_2^\nu = \Sigma_2^0 + \Sigma_2^\nu$. As a result, the tunneling resonance between the impurity level and the TSSs manifests itself as a peak in the DOS, with location determined by $\omega = \varepsilon_\nu + \text{Re} [\Sigma_2^\nu]$ and width by $\text{Im} [\Sigma_2^\nu]$. In the absence of a magnetic field, both $\Sigma_2^0$ and $\Sigma_2^\nu$ contain a factor $\omega + \mu$. Therefore, the tunneling resonance peak will change its location and width, when the chemical potential $\mu$ is varied. The resonance effect is fully suppressed at the Dirac point ($\omega + \mu = 0$).

The above inferences are confirmed by the numerical results shown in figure 1(a), where the DOS on the impurity is shown for three different values of chemical potential $\mu$. The DOS vanishes exactly at the Dirac point, as can be easily seen from the dark solid curve in figure 1(a), and the tunneling resonance peak becomes broader and lower as $\mu$ increases from 0 to 0.2. To further demonstrate the $\mu$-dependent resonance, we plot $\text{Re} [\Sigma_2^\nu]$ and $\text{Im} [\Sigma_2^\nu]$, respectively, in figures 1(b) and (c) for the same parameters as in figure 1(a). As shown in figure 1(b), with increasing $\mu$, the solution for $\omega = \varepsilon_\nu + \text{Re} [\Sigma_2^\nu]$, i.e., the intersection of the corresponding curve of $\text{Re} [\Sigma_2^\nu]$ and the straight line, moves leftward. As a result, the tunneling resonance peak shifts from its original position, as can be seen from figure 1(a). In figure 1(c), when the Dirac point is tuned away from the Fermi level, the value of $\text{Im} [\Sigma_2^\nu]$ gets bigger and bigger around the resonance energy, which broadens the tunneling resonance peak. Due to the normalization of $\rho_{\text{imp}}$, namely, $\int d\omega \rho_{\text{imp}} = 1$, the tunneling resonance peak will be lower when it becomes broader, as shown in figure 1(a).

Apart from the tunneling resonance, another narrow and sharp peak is also found exactly at the Fermi level in figures 1(a) and (b), which corresponds to the Kondo resonance. The Kondo resonance is also reflected in the sudden change of $\text{Im} [\Sigma_2^\nu]$ at the Fermi level. The appearance of the Kondo peak, resembling the scenario of an impurity deposited on a normal metal or graphene surface, is attributable to the singularities of $\Sigma_2^\nu$ at the Fermi level. Since the digamma function $\psi\left(\frac{1}{2} + \frac{\omega - E_F}{2\pi i T}\right)$ in $\Sigma_2^\nu$ peaks at $\omega = \varepsilon_\nu + \varepsilon_\nu = E_F$, the Kondo peak in fact develops at $\omega = E_F + \varepsilon_\nu = E_F$. If the impurity levels are not split, the Kondo peaks will appear exactly at the Fermi level for both spin species. From figures 1(b) and (c), it is found that the peak of the real part of $\Sigma_2^\nu$ tends to be much higher and sharper, and the sudden change of $\text{Im} [\Sigma_2^\nu]$ becomes much more severe with increasing the chemical potential. One may expect the Kondo peak to be higher and sharper with the variation of $\Sigma_2^\nu$. However, we see from figure 1(d) that with increasing the chemical potential, the LDOS at the Fermi level reduces after reaching a maximum. To understand this interesting behavior of the LDOS at the Fermi level, we may first define an effective impurity level $E_d$ by the equation: $E_d = \varepsilon_\nu + \text{Re} [\Sigma_2^0 + \Sigma_2^\nu]_d - E_F$. The solution can be obtained graphically, just as in figure 1(b). Then we estimate the Kondo temperature from the calculated impurity Green’s function. The relevant energy scale can be determined from the leading terms in the denominator of the impurity Green’s function, i.e., by the temperature at which the real parts of $G_{\text{imp}}^{\text{re}}(\omega)$ vanishes. When $|E_d - E_F| \gg k_B T$, using the approximate form $\text{Re} \left[ \psi\left(\frac{1}{2} + \frac{E_d - E_F}{2\pi i T}\right) \right] \approx \ln \frac{\sqrt{(E_d - E_F)^2 + (\pi T)^2}}{2\pi T}$, we find that the
temperature scales as $T_K^{\text{th}} \sim \frac{1}{\Lambda} \frac{\mu^2 T K}{\ln \left( \frac{E_d - E_f}{T K} \right)^2 + \left( \frac{E_d - E_f}{T K} \right)^2}$, such that the real part of the denominator of the impurity Green’s function near the effective impurity level becomes $\eta (E_d + \mu) \ln \left( \frac{E_d - E_f}{T K} \right)^2 + \left( \frac{E_d - E_f}{T K} \right)^2$. Note that $T_K^{\text{th}}$ is smaller than the true Kondo temperature $T_K$. The emergence of the Kondo resonance requires that there exists a solution near the Fermi level, i.e., $\omega \sim \varepsilon_0$. For a small value of $\mu$, only one solution near $\varepsilon_0$ can be found, so that the Kondo resonance is suppressed. When $\omega \gg T_K$, the Kondo resonance emerges, as can be seen from figures 1(a) and (b), and $T_K$ increases exponentially with increasing $\mu$ for $E_d \gg \varepsilon_0$. However, with further increasing $\mu$, $E_d$ will be pushed away from the Fermi level, and when $E_d \sim \varepsilon_0$, $T_K$ decreases with increasing $\mu$. Therefore, there exists a critical value of $\mu \sim -\varepsilon_0$, determined by the equation: $\varepsilon_0 - E_d = 0$, above which $T_K$ becomes smaller than $T$ and the Kondo peak vanishes again. As a result, the Kondo peak reduces its intensity after reaching a maximum value.

It is interesting to see that, for a finite LDOS of the TSSs at the Fermi level, i.e., $\mu + E_f = 0$, a Fermi liquid behavior at small enough temperatures can be obtained. At low temperatures, $\langle n_s \rangle = 1/2$ for $\mu + E_f = 0$ and $\varepsilon_0 < E_d$, so that $\langle G_{\text{th}}^{\omega} \rangle^{-1} = 2 (\omega - \varepsilon_0 - \Sigma_0^\text{th})^{-1}$. The system is in the deep Coulomb blockade regime. The numerical calculation shows that $\text{Im} \langle \Sigma_0^\text{th} \rangle^{-1} = \Gamma_e (\mu + E_f)$ for the Fermi liquid. The effective impurity level satisfies the relation $(\omega - E_d)_{\omega \sim \varepsilon_0} \rightarrow 0$ if $T \ll T_K$, because of the emergence of the Kondo effect. Consequently, $\text{Re} [G_{\text{th}}^{\omega} (E_d)]^{-1} = 0$, and the Friedel sum rule $\text{Re} [G_{\text{th}}^{\omega} (E_d)]^{-1} = -\Gamma_e (\mu + E_f) \cot (\pi n_s)$ is also satisfied.

5.2. Surface tunneling resonance and Kondo resonance

From the above analysis, we know that the tunneling resonance takes place around $\omega = \varepsilon_0 + \text{Re} [\Sigma_0^\text{th}]$ and the Kondo peak emerges at $\omega = E_f$ for Dirac point away from the Fermi level ($E_f + \mu = 0$). Both the tunneling...
Figure 2. The LDOS of the TI, $\rho_{\text{TI}}$, versus $\omega$ with $\mu = 0.05 \Lambda$, $r = (5, 0)$ and $r_{\text{imp}} = (0, 0)$. The other parameters are the same as figure 1.

resonance and Kondo resonance can affect the TSSs. In figure 2, we plot the total LDOS $\rho_{\text{TI}} (= \rho_{\text{TL,1}} + \rho_{\text{TL,2}})$ versus $\omega$ for some different values of $\varepsilon_0$. Obviously, there exists tunable low-energy tunneling resonance in the LDOS of the TI surface. With $\varepsilon_0$ increasing from $-0.15$ to $0.02$, the resonance peak first becomes sharper and closer to the Dirac point, and then it further passes through the Dirac point with decreasing height and broadening width. For a fixed $\varepsilon_0$, the strength of the low-energy tunneling resonance strongly depends on the energy difference between the Fermi level and the Dirac point, which is helpful for understanding the experimental observations, e.g., the low-energy resonances observed by STM performed on the surface of strong TI $\text{Bi}_2\text{Se}_3$ [28]. The low-energy resonances induced by a classic impurity were also studied before [21, 26, 27], but the physical mechanism is different from that of a quantum impurity investigated here. For a classical impurity, the low-energy resonances are bound states corresponding to the poles of the $T$-matrix, which can never be tuned to cross the Dirac point. The low-energy tunneling resonance observed here originates from the electron exchange interaction between the impurity and the TSSs, which is highly tunable by varying the internal energy level of the impurity. It can even pass through the Dirac point with changing the impurity level alone, as has been observed in figure 2.

In addition to the tunneling resonance in figure 2, one can notice that there emerges a narrow and sharp peak in the LDOS exactly at the Fermi level for $\varepsilon_0 = -0.025$. The new peak comes from the Kondo resonance, which vanishes if the Dirac point is tuned to be at the Fermi level. For a larger chemical potential, the Kondo resonance will be less noticeable because of the reduction of the impurity DOS at the Fermi level mentioned above.

Interestingly, although the Dirac dispersion of the TSSs is heavily destroyed by the resonances at low energies, especially near the Dirac point, the Dirac point itself is insensitive to the Anderson impurity, as the zero energy difference between the Fermi level and the Dirac point, which is helpful for understanding the DPR. Meanwhile, $\lim_{\omega \to -\mu}[(\omega + \mu)F_0] = 0$ and $\lim_{\omega \to -\mu}[(\omega + \mu)F_1] = \hbar v_F/r$. As a result, the Dirac point is robust against the Anderson impurity on the TI surface ($\delta \rho_{\text{TI}, 0} = 0$), as shown in figure 2.

5.3. DPR
As analyzed above, nonvanishing $\text{Im} \Sigma_{\omega}'$ at the Dirac point is a necessary requirement for generating the DPR. However, the requirement is impossible to meet for classic impurities, since the $T$-matrix, $T(\omega) = V[1 - G_{\text{TI}}(\omega) V^{-1}$, always satisfies $\text{Im}[T(-\mu)] = 0$. In contrast, for quantum impurities, it is easy to induce an additional imaginary part in the self-energy. For example, during the experimental measurement by STM [28], the quantum impurity could couple to the STM, which will contribute to the imaginary part of the self-energy. To further demonstrate this point, we introduce in the present model an additional coupling between the impurity and a STM tip with hybridization $H_{\text{tip}} = \sum_{\sigma} (T_{\text{TI}} d_{\sigma}^{\text{up}} a_{\sigma}^{\text{up}} + T_{\text{TI}}^{\text{up}} a_{\sigma}^{\text{up}} d_{\sigma})$ and dispersion $\varepsilon_k = (\hbar k)^2/2m$ for the STM tip. The same coupling has been extensively employed for impurities adsorbed on the surfaces of ordinary metals [36, 37].

We derive the impurity Green’s function, as an instance, in the deep Coulomb blockade regime, given by $G^d_{\text{TI}, \sigma}(\omega) = (1 - \langle n_\sigma \rangle)/(\omega - \varepsilon_\sigma - \Sigma^\omega_x - \Sigma^\omega_{\text{tip}})$, where $\Sigma^\omega_{\text{tip}}$ is the STM-induced self-energy, as given in the appendix. The expression for $\Sigma^\omega_{\text{tip}}$ is different from that for $\Sigma^\omega_x$, since the STM tip is considered to have a constant
DOS ($D_{\sigma}$). Because of the appearance of the self-energy $\Sigma^\sigma_{\text{tip}}$, the self-consistent equation for $\langle n_\sigma \rangle$ is changed to be

$$
\langle n_\sigma \rangle = -\int \frac{d\omega}{\pi} \text{Im}[G^\sigma_\text{tip,0}(\omega)] \frac{\Gamma^\sigma_{\text{tip}} f_{\text{tip}}(\omega) + |\Gamma^\sigma_{\tau}(\omega)| f_{\text{TI}}(\omega)}{\Gamma^\sigma_{\text{tip}} + |\Gamma^\sigma_{\tau}(\omega)|} \quad (15)
$$

with $\Gamma^\sigma_{\text{tip}} = 2\pi D_{\sigma}|T_{\text{tip}}|^2$.

We first consider the case, where the temperature is beyond the Kondo temperature, and the result is presented in figure 3(a). Obviously, the DPR is generated, and strongly depends on the STM tip-impurity tunneling resonance. For the impurity level far away from the Dirac point, e.g., for $\varepsilon_0 = -0.10$ and $0.05$ in figure 3(a), the LDOS of the TI surface peaks at the tunneling resonance energy, just slightly away from the Dirac point. With the impurity level approaching to the Dirac point, e.g., for $\varepsilon_0 = -0.037$ and $-0.05$, the DPR peak shifts toward the Dirac point, and gradually reaches its maximum when the peak coincides with the Dirac point. The behavior of the DPR observed here is quite different from that for a high-spin nanomagnet adsorbed on the TI surface, where the DPR strongly relies on the strength of magnetic anisotropy [16]. Here, the DPR is due to the interplay of the STM tip-impurity and TI-impurity interactions, and is strongly dependent on the location of the impurity level. In [16], the magnetic anisotropy ($D$) in high-spin nanomagnet is crucial. If the magnetic anisotropy vanishes, i.e., $D = 0$, the DPR in [16] will disappear, reducing to the present Anderson impurity case. Here, we show that the DPR can be induced simply by coupling the impurity to a STM tip, without requiring the magnetic anisotropy of the impurity.

To further clarify the origin of the DPR, we derive the spin-resolved LDOS modification at the Dirac point to be $\delta \rho_{\text{TI},\sigma} = N\eta_\sigma \text{Im} G^\sigma_{\text{tip},0}(-\mu)/2\pi^2 r^2$, by utilizing the relations $\lim_{\omega \to -\mu}[(\omega + \mu) F_0] = 0$ and $\lim_{\omega \to -\mu}[(\omega + \mu) F_1] = \hbar v_F/r$. It is interesting to see that the LDOS $\rho_{\text{TI},\sigma}$ of one spin $\sigma$ is modified by the opposite spin $\bar{\sigma}$, and shows an inverse-square $1/r^2$ attenuation law without Friedel oscillations, which is quite different from the Kondo resonance or the bound states [16, 29, 30]. More interestingly, when the temperature is below the Kondo temperature, the DPR can be significantly strengthened by the Kondo resonance. In figure 3(b), we plot the evolution of the DPR with the Kondo resonance. It is obvious that, with the Kondo peak approaching to the Dirac point, the DPR stands out rapidly. Moreover, by varying the Fermi energy of the STM, the Kondo resonance can be tuned to be exactly at the Dirac point, which strongly enhances the DPR.

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Figure 3. The LDOS of the TI, $\rho_{\text{TI}}$, versus $\omega$ with $E_{\text{tip}}^\tau = 0$, $k_B T_{\text{tip}} = 10^{-2}\Lambda$ for (a), and $\varepsilon_0 = -0.03\Lambda$, $k_B T_{\text{tip}} = 10^{-5}\Lambda$ for (b). Here, we set $\Gamma_{\text{tip}} = 0.01\Lambda$, $\mu = 0$ and $r = (2, 0)$. The other parameters are the same as figure 1.
6. Summary

We investigated the scattering of Dirac electrons with a STM-coupled Anderson impurity adsorbed on the TI surface, and proposed an effective method to deal with the mutual interactions between the TSSs and the Anderson impurity. It was found that the STM-coupled Anderson impurity can heavily destroy the Dirac spectrum by creating of the DPR, Kondo resonance, and tunneling resonance. The DPR can be significantly strengthened either by the low-energy tunneling resonance or Kondo resonance, even exactly at the Dirac point, in sharp contrast to the case of an impurity decoupled from the STM, where all the resonances are fully suppressed at the Dirac point. Our finding is helpful for understanding the experimental observations, e.g., the low-energy resonances observed by STM performed on the surface of strong TI Bi2Se3. Furthermore, the low-energy tunneling resonance induced by the Anderson impurity is tunable to cross the Dirac point, essentially different from the low-energy bound states induced by a classic impurity.

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Appendix A. STM tip-induced self-energies

Following the way mentioned in the main text, we derive the impurity Green’s function in the presence of a coupling between the impurity and STM tip, bringing about the additional tip-induced self-energies

\[
\Sigma_{\text{tip}}^{0\sigma} = \frac{N_n|T_{\text{tip}}|^2}{2\pi\hbar^2} \left[ \ln \left( \frac{\omega + \Lambda}{\omega - \Lambda} \right) - i\pi\theta(\Lambda - |\omega|) \right]
\]

\[
\Sigma_{\text{tip}}^{\sigma\sigma} = \frac{N_n|T_{\text{tip}}|^2}{2\pi\hbar^2} \left[ \ln \left( \frac{\omega_\sigma + \Lambda}{\omega_\sigma - \Lambda} \right) - i\pi\theta(\Lambda - |\omega_\sigma|) \right] + \frac{N_n|T_{\text{tip}}|^2}{2\pi\hbar^2} \left[ \ln \left( \frac{\omega_\tau + \Lambda}{\omega_\tau - \Lambda} \right) - i\pi\theta(\Lambda - |\omega_\tau|) \right]
\]

\[
\Sigma_{\text{tip}}^{2\sigma} = \frac{N_n|T_{\text{tip}}|^2}{2\pi\hbar^2} \left[ \ln \left( \frac{\omega_\sigma + \Lambda}{2\pi i T} \right) - \psi \left( \frac{1}{2} + \frac{\omega_\sigma - E_{\text{tip}}^0}{2\pi i T} \right) \right] - \frac{N_n|T_{\text{tip}}|^2}{2\pi\hbar^2} \left[ \ln \left( \frac{\omega_\tau + \Lambda}{2\pi i T} \right) - \psi \left( \frac{1}{2} + \frac{\omega_\tau - E_{\text{tip}}^0}{2\pi i T} \right) \right]
\]

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