Local moment formation in Dirac electrons

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Abstract. Elemental bismuth and its compounds host strong spin-orbit interaction which is at the heart of topologically non-trivial alloys based on bismuth. These class of materials are described in terms of $4 \times 4$ matrices at each $\mathbf{k}$ point where spin and orbital labels of the underlying electrons are mixed. In this work we investigate the single impurity Anderson model (SIAM) within a mean field approximation to address the nature of local magnetic moment formation in a generic Dirac Hamiltonian. Despite the spin-mixing in the Hamiltonian, within the Hartree approximation it turns out that the impurity's Green function is diagonal in spin label. In the three dimensional Dirac materials defined over a bandwidth $D$ and spin-orbit parameter $\gamma$, that hybridizes with impurity through $V$, a natural dimensionless parameter $\frac{V^2 D^2}{4 \pi \gamma^3}$ emerges. So neither the hybridization strength, $V$, nor the spin-orbit coupling $\gamma$, but a combination thereof governs the phase diagram. By tuning chemical potential and the impurity level, we present phase diagram for various values of Hubbard $U$. Numerical results suggest that strong spin-orbit coupling enhances the local moment formation both in terms of its strength and the area of the local moment region. In the case that we tune the chemical potential in a similar way as normal metal we find that magnetic region is confined to $\mu \geq \varepsilon_0$, in sharp contrast to 2D Dirac fermions. If one fixes the chemical potential and tunes the impurity level, phase diagram has two magnetic regions which corresponds to hybridization of impurity level with lower and upper bands.

1. Introduction

The low-energy features of the band structure in some materials are hyperbolic rather than parabolic. Graphene being an extreme example in two dimensions where the effective single-particle energy levels are described by a cone. Other examples in three dimensions have emerged a large class of which are based on elemental bismuth. In these class of materials, the low-energy effective theory around the Fermi level is described in terms of Dirac theory, namely the Hamiltonian at each point is of the form

$$H = v_F \mathbf{\alpha} \cdot \mathbf{p} + \beta m$$

(1)

where matrices $\alpha_i$, $\beta$ square to unit matrix and anti-commute among themselves. The above properties constrain the matrices to be even-dimensional. In three space dimension where we need three matrices $\alpha_i$, $i = 1, 2, 3$, one needs at least $4 \times 4$ matrices to satisfy the above algebra.

It was shown by Wolff [1] that the effective theory of the electronic states of bismuth near the L point of the Brillouin zone can be described by a Dirac theory. Within the isotropic
approximation this equation can be written as [2]

$$H_B = \sum_k \Psi^\dagger_k \begin{pmatrix} \Delta & i\gamma \vec{k}\sigma \\ -i\gamma \vec{k}\sigma & -\Delta \end{pmatrix} \Psi_k,$$

(2)

where the Hamiltonian matrix corresponds to the Dirac representation of the gamma matrices and the four component spinor is defined as $\Psi^\dagger_k = (c^\dagger_{\vec{k}\uparrow}, c^\dagger_{\vec{k}\downarrow}, d^\dagger_{\vec{k}\uparrow}, d^\dagger_{\vec{k}\downarrow})$. The above Hamiltonian describes two bands of positive and negative energy states corresponding to $c^\dagger_{\vec{k}\sigma}$ and $d^\dagger_{\vec{k}\sigma}$ operators. Obviously $\vec{k}$ is the Bloch momentum and $\sigma$ is the spin component. $2\Delta$ is the gap which in the case of bismuth is approximately 15.4 meV [3, 4] and $\gamma = \hbar v$ comes from spin-orbit interaction and sets the velocity scale [4], with $v/c \approx 10^{-3}$. The spectrum of this model is:

$$\varepsilon_k = \pm \sqrt{\gamma^2 k^2 + \Delta^2}.$$

(3)

In this paper we take the Dirac Hamiltonian (2) as the continuum of host material states, and couple it to an isolated impurity level within the single impurity Anderson model (SIAM) to investigate the nature of local moment formation in Dirac materials.

2. Anderson impurity in a Dirac host

Single impurity Anderson model for a host of Dirac fermions is given by,

$$H = H_B + H_{\text{imp}} + H_{\text{hyb}},$$

(4)

where $H_{\text{imp}}$ is given by:

$$H_{\text{imp}} = \sum_{\sigma} \varepsilon_0 f^\dagger_{\sigma} f_{\sigma} + U n_{\uparrow} n_{\downarrow},$$

(5)

where $f^\dagger$ represents creation operator in impurity orbital, $n_{\sigma} = f^\dagger_{\sigma} f_{\sigma}$, the energy $\varepsilon_0$ is the impurity energy level and $U$ is the on-site Coulomb repulsion. The hybridization between continuum states of the host and the impurity level is constructed as follows: The two bands of positive and negative energy states in the three dimensional Dirac Hamiltonian essentially comes from the combination of orbitals of two neighboring atoms in a unit cell. Therefore the even (or equivalently odd) combination of positive and negative energy states forms a state localized on lattice site. Hence we assume a local hybridization of the following form:

$$H_{\text{hyb}} = \frac{1}{\sqrt{V}} \sum_{\vec{k}} [V(c^\dagger_{\vec{k}\sigma} + d^\dagger_{\vec{k}\sigma}) f_{\sigma} + V^* f^\dagger_{\sigma} (c_{\vec{k}\sigma} + d_{\vec{k}\sigma})].$$

(6)

where $V$ is hybridization strength between impurity level and Bloch state and $V$ is the volume of the host material.

The local component of the retarded Green function is defined using the standard notation as follows:

$$\langle\langle f_\sigma(t) | f^\dagger_{\sigma'}(t') \rangle\rangle = -i\theta(t - t') \langle\{ f_\sigma(t), f^\dagger_{\sigma'}(t') \} \rangle.$$

(7)

Writing the equation of motion for the above Green function in frequency domain gives,

$$\langle \omega - \varepsilon_0 \rangle \langle\langle f_\sigma | f^\dagger_{\sigma'} \rangle\rangle = \delta_{\sigma\sigma'} + U \langle\langle f_\sigma n_{\bar{\sigma}} | f^\dagger_{\bar{\sigma}} \rangle\rangle + \sum_{\vec{k}} \frac{V^*}{\sqrt{V}} \langle\langle b^\dagger_{\vec{k}\bar{\sigma}} | f^\dagger_{\sigma} \rangle\rangle,$$

(8)
in which we define \( b_{k\sigma} = c_{k\sigma} + d_{k\sigma} \). Applying the Hartree approximation to Coulomb term amounts to the replacement \( \varepsilon_0 \rightarrow \varepsilon_{\sigma} = \varepsilon_0 + U\langle n_{\sigma}\rangle \). To close the equation of motion we write the equation of motion for \( \langle \langle b_{k\sigma} f_{\sigma'}^\dagger \rangle \rangle \) that gives,

\[
\langle \langle b_{k\sigma} f_{\sigma'}^\dagger \rangle \rangle = \frac{V}{\sqrt{V} \omega^2 - \varepsilon_k^\sigma} \langle \langle f_{\sigma} f_{\sigma'}^\dagger \rangle \rangle.
\] (9)

This result shows that within Hartree mean-field approximation, the Green function reads:

\[
(\omega - \varepsilon_{\sigma} - \Sigma_f(\omega)) \langle \langle f_{\sigma} f_{\sigma'}^\dagger \rangle \rangle = \delta_{\sigma\sigma'},
\] (10)

where the self-energy at the Hartree level is:

\[
\Sigma_f(\omega) = \frac{|V|^2}{\sqrt{V}} \sum_k \frac{2\omega}{\omega^2 - \varepsilon_k^\sigma}.
\] (11)

Equation (10) indicates that within the present Hartree decoupling, in spite of spin-mixing in the Hamiltonian, the impurity’s Green function remains diagonal in spin label; or equivalently the spin-flip correlation function is zero, i.e. \( \langle \langle f_\uparrow f_\downarrow^\dagger \rangle \rangle = 0 \). Doing the summation over \( \vec{k} \) in Eq. (10), the self-energy as a function \( \omega \) becomes:

\[
\Sigma(\omega) = \frac{\bar{\nu}}{\pi D} \sqrt{\omega^2 - \Delta^2} \left[ 2\omega \ln \left( \frac{\sqrt{D^2 - \Delta^2} + \sqrt{\omega^2 - \Delta^2}}{\sqrt{D^2 - \Delta^2} - \sqrt{\omega^2 - \Delta^2}} \right) - \frac{4\omega\sqrt{D^2 - \Delta^2}}{\sqrt{\omega^2 - \Delta^2}} - i\pi|\omega| \right].
\] (12)

In above equation \( D \) is the bandwidth. In contrast to normal metal where the dimensionless parameter \( \frac{\Delta^2}{\Delta D} \) emerges in Hartree approximation, here in Eq. (12) \( \bar{\nu} \equiv \frac{|V|^2}{2\pi\bar{\nu}} \) emerges naturally. We have to emphasize that in previous study of SIAM in two dimensional Dirac material (graphene), the conventional dimensionless parameters \( Y = \frac{\mu - \varepsilon_0}{\bar{\nu}} \) and \( X = \frac{\pi V^2}{\bar{\nu}^2} \) did not appear naturally, and they were employed based on analogy with normal metallic hosts. There the phase diagram was plotted in terms of these conventional parameters \( Y \) and \( X \) to contrast the effect of the Dirac nature of charge carriers on local moment formation and to contrast it to normal metals. As we will see in this work, the emergence of the above natural parameter leads to qualitative differences in the nature of local moment formation both compared to two dimensional ones, as well as the normal metals. Given this natural parameter, neither the hybridization strength, \( V \), nor the spin-orbit coupling, \( \gamma \) is the major player, but this peculiar combination of the parameters determines the phase diagram. This helps us to study the effect of spin-orbit interaction on local moment formation. In what follows, we will calculate the occupation of spin \( \uparrow \) and \( \downarrow \) at zero temperature. The occupation of impurity site for spin \( \uparrow \) is given as an integral over spectral function, which it depends on spin \( \downarrow \) occupation. As a result the occupation and magnitude of local moment is calculated self-consistently:

\[
\langle n_{\uparrow} \rangle = -\frac{1}{\pi} \int_{-\infty}^{\mu} d\omega \frac{I m \Sigma_f}{(Z^{-1}(\omega)\omega - \varepsilon_{\downarrow})^2 + I m (\Sigma_f)^2},
\] (13)

where the renormalization factor is:

\[
Z^{-1}(\omega) = 1 - \frac{2\bar{\nu}}{\pi D} \sqrt{\omega^2 - \Delta^2} \left[ \ln \left( \frac{\sqrt{D^2 - \Delta^2} + \sqrt{\omega^2 - \Delta^2}}{\sqrt{D^2 - \Delta^2} - \sqrt{\omega^2 - \Delta^2}} \right) - \frac{2\sqrt{D^2 - \Delta^2}}{\sqrt{\omega^2 - \Delta^2}} \right].
\] (14)
3. Numerical results

We solve Eq. (13) along with a similar equation obtained by replacing $↑→↓$ self-consistently. Local magnetic moment is characterized by $n_↑ - n_↓ \neq 0$ the intensity plots of which are presented. We construct the phase diagram of the magnetic moments in three dimensional Dirac systems in the plane of variables $X = \tilde{v} = |V|^2 D/(2\pi \gamma^3)$ and $Y = \frac{\mu - \varepsilon_0}{U}$. The first dimensionless parameter is naturally driven from the dynamics of the SIAM, while the second dimensionless parameter is usually used in the literature following Anderson’s work on local magnetic states in metals. Since in this case the variable $Y$ does not naturally arise from the dynamics of SIAM, $\mu$ and $\varepsilon_0$ will be two independent variables, tuning of which gives rise to qualitatively different regions for the local magnetic states. Let us independently tune them in the sequel.

3.1. Tuning $\mu$

Fig. 1-a shows the phase diagram for an impurity with impurity level at energy $\frac{\varepsilon_0}{D} = 0.02$ and Hubbard repulsion $U = 0.5D = 1$ eV. Note that the phase diagram which is obtained by tuning parameters $\mu$ and $X$ does not have the particle-hole symmetry around $Y = 0.5$, as in the two-band case, particle-hole symmetry holds when in addition to $Y = 0.5$, the chemical potential $\mu$ is also at the mid-gap in which case there would be no conduction in the system. In addition, the magnetic region is limited to $\mu \geq \varepsilon_0$. In this respect the local magnetic states in 3D massive Dirac materials are akin to those in normal metals. However, for 2D massless Dirac fermions in graphene the magnetic region extends to $\mu < \varepsilon_0$. This can be understood by the broadening of impurity level which asymptotically behaves like $\frac{1}{\mu^3}$. This means that the spectral function of local impurities embedded in the Wolff Hamiltonian decreases fast enough to avoid magnetic moments for $Y < 0$ region as happens for the local moments in normal metals.
Fig. 1-b is the same as Fig. 1-a, but with a different value of $\varepsilon_0 = -1.4$ eV. In both figures it can be seen that smaller values of $X$ that correspond to larger values of $\gamma$ give rise to larger local magnetic moments. The parameter $\gamma$ is controlled by the spin-orbit coupling, and also sets the velocity scale of the Dirac fermions. It is therefore curious to note that faster 3D Dirac fermions when hybridized with a local impurity level give rise to larger magnetic moments. Also it is noteworthy to mention that the sign of $\varepsilon_0$ determines whether the magnetic region bends upward ($\varepsilon_0 < 0$) or downward ($\varepsilon_0 > 0$) as one moves towards larger $X$ values. In this respect the region of magnetic states in graphene also displays similar behavior, but in graphene the boundaries are round, and also extend to negative $Y$ axis [5].

### 3.2. Tuning $\varepsilon_0$

Due to the experimental results on dielectric constant of bismuth and its compounds, which indicate a relative permeability about 10-40, the Coulomb repulsion could be substantially decreased [6]. In addition regarding the Haldane-Anderson mechanism for impurity in semiconductors, reduction of the charge accumulation on impurity site leads to a fall in on-site Coulomb repulsion up to 2 orders of magnitude [7, 8]. Therefore, we investigate the problem for smaller values of Coulomb interaction $U$. Since $\mu$ and $\varepsilon_0$ in the SIAM for Dirac materials are

![Figure 2](image_url)

**Figure 2.** Phase diagram of SIAM in three dimensional massive Dirac matter. The area enclosed by the curves and the $Y$-axis is magnetic region. The variables are defined by $X = \frac{V^2 D}{2\pi \gamma^3}$ and $Y = \frac{(\mu - \varepsilon_0)}{U}$. The Coulomb repulsion and chemical potential are $U = 1$ eV and $\mu = 35$ meV.
Figure 3. Phase diagram of SIAM in massless Dirac matter. The area enclosed by the curves and the $Y$-axis is magnetic region. The variables are defined by $X = \frac{|V|^2 D}{2\pi\gamma^3}$ and $Y = \frac{(\mu - \varepsilon_0)}{U}$. The Coulomb repulsion and chemical potential are $U = 1$ eV and $\mu = 35$ meV.

independent parameters, we choose to fix $\mu = 35$ meV which is relevant to bismuth and tune $\varepsilon_0$ in order to construct a phase diagram in the plane of $X$ and $Y$. In general, for smaller values of Hubbard $U$ one expects narrower magnetic region as double occupancy becomes less costly. When we tune $\varepsilon_0$ for a fixed $\mu$, curiously the local moment region of the phase diagram splits into two pieces shown in Fig. 2. The two pieces correspond to the hybridization of impurity level with negative and positive energy states of the Dirac continuum. Saying it in another way, the upper magnetic region comes from the situation where the impurity level lies within the valence band ($\varepsilon_0 < -\Delta$) and the lower magnetic region arises from the case where the impurity level is above the gap ($\varepsilon_0 > \Delta$). As indicated in the legend, the red color stands for fully spin polarized impurity level and the white color represents the non-magnetic state.

3.3. Massless($\Delta = 0$)
The 3D Dirac fermions in materials such as $Na_3Bi$ or $Bi_{1-x}Sn_x$ for $x \approx 0.04$ [9] become massless. Therefore it is interesting to check what happens to the local magnetic moments when the gap parameter of the host Dirac material vanishes. The phase diagram of local magnetic states in a host of massless Dirac fermions is depicted in Fig 3. The elbow-like upper branch of the magnetic region in the massless case is narrowed and smoothened.

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