Dirac-Kondo semimetals and topological Kondo insulators in the dilute carrier limit

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Heavy fermion systems contain not only strong electron correlations, which promote a rich set of quantum phases, but also a large spin-orbit coupling, which tends to endow the electronic states a topological character. Kondo insulators are understood in terms of a lattice of local moments coupled to conduction electrons in a half-filled band, i.e. with a dense population of about one electron per unit cell. Here, we propose that a new class of Kondo insulator arises when the conduction-electron band is nearly empty (or, equivalently, full). We demonstrated the effect through a honeycomb Anderson lattice model. In the empty carrier limit, spin-orbit coupling produces a gap in the hybridized heavy fermion band, thereby generating a topological Kondo insulator. This state can be understood in terms of a nearby phase in the overall phase diagram, a Dirac-Kondo semimetal whose quasiparticle excitations exhibit a non-trivial Berry phase. Our results point to the dilute carrier limit of the heavy-fermion systems as a new setting to study strongly correlated insulating and topological states.

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I. TOPOLOGICAL ELECTRONIC STATES AND KONDO EFFECT

A simple platform for topological electronic states is the honeycomb lattice as in graphene. In the absence of the SOC, the system at half filling or with one electron per site realizes a Dirac semimetal with the conduction and valence bands touching at a point in momentum space, the Dirac point, where the quasiparticles show linear dispersions of Dirac fermions. This semi-metallic phase can be topologically non-trivial if the corresponding quasiparticle wavefunction carries a destructive Berry phase. The topological effect gives rise to unconventional quantum Hall plateaus when a magnetic field is applied as manifested in graphene. Remarkably, such topological semimetal can be viewed as a parent phase of topological band insulators, in the sense that it can open a bulk band gap and exhibit gapless surface states in the presence of intrinsic SOC. An important open issue is what happens to such topological semimetallic or insulating phases when the electron correlations are strong.
able parameter. Motivated by the recent experiments on the dilute-carrier heavy fermion materials, as well as by an earlier study about the role of SOC in Kondo lattice systems, in this paper we explore the interplay between the Kondo effect and SOC in the DCL regime. We investigate the paramagnetic phases in a honeycomb Anderson lattice model at arbitrary electron fillings. We study the model when the f-electron Coulomb repulsion is strong, and compare the results with their counterparts when the interaction is weak. We demonstrate the existence of the paramagnetic semimetallic phase, the DSKM, in the absence of the SOC. When the SOC becomes nonzero, this phase becomes the $Z_2$-TKI or -topological mixed valence insulator. We also discuss the role of topological Berry phase and the Dirac fermion behavior of low energy excitations.

II. ANDERSON LATTICE MODEL

We start from the Hamiltonian for a honeycomb Anderson lattice:

$$H = H_0 + H_{cd} + H_d.$$  \hspace{1cm} (1)

Here, $H_0 = -t \sum_{\langle i,j \rangle} \left( c_{i,\sigma}^\dagger c_{j,\sigma} + h.c. \right)$ is the kinetic term of the conduction $c$ electrons with the nearest-neighbor (n.n.) hopping, $H_d = E_0 \sum_{\alpha} n_{\alpha d\sigma} + U \sum_{\alpha} n_{\alpha d\sigma} n_{\alpha c\sigma}$ describes the energy level $E_0$ and on-site Coulomb repulsion $U$ of the local $d$ electrons, and $H_{cd} = V \sum_{j\sigma} \left( c_{j,\sigma}^\dagger d_{j,\sigma} + h.c. \right)$ is the hybridization between the $c$ and $d$ electrons. We will consider $E_0$ to be well below the Fermi energy. Our primary interest is for large $U$, where the model is mapped to a Kondo lattice. To gain insights into the topological characteristics of the electronic states, we will first consider the small $U$ regime.

In the momentum $k$-space, the conduction electron part shifted by the chemical potential $\mu$ takes the form

$$H_0 = \sum_{\mathbf{k}\mathbf{\alpha}} \left( \epsilon_{\mathbf{k}\mathbf{\alpha}}^c + \mu \right) c_{\mathbf{k}\mathbf{\alpha}}^\dagger c_{\mathbf{k}\mathbf{\alpha}},$$

where $\epsilon_{\mathbf{k}\mathbf{\alpha}}^c = t \left[ 1 + e^{-i\mathbf{k}\cdot\mathbf{a}_\alpha} \right]$, with $\mathbf{k}$ valued in the first Brillouin zone (BZ). The subscripts $a$ and $b$ denote two sublattices of the honeycomb lattice where the primitive vectors are represented by $\mathbf{a}_1$ and $\mathbf{a}_2$, respectively.

III. SEMIMETAL PHASE: THE CASE OF WEAK COUPLING

We first consider the weak-coupling regime where the effect of $U$ can be treated perturbatively. We assume that the $d$-orbital (with $E_0 < E_F$) is half-filled in the absence of the $c$-$d$ hybridization. While a finite $V$ could delocalize the $d$ electrons, a small $U$ will lead to a renormalization of quasi-particle weight $Z = \frac{1}{1 - \eta \epsilon_k}$ for $d$-electrons. Here, the self-energy of $d$-electrons is assumed to be momentum-independent, $\Sigma_d(k, \omega) \approx \Sigma_d(\omega)$, since the $d$-electrons are predominately localized in the absence of the $c$-$d$ hybridization. The value of $0 \leq \epsilon \leq 1$, which could be calculated perturbatively, leads to an effective hybridization $\tilde{V} = \sqrt{Z}V$. A crucial feature of the honeycomb lattice is that, at the half-filling, $\tilde{V}$ is nonzero only when $V$ is larger than a threshold value, $V_c$, due to the Dirac-like dispersion of the conduction band. Usually, away from half-filling, $V$ is significantly reduced due to an enhanced density of states near the Fermi energy. The situation with a finite effective hybridization or Kondo effect corresponds to the regime where $\tilde{V} > V_c$.

In this hybridization phase, the dressed $d_{k\sigma} = ZV d_{k\sigma}$ is used for both sublattices. Then, the Hamiltonian can be re-expressed by $H = \sum_{k\sigma} \Psi_{k\sigma} \hat{H}_{k\sigma}^{(weak)} \Psi_{k\sigma}$, with

$$H_{k\sigma}^{(weak)} = \left( M_k \tilde{V} - I_{2x2} \right).$$  \hspace{1cm} (3)

Here, $\Psi_{k\sigma} = (c_{a,\sigma}^\dagger, c_{b,\sigma}^\dagger, \tilde{d}_a^\dagger, \tilde{d}_b^\dagger)$, $I_{2x2}$ is a $2 \times 2$ identity matrix, $\epsilon_d = Z(E_0 + \Sigma_d(0))$ is the renormalized $d$ electron level. The eigenstates of the above Hamiltonian are degenerate for the two spin components. Each of them has four quasiparticle bands with energies

$$E_k^{(\eta, \tau)} = \frac{1}{2} \left[ \epsilon_\eta - \epsilon_d \eta + \sqrt{\left( \epsilon_d - \epsilon_k^{(\eta)} \right)^2 + 4V^2} \right].$$  \hspace{1cm} (4)

Where, $\epsilon_k^{(\eta)} = \eta g_k - \mu$, $\eta = (+, -)$ indicates the band index due to the superposition of the (a,b) sublattices, $\tau = (+, -)$ the band index due to the c-d hybridization.

The order of the bands is related to the sign of $\epsilon_d - \epsilon_k^{(\eta)}$. For convenience, we denote $E_1^{(1)} = E_k^{(+, +)}$, $E_2^{(-, +)}$, $E_3^{(-, -)}$, and $E_4^{(+, -)}$. Without losing generality, we assume the order $E_1^{(1)} \geq E_2^{(2)} \geq E_3^{(3)} \geq E_4^{(4)}$ in the absence of hybridization. This is satisfied if the bare d-electron level $E_d$ is at or below the bottom of the conduction band, because for $\tilde{V} = 0$ and $\epsilon_d < \epsilon_k^{(\eta)}$ we have $E_1^{(1)} = \epsilon_k^{(+)}$, $E_2^{(2)} = \epsilon_k^{(-)}$, $E_3^{(3)} = E_4^{(4)} = \epsilon_d$.

At the half-filling, $\mu = 0$, $\epsilon_k^{(+)}$ and $\epsilon_k^{(-)}$ contact at the Dirac points, $\pm \mathbf{k}_D = \pm \frac{\pi}{a_0} \left( \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, 0 \right)$ ($a_0$ is the distance of the two n.n. sites), so that $g_{\pm \mathbf{k}_D} = 0$. In the hybridization phase $\tilde{V} > 0$, the four bands deform differently. An important observation is that the order of bands $E_1^{(1)} \geq E_2^{(2)} \geq E_3^{(3)} \geq E_4^{(4)}$ holds for arbitrary $\tilde{V} > 0$ and $\mathbf{k}$ in BZ. The equality holds only at the Dirac points $\pm \mathbf{k}_D$. Hence the two upper bands $E_1^{(1)}$ and $E_2^{(2)}$, as well as the two lower bands $E_3^{(3)}$ and $E_4^{(4)}$, contact at the Dirac points respectively. Such band touching behavior is robust for any $\tilde{V} > 0$ since the hybridization keeps the required discrete symmetries like those in graphene.
average particle number per unit cell $n$ is not conserved when $\tilde{\pm}$ coupling regime where the symmetry points (Γ → M → K → Γ) are one of the Dirac points by tuning the chemical potential $\mu > 0(0)$ in Case (I) and Case (II) accordingly.

However, the two intermediate bands $E^{(2)}_k$ and $E^{(3)}_k$ are always separated by a finite gap $\Delta = \sqrt{(\varepsilon_d + \mu)^2 + 4V^2}$. This is the hybridization gap which leads to the Kondo or mixed valence insulating phase at the half filling ($\mu = 0$).

If we tune the chemical potential upward to $\mu = \mu_c = \tilde{\epsilon}_d$, the Fermi energy is shifted to the Dirac points so that $E^{(1)}_{\pm \pm \vec{k}_D} = E^{(2)}_{\pm \vec{k}_D} = 0$. The total electron filling factor is then $n = (n_c + n_d)/2 = 3/4$. Notice that the average particle number per unit cell $n_c$ (or $n_d$) alone is not conserved when $\vec{V} \neq 0$, and can be calculated by $n_c = -\frac{1}{2N} \frac{\partial}{\partial \mu} \sum_{k,i=2,3,4} E^{(i)}_k$ with $N$ being the total number of unit cells. When $\vec{V} = 0$, the total electron filling $n/2 = 3/4$ corresponds to the case with $n_c = 2$ (the half-filling for c electrons) and $n_d = 1$ (the half-filling for d electrons).

Figure 1(a) shows the band structure along some high symmetry points (Γ → M → K → Γ) in the weak-coupling regime where the K-point is one of the Dirac points $\pm \vec{k}_D$. Here the parameters $t = 1$ and $E_0 = -3$ are fixed. Without loss of generality, we also choose $\varepsilon_d = -2.5, \tilde{\epsilon}_d = 0.9$ as due to the renormalization effect of the hopping $U$. In Fig.1(a) we shift the Fermi energy at the Dirac points in between the two upper bands (where $E_F = 0$).

This is realized by increasing the chemical potential to $\mu_c = 0.324$. The hybridization gap opens in between the second and third bands. The flat band nature of the $d$-level is mainly reflected in the two lower bands.

In principle the Fermi energy can be also shifted downward by tuning the chemical potential. It would be expected that we can tune the total electron filling factor to $n = (n_c + \frac{1}{2})/2 = 1/4$ so that the Fermi energy is shifted to $E^{(3)}_{\pm \pm \vec{k}_D} = E^{(4)}_{\pm \vec{k}_D}$. But this value is always negative as $\varepsilon_d < 0$ and $\mu > \varepsilon_d$ in the weak-coupling regime. We will see below that the Fermi energy can be tuned to zero exactly in the strong-coupling regime.

IV. SEMIMETAL PHASE: THE CASE OF STRONG COUPLING

We turn next to the strong-coupling regime where $U$ is large enough so that no double occupancy is allowed on each sites of the $d$-sublattice. We utilize the slave-boson method, and express $\hat{c}^\dagger_\sigma \hat{f}^{\dagger \sigma}_{\vec{k}} b_{\vec{k}}$, with $\hat{f}^{\dagger \sigma}_{\vec{k}}$ and $b_\vec{k}$ being respectively fermionic and bosonic operators satisfying the constraint $b_\vec{k}^\dagger b_\vec{k} + \sum_{\sigma} \hat{f}^{\dagger \sigma}_{\vec{k}} \hat{f}^{\sigma}_{\vec{k}} = 1$. Introducing the basis $\Psi^{\pm}_{\vec{k} \sigma} = \langle \epsilon^i_{a,\vec{k} \sigma}, \epsilon^i_{b,\vec{k} \sigma}, \hat{f}^i_{a,\vec{k} \sigma}, \hat{f}^i_{b,\vec{k} \sigma} \rangle$, the mean-field Hamiltonian is expressed as $H_{MF} = \sum_{\vec{k}\sigma} \Psi^{\dagger}_{\vec{k} \sigma} H^{(strong)}_{\vec{k} \sigma} \Psi_{\vec{k} \sigma}$ with

$$H^{(strong)}_{\vec{k} \sigma} = \left( \frac{M_\vec{k}}{r V} \right) \nu \cdot I_{2x2} \left( E_0 + \xi \right) \cdot I_{2x2}^T.$$ (5)

Here, $r = \langle \hat{b} \rangle$ is the condensation density of the bosons, and $\xi$ is the Lagrange multiplier imposing the constraint.

The structure of the strong-coupling Hamiltonian Eq. (5) is similar to that in the weak-coupling regime, Eq. (4). The quasiparticle bands are then obtained as in Eq. (4) with replacements $\varepsilon_d \to E_0 + \xi$ and $\sqrt{\tilde{Z}} \to r$. Hence in the hybridization phase $V^* = r V \neq 0$, or $r > 0$, there are four quasiparticle bands, with two upper bands and two lower bands contact respectively at the Dirac points. Different from the weak-coupling regime, the parameters $r$ and $\xi$ should be determined self-consistently by $\frac{1}{2N} \sum_{k,\alpha=a,b} \langle \epsilon^i_{a,\vec{k} \sigma}, \epsilon^i_{b,\vec{k} \sigma}, \hat{f}^i_{a,\vec{k} \sigma}, \hat{f}^i_{b,\vec{k} \sigma} \rangle + r^2 = 1$, $\frac{1}{2N} \sum_{k,\alpha=a,b} \nu \langle \epsilon^i_{a,\vec{k} \sigma}, \epsilon^i_{b,\vec{k} \sigma}, \hat{f}^i_{a,\vec{k} \sigma}, \hat{f}^i_{b,\vec{k} \sigma} \rangle + r \xi = 0$, with $\nu$ indicating the real part. Here we numerically solve these equations for $t = 1, E_0 = -3$ for various $V$ at the fractional fillings of the total electron $n/2 = (n_c + n_d)/2$ per unit cell, with $n_c = -\frac{1}{2N} \frac{\partial}{\partial \mu} \sum_{k,i} E^{(i)}_k$ and $n_d = \frac{1}{2N} \frac{\partial}{\partial \mu} \sum_{k,i} E^{(i)}_k$ for occupied band(s) $i$.

Similar to the half-filling case where a finite value of $V_c$ is required for the Kondo phase, we find that at the 1/4-filling the solution for $r > 0$ exists when $V > V_c \sim 2.6$. To shift the Fermi energy to zero at the Dirac points, we can tune the chemical potential to $\mu_c = -\frac{r^2 \nu^2 V^2}{E_0 + \xi}$ so that $|\mu|$ is relatively large in the strong-coupling regime. In this regime, $E_0 + \xi$ is slightly above the Fermi energy so that the Kondo phase is stabilized. For example, a set of self-consistent parameters $\xi = 3.129, r = 0.241$, and $\mu = -4.903$ is obtained when we fix $V = 3.3$. The resulting band structure is shown in Fig.1(b) where the four bands for high symmetry points are plotted. Although the two lower bands are relatively narrow, they contact at the Dirac points where the Fermi energy locates realizing the DKSFM phase. In principle, the Fermi energy can be also shifted upward. But precisely at the 3/4-filling, only the trivial solution $r = 0$ exists, indicating that the ground state is always in the decoupled phase. This is due to the strong on-site $U$. 

![Figure 1](image-url)
Having established its existence in the weak- and strong-coupling regime, we expect that the semimetal phase also exist for intermediate values of $U$. On general grounds, the symmetry-preserving nature of the hybridization we consider ensures that the location of the Dirac points is protected by the inversion symmetry of the lattice, as in graphene. More microscopically, in the Kondo-hybridized phase, the strength of hybridization is expected to interpolate between the results calculated in the small and large $U$ limits. In other words, within the hybridized phase, the main effect of varying $U$ is expected to renormalize the model parameters.

V. TOPOLOGICAL BERRY PHASE AND DIRAC HEAVY FERMIONS

Our analysis so far establishes the existence of the paramagnetic semimetal phase in the present honeycomb Anderson lattice away from half-filling. The extreme situations include Case (I): in the weak-coupling regime at the $3/4$-filling, and Case (II): in the strong-coupling regime at the $1/4$-filling. In these two cases the Fermi energy can be tuned exactly to zero. The next issue is whether the semimetallic phase is topologically nontrivial. We thus calculate the Berry phase of the quasiparticle wavefunctions around the Dirac points. For instance, let $|\Phi_k\rangle = \{\Phi_k^{(1)}, \ldots, \Phi_k^{(4)}\}^T$ be the eigenstate of $h_k$, with $\Phi_k^{(i)}$ given explicitly in the SM. When the crystal momentum $k$ rotates adiabatically with a time-like parameter $\lambda$ in a loop $C$, $|\Phi_k\rangle$ is always single-valued, while the corresponding Berry phase is given by

$$\theta = -i \int_C \langle \Phi_k | \frac{\partial}{\partial \lambda} |\Phi_k\rangle d\lambda.$$  

We find that when $C$ encloses the Dirac point $k_D$, $\theta = 2\pi$; $|\langle \Phi_k^{(1)} |^2 + |\Phi_k^{(3)} |^2 | = \pi$. Similarly, $\theta = -\pi$ when $C$ encloses the Dirac point $-k_D$. Notice that the above derivation holds for both weak- and strong-coupling regimes. Such a non-trivial Berry phase will cancel the contribution from the zero-point quantum fluctuation, leading to the shifted quantum Hall plateaus as observed in graphene.  

It is also interesting to ask whether the low energy excitations near the Dirac points are Dirac fermions. In the Kondo-destroyed phase, the semimetal appears at half-filling like in graphene so that the low energy excitations are Dirac fermions, exhibiting the relativistic dispersion $E_q^\pm = m_F q + m_D^0 q^2$ for small $|q|$ shifted from $\pm k_D$ with the velocity $v_F = \frac{m_F}{m_D^0}$. In the Kondo hybridized phase, the corresponding low energy excitations show different behavior. In general, quadratic dispersions emerge due to the finite effective hybridization. For illustration, we consider the situation where $V$ is close to the phase boundary in Case (I) or Case (II) where $V$ or $V^*$ is small. The particle- and hole-like excitations take the form $E_q^{(\pm)} = \pm \tilde{v}_F |q| + \tilde{a} q^2$ up to $O(|q|^4)$ in Case (I), and $E_q^{(\pm)} = \pm v_F^* |q| - a^* q^2$ in Case (II), with the corresponding renormalized Fermi velocities $v_F^*$ and the momentum-dependent coefficients $\tilde{a}$, $a^*$ given explicitly in the Supporting Information.

In the immediate vicinity of the momentum space near the Dirac points, the linear term dominates so that the low energy excitations are approximately Dirac fermions. For Case (I), when hybridization increases, the renormalized Fermi velocity $v_F^*$ decreases and the quadratic term $a^*$ increases. Hence, the range of the shifted momentum $q$, where the linear dispersion dominates is reduced by the effective hybridization. This implies that the excitations gain a finite effective mass beyond this range. For Case (II), the suppression of the renormalized Fermi velocity $v_F^*$ is stronger so that $a^*$ is effectively enhanced. As a result, the quasiparticle band $E_k^{(3)}$ (or quasihole band $E_k^{(4)}$) is significantly flattened due to the $f$-electron feature, indicating that the momentum range where the energy dispersion exhibits linear behavior is narrowed. Therefore the effective mass is enhanced in the DKSM phase. For this reason, we can also call the quasiparticles in the DKSM as Dirac heavy fermions (DHFs).

VI. TOPOLOGICAL KONDO INSULATOR

We now discuss the influence of the conduction electrons’ SOC on the semimetal phase. We add $H_{SO} = i\lambda_{so} \sum_{i,j<\sigma} c_{i\sigma}^{\dagger} \sigma_i \sigma_{j\sigma'} c_{j\sigma'}$ to Eq. (1), with $\lambda_{so}$ being the strength of the intrinsic (Dresselhaus-type) SOC of the conduction electrons and $\lambda_{so}$ depends on the direction of hopping between the next-nearest-neighbor sites. In general, $\lambda_{so}$ will open a gap in the semimetal phase and produce edge states. For example, in Case (II), we show in Fig. 2 the energy spectra of a stripe.
of the finite system with a zigzag geometry by using the same set of model parameters as discussed previously. A finite band gap in the two lower (or two upper) bands opens immediately with metallic edge states.

The above calculation demonstrates that the DKSM or hybridization semimetal can be driven to TKI or topological mixed valence insulator by turning on the SOC, as schematically shown in Fig. 3. As demonstrated previously, there is a phase transition from the TI to KI phases when going across the dotted line on the \( \mu = 0 \) (or \( n_c = 1 \))-plane corresponding to the half-filling case. However, no direct transition can take place from the TI to TKI phases by tuning only one of the three parameters. Of course, the TKI phase could also be realized from the topological trivial KI phase in the presence of the SOC by tuning the chemical potential, or from the helical metal phase by tuning both the chemical potential and Kondo coupling.

**NEW PHYSICS IN THE DILUTE LIMIT: DISCUSSIONS**

Fig. 4 illustrates the DCL regime we are considering, with the local moments represented by a Mott-insulator component and the conduction electrons given by a band-insulator component. Our results highlight several important features in this DCL regime of heavy fermion systems. First, a relatively large \( V_c \) as shown for Case (II) is required in the Kondo phase, indicating the delayed Kondo screening as a natural consequence of the so-called Nozières exhaustion problem in this limit. This conclusion is consistent with the recent experiments, which show the depletion of the coherent Kondo energy scale\(^{32,42}\). Second, the band touching and topological features are both inherited from those of the itinerant and local components of the lattice model due to the symmetry preserving hybridization. The band curvature deforms drastically due to the finite hybridization, rendering the linear Dirac dispersion valid only in a narrowed momentum region in the vicinity of the Dirac points. Third, in the Kondo phase, the SOC of conduction electrons can generate a bulk gap at the Dirac points leading to a correlated TI state. Fourth, the surface states of the TKI phase could be either light or heavy fermions, depending on the details of the hybridization and the quasiparticle momentum. In this connection, we notice that both light and heavy quasiparticles as well topological non-trivial or trivial surface states are observed in SmB\(_6\) and YbB\(_6\) depending on surface directions in several recent magneto-thermoelectric transport and pressure measurements\(^{38,52}\). Finally, while we have emphasized the SOC of the conduction electrons, an SOC of \( f \) electrons will also open a bulk gap driving the semimetal phase to the TKI phase.

So far we considered the paramagnetic state, which has a prevailing interest in understanding the fundamental underlying principle of the electronic structures and can be stabilized by both SOC and quantum fluctuations. In the absence of SOC, on the other hand, the system could be ferromagnetically ordered in the DCL regime. We can qualitatively explore the influence of the ferromagnetic order by \( H_F = \sum_{\alpha} \sigma M [ J_{RI} f_{n_k \sigma} c_{n_k \alpha} - I_R f_{n_k \sigma} f_{n_k \alpha} ] \), with parameters \( J_{RI} \), \( I_R \) and \( M \) being the effective Kondo coupling, the RKKY interaction, and the magnetization, respectively. The non-zero \( M \) splits the spin degeneracy, leading to the shifts \( \mu \rightarrow \mu_\sigma = \mu - \sigma M J_{RI} \) and \( E_0 \rightarrow E_{0,\sigma} = E_0 - \sigma M I_R \). Therefore, in each spin channel, the order of four bands does not alter and the band touching feature at the Dirac points \( k_D \) is still robust. This feature ensures the existence of the ferromagnetic Dirac semimetal phase by properly tuning the spin-dependent chemical potentials. The relative band fillings of each spin channel are delicately dependent on the effective parameters \( J_K \), \( I_R \), and \( M \). The consequence of these deserves future investigations.

We close this section by discussing the experimental realizations of our results. Given the recent emergence of heavy fermion systems in the DCL regime, it is quite plausible to realize the novel type of Kondo insulator states in heavy fermion compounds whose conduction-electron band is insulating, especially those with the non-\( f \) electrons being hosted by heavy elements\(^{32}\). In addition, Fig. 4 also inspires us to propose a new type of structure to realize the physics we have discussed. This corresponds to building a heterostructure between a Mott insulator and a band insulator. Such structures can be engineered so that i) for the band insulator, the chemical potential is close to the top of the valence band or the bottom of the conduction band and ii) the barrier at the interface will be relatively small so that a nonzero hybridization will operate between the electronic states.
illustrated in Fig. 4.

VIII. SUMMARY AND OUTLOOK

To summarize, we have shown that the correlated semimetal phases exist in the honeycomb Anderson lattice in the dilute limit of charge carriers where the conduction electron band is nearly empty or full. They could be realized in heavy fermion compounds in the dilute-carrier limit, or at the interface between trivial band and Mott insulators due to a proximity effect. The low energy excitations in such semimetals are approximately linear in the vicinity of the Dirac points. For the case with a large \( f \)-electron’s correlation and almost empty band of conduction electrons, the DKSM is realized and the corresponding quasiparticles are the DHFs because the \( f \)-electron’s contribution is inextricable. In particular, when the quasiparticle’s momenta are moderately away from the Dirac points, such DHFs will gain a finite (cyclotron) mass due to the quadratic correction to the energy dispersion, and manifest the heavy-fermion behavior.

We have also demonstrated that when turning on the SOC, the hybridization semimetal or DKSM phase will open a bulk gap while with metallic surface states. This phase is different to either KI or TI phases at the half-filling case\(^\dagger\). Thus, the present study has established an alternative route towards the formation of TKIs. In this scenario, a TKI is driven from the DKSM phase by the SOC of conduction electrons. Our findings underscore that the interplay between the Kondo coupling and SOC can in general nucleate new quantum phases and their transitions in strongly correlated settings.

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In this Supporting Information, we provide additional derivations for the details of the band dispersion, demonstrate the robustness of the Dirac points in the hybridization phase in the absence of the SOC, and further discuss the formation of topological Kondo or mixed valence insulating state in the presence of the SOC of conduction electrons. The dispersion relations of the low-energy excitations near the Dirac points in the semimetal phase are also presented explicitly.

The Hamiltonian we study is the Honeycomb Anderson lattice with the intrinsic SOC of conduction electrons, described by

\[ H = -t \sum_{\langle ij \rangle \sigma} c_{i \sigma}^{\dagger} c_{j \sigma} + V \sum_{\langle i \sigma \rangle} (c_{i \sigma}^{\dagger} d_{i \sigma} + h.c.) + E_0 \sum_{i \sigma} d_{i \sigma}^{\dagger} d_{i \sigma} + U \sum_{i \sigma} n_{i \uparrow} n_{i \downarrow} + i \lambda_{so} \sum_{\langle \langle ij \rangle \rangle \sigma \sigma'} v_{ij}^\sigma c_{i \sigma}^{\dagger} \sigma_{\sigma} \sigma_{\sigma'} c_{j \sigma'}. \]  

(S1)

The first two lines correspond to the Hamiltonian Eq. (1) given in the main text, the third line is the SOC of conduction electrons.

In the weak-coupling regime, there are totally eight bands of eigenstates, with the following eigenenergies

\[ E^{(\eta, \tau, \sigma)}_k = \frac{1}{2} \left( \epsilon_d + h^{(\eta)}_k - \mu + \tau \sqrt{[\epsilon_d - h^{(\eta, \sigma)}_k + \mu]^2 + 4V^2} \right). \]  

(S2)

Where, \( h^{(\eta, \sigma)}_k = \eta \sqrt{|g(k)|^2 + 4k_{\sigma}} \), \( g_k = t[1 + e^{-ik a_1} + e^{-ik a_2}] \), \( k_{\sigma} = 2\sigma \lambda_{so} \sin|k \cdot a_1| - \sin|k \cdot a_2| - \sin|k \cdot (a_1 - a_2)| \). \( \sigma = (+1, -1) \) indicates the spin index due to the spin up and spin down components, \( \eta = (+, -) \) indicates the band index due to the superposition of the \((a, b)\) sublattices, and \( \tau = (+, -) \) the band index due to the \(c-d\) hybridization. The eigenstates with \( \sigma = (+1, -1) \) are degenerate due to the time reversal symmetry, resulting in four energy bands \( E^{(\iota)}_k \) ( \( \iota = 1, \cdots, 4 \)) in each spin sector, as given explicitly in Eq. (S3) where the index \( \sigma \) in Eq. (S2) is dropped in the following discussions. For a given band \( E^{(\iota)}_k \), the corresponding eigenstate can be solved as \( |\Phi_k^{(\iota)}\rangle = \{\Phi_k^{(\iota)(1)}, \cdots, \Phi_k^{(\iota)(4)}\}^T \), where

\[ \Phi_k^{(1)} = \frac{1}{m_k} \left( \sqrt{V^2 - (E^{(\iota)}_k + \mu)(E^{(\iota)}_k - \epsilon_d)} \right), \quad \Phi_k^{(2)} = \frac{1}{m_k} \left( \sqrt{V^2 - (E^{(\iota)}_k + \mu)(E^{\iota}_k - \epsilon_d)} \right), \]

\[ \Phi_k^{(3)} = \frac{1}{m_k} \left( \sqrt{V^2 - (E^{(\iota)}_k + \mu)(E^{(\iota)}_k - \epsilon_d)} \right), \quad \Phi_k^{(4)} = \frac{1}{m_k}, \]  

with \( m_k \) being a normalization coefficient.

In the strong-coupling regime, the quasiparticle bands can be solved in a similar manner following the weak-strong correspondence illustrated in the main text. The situation \( \mu = 0 \) in the strong-coupling regime was considered in Ref. 14, corresponding to the half-filling of both conduction and local electrons. We emphasize here that in the strong-coupling regime, the solutions obtained at \( \mu = 0 \) do not necessary apply to the case of \( \mu \neq 0 \) because the mean-field parameters such as the boson density \( r \) and the Lagrangian multiplier \( \xi \), which must be solved self-consistently, are strongly dependent on the chemical potential \( \mu \). On the other hand, the rigid band shift of band structure, which usually applies to the weak-coupling regime, does not applies to the strong-coupling regime. Indeed, the band structures display drastic deformation at the 1/4- or 3/4-filling and no solution exists at the strong-coupling for the 1/4-filling case where the Fermi energy is precisely at the Dirac points. We here mainly focus on the semimetal phase and the related quasiparticle properties assuming the existence of the aforementioned mean-field parameters.

In the absence of spin-orbital coupling

In the absence of the SOC, we denote

\[ E^{(1)}_k(\tilde{V}) = \frac{1}{2} \left( \epsilon_d + |g_k| - \mu + \sqrt{\epsilon_d - |g_k| + \mu}^2 + 4\tilde{V}^2 \right), \]

\[ E^{(2)}_k(\tilde{V}) = \frac{1}{2} \left( \epsilon_d - |g_k| - \mu + \sqrt{\epsilon_d + |g_k| + \mu}^2 + 4\tilde{V}^2 \right), \]

\[ E^{(3)}_k(\tilde{V}) = \frac{1}{2} \left( \epsilon_d + |g_k| - \mu - \sqrt{\epsilon_d - |g_k| + \mu}^2 + 4\tilde{V}^2 \right), \]

\[ E^{(4)}_k(\tilde{V}) = \frac{1}{2} \left( \epsilon_d - |g_k| - \mu - \sqrt{\epsilon_d + |g_k| + \mu}^2 + 4\tilde{V}^2 \right). \]  

(S3)

Where, \( E^{(1)}_k \) are \( E^{(0)}_k \) for \( k \in BZ \), \( E^{(2)}_k \) are \( E^{(0)}_k \) for \( k \not\in BZ \), \( E^{(3)}_k \) are \( E^{(0)}_k \) for \( k \not\in BZ \), \( E^{(4)}_k \) are \( E^{(0)}_k \) for \( k \not\in BZ \). Then, we have the following propositions.

**Proposition I.** If \( E^{(1)}_k(0) \geq E^{(2)}_k(0) \geq E^{(3)}_k(0) \geq E^{(4)}_k(0) \) for any \( k \in BZ \), then \( E^{(1)}_k(\tilde{V}) \geq E^{(2)}_k(\tilde{V}) > E^{(3)}_k(\tilde{V}) \geq E^{(4)}_k(\tilde{V}) \) for any finite \( \tilde{V} \) and \( k \in BZ \).

**Proposition II(a).** In the weak-coupling regime and at 3/4-filling, when \( \tilde{V} \) is sufficiently small, the particle- and hole-like excitations take the form

\[ E^{(\pm)}_q = \pm \tilde{v}_F |q| + \tilde{a}q^2. \]  

(S4)
up to $\mathcal{O}(|\frac{\mathbf{q}}{\mathbf{k}_D}|^2)$, with $\bar{v}_F = [1 - \frac{\bar{V}^2}{|\epsilon_d + \mu|^2}]v_F$, $\tilde{a} = [\frac{\bar{V}^2}{|\epsilon_d + \mu|^2}] + (1 - \frac{\bar{V}^2}{|\epsilon_d + \mu|^2})\sin(3\theta_a)|v_F|$, and $\theta_a = \arctan(\frac{\mathbf{q}}{\mathbf{q}/|\mathbf{k}_D|})$.

**Proposition II(b).** In the strong-coupling regime and at $1/4$-filling, when $V^*$ is sufficiently small, the particle- and hole-like excitations take the form

$$E_{\mathbf{q}}^{(\pm)} = \pm v_F^*|\mathbf{q}| - a^*q^2,$$

(S5)

with $v_F^* = \frac{V_{sc}^2}{|E_{0} + \xi + \mu|^2}v_F$, $a^* = \frac{V_{sc}^2}{|E_{0} + \xi + \mu|^2}\pm \frac{|E_{0} + \xi + \mu|^2}{|E_{0} + \xi + \mu|^2}\sin(3\theta_a)|v_F|$.

Proof. The effective hybridization $V$ keeps the discrete symmetries such as the time reversal symmetry, the lattice inversion symmetry as well the $C_{3h}$ rotation symmetry. Therefore, the existence of the Dirac points $\mathbf{k}_D$ is robust, where

$$E_{\mathbf{k}}^{(1)} = E_{\mathbf{k}}^{(2)} = \frac{1}{2}[\epsilon_d - \mu + \sqrt{(\epsilon_d + \mu)^2 + 4V^2}],$$

$$E_{\mathbf{k}}^{(3)} = E_{\mathbf{k}}^{(4)} = \frac{1}{2}[\epsilon_d - \mu - \sqrt{(\epsilon_d + \mu)^2 + 4V^2}].$$

So at the Dirac points, the two pairs of bands $E_{\mathbf{k}}^{(1)}$ and $E_{\mathbf{k}}^{(2)}$, $E_{\mathbf{k}}^{(3)}$ and $E_{\mathbf{k}}^{(4)}$ contact to each other. But the bands $E_{\mathbf{k}}^{(1)}$ and $E_{\mathbf{k}}^{(3)}$ are separated at the Dirac points by a finite gap $\Delta = \sqrt{(\epsilon_d + \mu)^2 + 4V^2}$.

It is further observed that when tuning the chemical potential $\mu$ so that the Fermi energy is shifted to $E_{\mathbf{k}}^{(1)} = E_{\mathbf{k}}^{(2)} = 0$, one must have $\mu > \epsilon_d$. This is realized when $\mu_c = -\frac{\bar{V}^2}{\epsilon_d}$, corresponding to the case of $3/4$-filling of conduction band. Similarly, the Fermi energy can be shifted to $E_{\mathbf{k}}^{(3)} = E_{\mathbf{k}}^{(4)} = 0$ only when $\mu < \epsilon_d$ where the conduction band filling is $1/4$. This can be realized in the strong-coupling regime where $E_{0} + \xi > 0$ and $E_{0} + \xi + \mu < 0$. The chemical potential is $\mu_c = -\frac{\bar{V}^2}{E_{0} + \xi}$.

Now we consider $\mathbf{k}$ near the Dirac points so that $|g_k/A|$ is sufficiently small, where $A = \epsilon_d + \mu$ (or $A = E_{0} + \xi + \mu$ in the weak-coupling regime (or the strong-coupling regime). Up to the order of $\mathcal{O}(|g_k/A|^2)$, we have

$$E_{\mathbf{k}}^{(\lambda, \tau)} = \frac{A + \tau \sqrt{A^2 + 4V^2}}{2} - \mu$$

(S6)

$$+ \frac{\lambda}{2} (1 - \frac{\tau A}{\sqrt{A^2 + 4V^2}})g_k - \frac{\tau V^2}{(A^2 + 4V^2)^3/2}g_k^2.$$

Then we consider $\bar{V}$ near the boundary from the side of hybridization phase where $|\bar{V}/A|$ is very small. Here two situations must be distinguished. When $A > 0$, we have

$$E_{\mathbf{k}}^{(1)} = A + \frac{\bar{V}^2}{A} - \mu + \frac{V^2}{A^2}g_k + \frac{V^2}{A^3}g_k^2 + \cdots$$

$$E_{\mathbf{k}}^{(2)} = A - \frac{\bar{V}^2}{A} - \mu - \frac{V^2}{A^2}g_k + \frac{V^2}{A^3}g_k^2 + \cdots$$

$$E_{\mathbf{k}}^{(3)} = -\frac{\bar{V}^2}{A} - \mu + (1 - \frac{V^2}{A^2})g_k - \frac{V^2}{A^3}g_k^2 + \cdots$$

$$E_{\mathbf{k}}^{(4)} = -\frac{\bar{V}^2}{A} - \mu - (1 - \frac{V^2}{A^2})g_k - \frac{V^2}{A^3}g_k^2 + \cdots.$$

While when $A < 0$, we have

$$E_{\mathbf{k}}^{(1)} = \frac{\bar{V}^2}{|A|} - \mu + (1 - \frac{V^2}{A^2})g_k + \frac{V^2}{|A|^3}g_k^2 + \cdots$$

$$E_{\mathbf{k}}^{(2)} = \frac{\bar{V}^2}{|A|} - \mu - (1 - \frac{V^2}{A^2})g_k + \frac{V^2}{|A|^3}g_k^2 + \cdots$$

$$E_{\mathbf{k}}^{(3)} = -\frac{\bar{V}^2}{|A|} - \mu + \frac{V^2}{|A|^2}g_k - \frac{V^2}{|A|^3}g_k^2 + \cdots$$

$$E_{\mathbf{k}}^{(4)} = -\frac{\bar{V}^2}{|A|} - \mu - \frac{V^2}{|A|^2}g_k - \frac{V^2}{|A|^3}g_k^2 + \cdots.$$

Notice that this situation applies to both weak-coupling regime at the $3/4$-filling and strong-coupling regime at the $1/4$-filling if we only focus on the Fermi energy close to the band touching points.

By taking into account the trigonal warping effect of the spectrum near $\mathbf{k} = \mathbf{k}_D + \mathbf{q}$, with $|\mathbf{q}|/|\mathbf{k}_D| \ll 1$, we have

$$\frac{|g_k|}{t} = \frac{3a_0}{2} |\mathbf{q}| - \frac{3a_0^2}{8} \sin(3\theta_a)|\mathbf{q}|^2 + \mathcal{O}(|\mathbf{q}|/|\mathbf{k}_D|^3)$$

(S7)

with $\theta_a = \arctan(\frac{\mathbf{q}}{\mathbf{q}/|\mathbf{k}_D|})$. Then Eq.(S4) and Eq.(S5) are obtained by substituting above expression into Eq.(S6) for the weak- and strong-coupling regimes respectively.

**In the presence of spin-orbital coupling**

In the presence of the intrinsic SOC, the M-matrix appears in Eq.(2) becomes

$$M_{\mathbf{k}\sigma} = \begin{pmatrix} \sigma \Lambda_k - \mu & \epsilon_k \\ \epsilon_k & -\sigma \Lambda_k - \mu \end{pmatrix},$$

(S8)

where, $\sigma = 1$ and $-1$ refers to spin up and spin down. $\Lambda_k = 2\lambda_{so}[\sin k_1 - \sin k_2 - \sin (k_1 - k_2)] = 2\lambda_{so}f_k$, $k_1 = k \cdot \mathbf{a}_1$, $k_2 = k \cdot \mathbf{a}_2$. Because the spin-up and spin-down components are degenerate and the time reversal symmetry is preserved under $\lambda_{so}$, we only need to consider one of the component, the spin-up component. So in the following we focus on the semimetal phase in weak-coupling regime where the two relevant bands for the spin-up component are
\[ E_{k\uparrow}^{(1)} = \frac{1}{2} \left( \varepsilon_d - \mu + \sqrt{g_k^2 + 4\lambda_{so} f_k^2} \right) + \sqrt{\left( \varepsilon_d + \mu - \sqrt{g_k^2 + 4\lambda_{so} f_k^2} \right)^2 + 4\tilde{V}^2}, \]

\[ E_{k\uparrow}^{(2)} = \frac{1}{2} \left( \varepsilon_d - \mu - \sqrt{g_k^2 + 4\lambda_{so} f_k^2} \right) + \sqrt{\left( \varepsilon_d + \mu + \sqrt{g_k^2 + 4\lambda_{so} f_k^2} \right)^2 + 4\tilde{V}^2}. \]

At the Dirac points, we have \( \Delta_{12} \equiv E_{k\uparrow}^{(1)} - E_{k\uparrow}^{(2)} = 3\sqrt{3}\lambda_{so} + \frac{1}{2} \left( \left[ \varepsilon_d + \mu - 3\sqrt{3}\lambda_{so} \right]^2 + 4\tilde{V}^2 \right) - \sqrt{\left[ \varepsilon_d + \mu - 3\sqrt{3}\lambda_{so} \right]^2 + 4\tilde{V}^2} \). When \( \lambda_{so} \) is very small, \( \Delta_{12} = 3\sqrt{3}\lambda_{so}(1 - \frac{|\varepsilon_d + \mu|}{\Delta_{12}}) + O(\lambda_{so}^2). \)

Therefore, a bulk band gap opens immediately by turning on the SOC. Obviously, the similar conclusion applies to the strong-coupling regime at the 1/4-filling. Because in the absence of the SOC the semimetal phase is topological non-trivial owing the \( \pi \)-Berry phase around the Dirac points, gap opening which does not destroy the time reversal symmetry will lead to non-vanishing flow of the Berry curvature from the band \( E_{k\uparrow}^{(1)} \) to the band \( E_{k\downarrow}^{(2)} \) or vice versa, from the band \( E_{k\downarrow}^{(2)} \) to the band \( E_{k\uparrow}^{(1)} \). This will result in the edge states protected by the time reversal symmetry. The spectra obtained for a finite strip system with the zig-zag geometry in the strong-coupling regime at the 1/4-filling do exhibit the surface states as shown in Fig.(2).