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Quantum impurities develop fractional local moments in spin-orbit coupled systems

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Systems with spin-orbit coupling have the potential to realize exotic quantum states which are interesting both from fundamental and technological perspectives. We investigate the physics that arises when a correlated spin-$\frac{1}{2}$ quantum impurity hybridizes with a spin-orbit coupled Fermi system. The intriguing aspect uncovered is that, in contrast to unit local moments in conventional systems, the impurity here develops a *fractional local moment* of 2/3. The concomitant Kondo effect has a high Kondo temperature (T_K). Our theory explains these features including the origins of the fractional local moment and provides a recipe to use spin-orbit coupling (λ) to enhance the Kondo temperature ($T_K \sim \lambda^{4/3}$). Even as our finding of such rich phenomena in a simple looking many-body system is of interest in itself, we also point out opportunities for systems with tunable spin-orbit coupling (such as cold atoms) to explore this physics.

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Systems with Rashba spin-orbit coupling (RSOC) have emerged as hosts of many new developments in condensed matter physics [1]. Examples include materials with topological bands [2,3], electron gases at oxide interfaces [4,5], cold atomic gases [6], etc. The study of quantum impurities in these systems, therefore, is of importance both from basic and applied perspectives.

A correlated quantum impurity in a Fermi gas (without RSOC) can give rise to the Kondo effect—screening of the impurity magnetic moment below a characteristic Kondo temperature T_K [7]. The Kondo effect and associated T_K in spin-orbit coupled systems have had their share of attention. Malecki pointed out that the Kondo effect is not destroyed by RSOC [8], which has been confirmed in a variational calculation [9]. Žitko and Bonča [10] reported that the increase/decrease of T_K depends on microscopic parameters and attributed it to the change in density of states (DOS) engendered by RSOC. Zarea *et al.* reported an enhancement of T_K using an effective projected *s*-*d*-like model [11] (see also Refs. [12–14]). In a broader context, the effects of nonuniform (even diverging) DOS on impurity physics have been investigated in metals [15,16], semiconductors [17], and superconductors [18]. Although the above discussion may suggest that quantum impurity problems with RSOC and other systems with structured DOS have been comprehensively addressed, in this Rapid Communication we demonstrate a surprising result not found in the works cited hitherto.

We study a quantum impurity (with a repulsive correlation energy for double occupancy) that hybridizes with a Fermi gas with RSOC (strength λ). When RSOC and the correlation energy are large enough, unlike the conventional unit local moment, we find here that the impurity develops a *fractional local moment* (the fraction is 2/3). This moment couples *antiferromagnetically* with the Fermi gas, and forms a Kondo-like ground state where the gas screens the fractional moment. Remarkably, the resulting T_K (where the screening stops to be operative upon increase of temperature) is large—a significant fraction of the Fermi energy—and can be tuned with increasing RSOC ($T_K \sim \lambda^{4/3}$). We establish these results using a variety of methods from mean-field theory, variational approach, and quantum Monte Carlo numerics. That many-body effects produce an unexpected fractional moment state in such a seemingly rudimentary model is itself of fundamental interest. We not only elucidate the physics of the fractional local moment in the context of RSOC systems, but we further identify the essential ingredients (power of infrared divergence of DOS) in any system necessary to realize this physics (including the size of the fractional moment). We also discuss possible experimental systems that can realize these phenomena, e.g., cold atomic systems.

Preliminaries. We consider a gas ("conduction bath") of two-component (spin-$\frac{1}{2}$, $\sigma = \uparrow, \downarrow$) fermions in three dimensions (3D) with density $n_0 \equiv \frac{k_F^3}{3\pi^2}$, and an associated Fermi energy $E_F = \frac{k_F^2}{2}$ [19]. With a RSOC of strength λ, the spin of a fermion is locked to its momentum $\boldsymbol{k}$, resulting in "helicity" $\alpha = \pm 1$ states. In terms of fermion operators $c^\dagger_{\boldsymbol{k}\alpha}$, the conduction bath kinetic energy is

$$H_c = \sum_{\boldsymbol{k}\alpha} [\varepsilon_\alpha(\boldsymbol{k}) - \mu] c^\dagger_{\boldsymbol{k}\alpha} c_{\boldsymbol{k}\alpha}, \tag{1}$$

where [20] $\varepsilon_\alpha(\boldsymbol{k}) = \frac{k^2}{2} - \alpha\lambda|\boldsymbol{k}|$ and μ is the chemical potential. The spin is polarized along $\boldsymbol{k}$ for $\alpha = 1$ and opposite to $\boldsymbol{k}$ for $\alpha = -1$. Thus, $c^\dagger_{\boldsymbol{k}\sigma} = \sum_\alpha f^\alpha_\sigma(\boldsymbol{k}) c^\dagger_{\boldsymbol{k}\alpha}$ where coefficients $f^\alpha_\sigma(\boldsymbol{k})$ are determined by $\boldsymbol{k}$ [see Supplemental Material (SM) [21]]. We introduce a quantum impurity d, with Hamiltonian

$$H_d = \sum_\sigma (\tilde{\varepsilon}_d - \mu) n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}, \tag{2}$$

at the origin of the box of volume Ω containing the RSOC fermionic bath. Here, $n_{d\sigma} = d^\dagger_\sigma d_\sigma$, $\tilde{\varepsilon}_d$ is the "bare" impurity energy (see below), and U ($\sim$ correlation energy) is the local repulsion between two $\uparrow$-$\downarrow$ fermions at the impurity. A crucial aspect is the local hybridization of the bath fermions with the impurity state given by

$$H_h = \frac{V}{\sqrt{\Omega}} \sum_{\boldsymbol{k}\sigma} (c^\dagger_{\boldsymbol{k}\sigma} d_\sigma + d^\dagger_\sigma c_{\boldsymbol{k}\sigma}). \tag{3}$$

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The Hamiltonian $H = H_c + H_d + H_h$ describes (see SM) the Anderson impurity problem [22] in a RSOC fermionic bath. We study the ground state and finite temperature properties of this system using various techniques. Our results (3D setting) are also applicable to other spatial dimensions (particularly 2D), and also to more general anisotropic RSOC of cold atomic systems [23].

It is useful to note that the RSOC Fermi gas itself (no impurity) undergoes changes with changing λ. For the given density n_0, increasing λ causes the topology of the Fermi surface [23] to change at $\lambda_T = \frac{k_F}{\sqrt[3]{4}}$. For $\lambda > \lambda_T$, the Fermi sea is a spherical annulus solely of $+$ helicity fermions. For $\lambda \ll \lambda_T$, μ varies as $\frac{\mu(\lambda)}{E_F} = 1 - \frac{1}{\sqrt[3]{2}}(\frac{\lambda}{\lambda_T})^2$, and as $\frac{\mu(\lambda)}{E_F} = \frac{2^{8/3}}{9}(\frac{\lambda_T}{\lambda})^4$ for $\lambda \gg \lambda_T$.

Ground state [Hartree-Fock (HF) mean-field theory]. A ground state with a broken rotational symmetry is assumed, such that $M = \langle n_{d\uparrow} - n_{d\downarrow}\rangle$ is nonzero. M is self-consistently determined by minimizing the ground state energy [22].

This calculation (and all others that we present below) requires an important technical input. Unlike the usual case where the bath has a finite bandwidth, the continuum fermions considered here do not. This leads to ultraviolet divergences (due to fermions at large momenta) requiring regularization. Our approach is to make the impurity energy $\tilde{\varepsilon}_d$ a bare parameter (see SM for details), trading it for the physical value ε_d of the impurity level via the relation

$$\varepsilon_d = \tilde{\varepsilon}_d - \frac{2V^2}{\Omega}\sum_{|\boldsymbol{k}|\leqslant\Lambda}\frac{1}{|\boldsymbol{k}|^2} = \tilde{\varepsilon}_d - \frac{V^2\Lambda}{\pi^2}, \tag{4}$$

where Λ is an ultraviolet cutoff. This procedure provides a route to make all interesting observables to be independent of cutoff Λ.

Figure 1(a) shows "magnetization" M of the impurity in the U-λ plane, showing three distinct regimes. For any λ, M vanishes when $U < U_c$ [$U_c(\lambda)$ is shown by the dashed line in Fig. 1(a)]. For $U > U_c$, $M \approx 1$ when $\lambda/k_F \lesssim 1$, consistent with known results [22]. Most interestingly, for $\lambda/k_F \gtrsim 1$ and $U > U_c$, we find that $M \approx 2/3$, motivating the more detailed investigations below.

Ground state (variational). To obviate any artifacts due to the artificially broken symmetry of the HF calculation, we now construct a variational ground state (see Ref. [24]) with a "rigid" Fermi sea of bath fermions and two added particles whose spin states are unbiased (see SM). We find that the ground state for all λ and U is rotationally invariant with a zero total (spin+orbital) angular momentum ($J = 0$, singlet). The size of the impurity local moment, characterized by $S_z^2 \equiv \langle(n_{d\uparrow} - n_{d\downarrow})^2\rangle$, depends on λ and U. As seen from Fig. 1(b), there are four distinct ground states. (i) For $\lambda \lesssim k_F$ and $U < U_c$ [U_c depends on λ, and is shown by a dashed line in Fig. 1(b)], S_z^2 vanishes and the impurity is doubly occupied. (ii) For $\lambda \lesssim k_F$ and $U > U_c$, $S_z^2 \simeq 1$, corresponding to the Kondo state where the impurity has a well-formed local moment that locks into a singlet with the bath fermions. Interestingly, in this regime of λ, U_c falls with increasing λ, i.e., small λ aids the formation of the Kondo state (see also Ref. [11]). The other two states occur for $\lambda \gtrsim k_F$, where U_c increases with increasing λ. (iii) For $U > U_c$, we find a strongly correlated state (vanishing double occupancy) with a *fractional* local moment of $S_z^2 = 2/3$. (iv) For $U < U_c$, an intriguing state is seen with an impurity occupancy of 4/3, moment 4/9, and double occupancy $\langle n_{d\uparrow}n_{d\downarrow}\rangle = 4/9$. The crossovers between these states are clearly demonstrated in Fig. 1(c), which shows various quantities evolving with λ for $U = 0.4E_F$, and in Fig. 1(d) for $U = E_F$. Indeed, the HF results discussed before are consistent with those of the variational calculations (VCs). We note that the first excited state of the VC is a triplet state ($J = 1$). The energy of this excited state compared to the singlet ground state gives an estimate of the Kondo scale T_K, which is discussed in detail below.

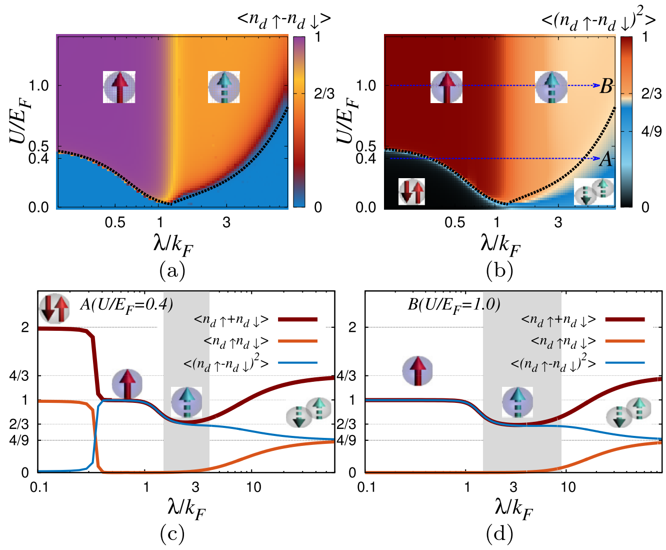

FIG. 1. Ground state in U-λ plane: Results for $V/E_F^{1/4} = 0.1$, $\varepsilon_d = \mu(\lambda)/2$. (a) Impurity moment $M = \langle n_{d\uparrow} - n_{d\downarrow}\rangle$ in the Hartree-Fock (HF) ground state. (b) Size of impurity moment $S_z^2 = \langle(n_{d\uparrow} - n_{d\downarrow})^2\rangle$ in the variational ground state. (c) and (d) Results along slices $A(U/E_F = 0.4)$ and $B(U/E_F = 1.0)$ shown in (b). Both HF and variational ground states show a *fractional* local moment (shown schematically by the broken vector) of 2/3 for $\lambda/k_F \gtrsim 1$, and U/E_F larger than a λ-dependent critical value shown by the dashed line in (a) and (b).

Finite temperature (quantum Monte Carlo). Several natural questions arise, including how the fractional local moment reveals itself at finite temperatures. We address this using the quantum Monte Carlo (QMC) method of Hirsch and Fye [25] (see SM for details) which, in addition, also provides an unbiased corroboration of the results of the previous sections. Figures 2(a)–2(c) show the temperature-dependent results (including the impurity magnetic susceptibility χ) obtained from QMC for a λ and U that possesses a fractional local moment in the ground state. Three temperature regimes are clearly seen. At high temperature $T \gg U$, we have the free orbital regime [26,27] where $T\chi(T) \approx \frac{1}{2}$ [Fig. 2(b)], followed by a regime where $T\chi(T) \approx \frac{2}{3}$ at lower temperatures. At even lower temperatures (temperature scale T_K) there is a crossover to the Kondo state. The interesting aspects of these results is that the impurity local moment S_z^2 attains a value of 2/3 in the same temperature regime where $T\chi(T) \sim \frac{2}{3}$ and remains so at low temperatures, even below the Kondo temperature

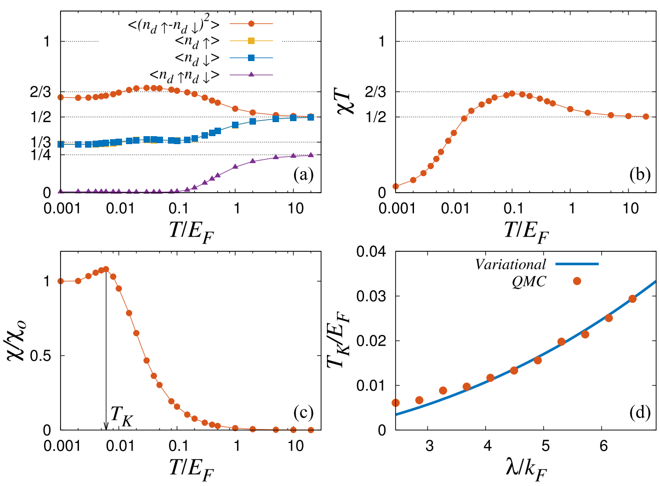

FIG. 2. Finite T physics: QMC results for $U/E_F = 0.5, \lambda/k_F = \frac{5}{\sqrt{6}}$, and $V/E_F^{1/4} = 0.1$. (a) Impurity observables, and (b) and (c) impurity magnetic susceptibility χ as a function of temperature T. χ_0 in (c) is the low temperature susceptibility. The Kondo temperature T_K is estimated from QMC results by the location of the peak in χ as shown in (c). (d) Dependence of T_K on λ ($U/E_F = 1.0$). Results (a)–(c) are obtained using $L = 512$ imaginary time slices, while $L = 128$ is used to obtain the T_K for various values of λ in (d). Sampling error bars are smaller than the symbol sizes.

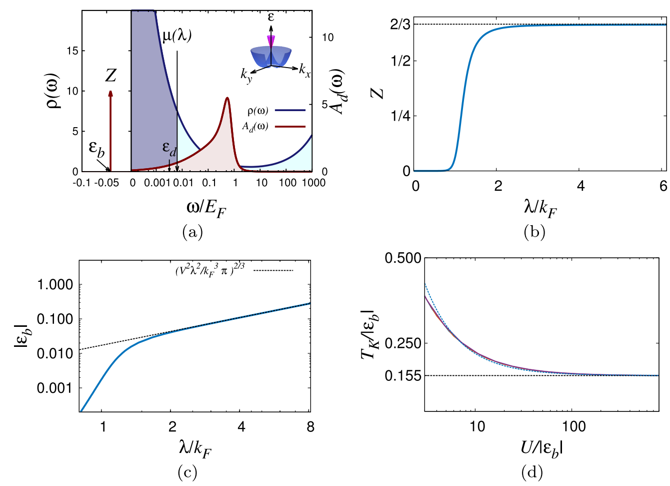

FIG. 3. Fractional local moment and high T_K: (a) Density of states of the bath $\rho(\omega)$ with filled states up to $\mu(\lambda)$. The spectral function $A_d(\omega)$ of the d state at ε_d after hybridization with the bath is also shown. (b) Weight (Z) of the impurity d state in the bound state, and (c) energy of the bound state ε_b, as function of λ. (d) "Universal" Kondo T_K scale as a function of U estimated from the variational calculation where $\frac{T_K}{|\varepsilon_b|} \approx 0.155 + \frac{|\varepsilon_b|}{U}$.

T_K. This clearly indicates the formation of a fractional local moment of 2/3 at the impurity, and screening of the same by the bath fermions at lower temperatures, confirming our ground state results. QMC also allows us to extract T_K as shown in Fig. 2(c), and its dependence on λ is shown in Fig. 2(d). The remarkable aspect is the large Kondo temperature scale that is a significant fraction of E_F, which interestingly increases with increasing λ in the fractional local moment regime [28]. Reassuringly, the energy scale obtained from VC also agrees with the QMC result (up to a factor of $\frac{1}{2}$, $T_K^{\rm QMC} \approx \frac{1}{2} T_K^{\rm VC}$), as shown in Fig. 2(d).

Discussion. What is the physics behind these results? In the absence of RSOC ($\lambda = 0$), the sole one-particle effect of hybridization on the impurity is to broaden its spectral function $A_d(\omega)$ from a Dirac delta at ε_d to a Lorentzian of width $\Delta \sim V^2\rho(\mu)$, where $\rho(\omega)$ ($\sim \sqrt{\omega}$ for $\lambda = 0$) is the DOS of the bath. Matters take a different turn when $\lambda \neq 0$ due to the infrared divergence of the DOS of the bath [$\rho(\omega) \sim \frac{\lambda^2}{\sqrt{\omega}}$ at near $\omega = 0$; see Fig. 3(a)]. A bound state appears for *any* V for $\lambda \neq 0$, i.e., the states $\{c^\dagger_{\boldsymbol{k}\alpha}, d^\dagger_\sigma\}$ reorganize themselves into a set of scattering states created by $a^\dagger_{km}$ and a one-particle *bound state* $b^\dagger_m$ (quantum numbers: $k = |\boldsymbol{k}|$, and $m = \pm\frac{1}{2}$ is the z projection of the total angular momentum $J = 1/2$.). In particular,

$$b^\dagger_{\frac{1}{2}} = \sqrt{Z} d^\dagger_\uparrow + \sum_{\boldsymbol{k}\alpha} B_{\boldsymbol{k}\alpha} c^\dagger_{\boldsymbol{k}\alpha}, \tag{5}$$

where Z is the weight of the d-impurity state in the bound state b, and B's are coefficients of the bath states. Now, Z depends on λ in a most interesting way. For a given ε_d and V, Z is vanishingly small for λ smaller than a critical value [see Fig. 3(b)]. For larger λ, Z attains a constant value (of $\frac{2}{3}$ for the 3D RSOC) *independent* of λ. The energy of the bound state ε_b also has interesting characteristics as shown in Fig. 3(c). For small λ, the binding energy is small and ε_d dependent, while for large λ, $\frac{\varepsilon_b}{E_F} \approx -(\frac{V^2\lambda^2}{k_F^3\pi})^{2/3}$ and becomes independent of ε_d.

The one-particle physics just discussed provides crucial clues to the physics even when U is nonzero. Clearly, the natural basis for analysis is provided by the b-bound state and the a-scattering states. For small λ, the bound state has very little d character and the physics is quite similar to the system without RSOC. The fall in U_c seen in Figs. 1(a) and 1(b) owes to the falling chemical potential of the gas for our choice of $\varepsilon_d = \mu(\lambda)/2$. At larger λ, the bound state b is deep. Since the b state has only a fraction $\sqrt{Z}$ of d state, even a large U on the d state does *not* entirely forbid double occupancy of the b state. Physically, the part of the b state with d character will "feel" a correlation energy Z^2U, while the other part remains uncorrelated. At large U, the "d part" of b will thus be singly occupied, forming a fractional local moment. This argument provides an expression for the critical U_c required to form a fractional local moment, as $U_c \sim \frac{1}{Z}|\varepsilon_b|$ and indeed matches (up to a multiplicative factor of ≈ 2) the result at large λ shown in Figs. 1(a) and 1(b). In fact, these observations also explain the regime of $U < U_c$ at large λ. Here, the b state is doubly occupied, and this corresponds to a d occupancy of $2Z$, and $\langle n_{d\uparrow}n_{d\downarrow}\rangle = Z^2$ and $S_z^2 = 2Z(1-Z)$, all in agreement with results of Fig. 1.

Turning again to $U > U_c$, the origin of the high T_K of the Kondo state formed by the fractional local moment can be understood from the variational calculation. As noted, the first excited state in VC is a triplet state made of a *singly occupied* b state and a scattering state at the chemical potential. This state is clearly a scale ε_b above the ground state. Thus in the large U limit we expect the Kondo scale T_K to be proportional to ε_b, as indeed found by explicit calculation [see Fig. 3(d)].

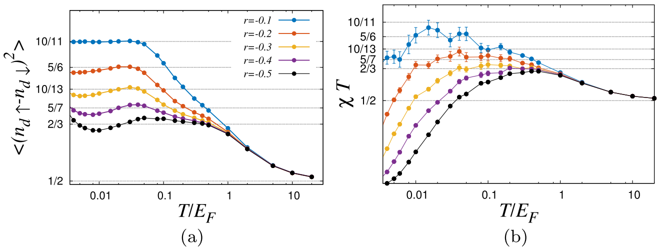

FIG. 4. Generic fractional local moments: QMC results for an impurity hybridizing with a conduction bath with $\rho(\omega) = \frac{1}{\pi^2}(\sqrt{2\omega} + \frac{\lambda}{\sqrt{2}}\frac{\omega^r}{\lambda^{2r}})$ $[V/E_F^{1/4} = 0.1, \lambda/k_F = \frac{1}{\sqrt{2}}(\frac{10}{\sqrt{3}})^{\frac{2}{1-2r}}, U/E_F = 2, \varepsilon_d = \mu_r(\lambda)/2, L = 128]$ for different values of r. (a) Impurity observables and (b) susceptibility χ as a function of temperature. The values of $\varepsilon_b/E_F \approx -0.1$ for all cases.

This provides a route to obtain large Kondo temperatures as $T_K \sim \lambda^{4/3}$. Also note that the physics of the fractional local moment formation in this system is very different from that noted in Ref. [29] which occurs in a *s*-*d* system that has a *ferromagnetic* coupling to the bath.

Finally, why is Z numerically equal to $\frac{2}{3}$? What controls this? Can it be tuned? We show that Z is *entirely determined by the exponent that characterizes the infrared divergence of the density of states*, independent of details such as spatial dimensions. For a system with

$$\rho(\omega) = \frac{1}{\pi^2}\left(\sqrt{2\omega} + \frac{\lambda}{\sqrt{2}}\frac{\omega^r}{\lambda^{2r}}\right), \tag{6}$$

we show (see SM) that $Z(r) = \frac{1}{1-r}$. We have performed QMC calculations with the impurity hybridizing to a bath with the given DOS in Eq. (6), and indeed find the anticipated fractional local moments [see Fig. 4(a)]. We further see [Fig. 4(b)] that there are two distinct intermediate temperature regimes, $T_K \lesssim T \lesssim |\varepsilon_b|$, which is the "fractional local moment regime" with $T\chi \approx Z(r)$, and the asymmetric local moment regime between $|\varepsilon_b| \lesssim T \lesssim U$, where $T\chi \approx \frac{2}{3}$. Interestingly, for the 3D RSOC, the susceptibility alone cannot discern these two.

This system can be realized in a cold atom setting by combining approaches described in Ref. [30] for the 3D RSOC, and [31] for the impurity (see also Refs. [32–34]). Signatures of the fractional local moment formation can be probed using radio-frequency (rf) spectroscopy [35] on the impurity. A finite concentration of well-separated quantum impurities would show a well-separated peak in the rf spectrum of $\uparrow$ spin, proportional to the concentration and the weight Z. The bath states make up a fraction of $(1 - Z) \sim \frac{1}{3}$ of the bound state, with an equal quantum mechanical admixture of $\uparrow$ and $\downarrow$ states of the bath. If the rf spectrum of the bath atoms is probed, this will again result in a well-separated peak (at the bound state energy) $\propto (1 - Z)$. A combination of these two measurements can provide evidence for the physics discussed here.

Analogous physics applies to the 2D system with RSOC which has a similar infrared divergence of $\rho(\omega)$ $(\sim \frac{1}{\sqrt{\omega}})$. Such 2D systems with strong spin-orbit coupling have been realized in interfaces [4,36] and surfaces [37] where the RSOC scale is comparable to the Fermi energy. It will be interesting to explore ways to realize the physics of the fractional local moments in these systems as well.

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