Fragility of the Kondo insulating gap against disorder: a resolution to recent puzzles in topological Kondo insulators

Sudeshna Sen, N. S. Vidhyadhiraja, Eduardo Miranda, Vladimir Dobrosavljević, and Wei Ku

1 Tsung-Dao Lee Institute, School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China
2 Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore-560064, India
3 Instituto de Física, Universidade Federal de Goiás, 74.001-970, Goiânia-GO, Brazil
4 Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA
5 Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), Shanghai 200240, China

Abstract

Kondo insulators are strong correlated system in which a clean insulating gap emerges only at very low temperature due to many-body effects involving localized f-electrons. However, certain Kondo insulators, like SmB₆ and CePt₃Bi₄, display metallic behaviors at extremely low temperature, that have defied current understanding. Recent advances in topological effects in materials has raised the attention on the protected surface states in these “topological Kondo insulators” as a potential resolution to some of the puzzling behaviors. Here we resolve these puzzles via a different route, by showing that the emergent Kondo insulating scale is extremely vulnerable against moderate degree of disorder, such that the gap is filled with small number of states. Therefore, the real samples are probably never truly insulating and this in turn compromises the essential building block of topological considerations. Our results suggests strongly that systems like the Slater insulators would be a more promising direction to extend the realm of topology to strongly correlated systems.
In recent years, topological Kondo insulators have emerged as a new class of materials where both the physics of strong electron correlations and/or topology could play a significant role. Interestingly, in great contrast to typical topological insulators, these systems exhibit seemingly contradictory behaviors, for example, a low-temperature metallic specific heat and an insulating-like activated transport at high temperatures. Even more puzzling is the observation of a saturated low-temperature resistivity. Naturally this can be interpreted from the conducting topological surface states. However, very recent observations strongly suggest bulk conduction instead, and advocate the essential role of disorder.

Thereby, several experimental observations in some of these systems have called for unconventional theoretical interpretations. Not only are the low temperature thermodynamic properties of this bulk insulator at odds with conventional knowledge, this material was recently found to exhibit 3D quantum oscillations typically associated with metals. To date, while several propositions have been attempted to understand such puzzling observations, including charge neutral quasi-particles and conducting surface states, no overall consistent picture has been obtained.

One long-standing key issue is the role of disorder. Even before realizing the connection with topological characteristics, disorder had already been speculated to be responsible for the saturation of low-temperature resistivity. More recent studies further found significant sample variation in the low-temperature properties of these systems, depending on the synthesis methods and seed materials used. Careful characterization of such samples indeed indicates that even in the nominally purest samples, minimal yet detectable amount (< 1%) of disorder is present, the amount of which appears to be correlated with their saturated value of resistivity and specific heat.

But, how can such a small amount of disorder overcome the insulating gap of 0.01eV scale, and are they necessarily itinerant? It is exactly this question that we address in this work and provide a microscopic physical mechanism explaining this issue.

1. RESULTS

Figure 1 gives an example of typical effect of minute amount of disorder on band insulators, containing a bulk insulating gap of full width $\Delta_g \approx 0.01$eV. In all our subsequent
FIG. 1. **Effect of disorder in a non-interacting band insulator:** The ground state density of states (DOS) of a non-interacting band insulator, is plotted as a function of energy, for different values of standard Anderson-type disorder in site-energies. $W$ is a measure of the fluctuation of site energy with values $W = 0, 0.05, 0.2$ eV. Clearly, disorder has negligible effect on the hybridization gap straddling around the chemical potential located at zero energy.

discussions based on the electronic density of states, we choose the $d$-electrons, as they are the ones involved in the transport. We simulate the disorder effects via a standard Anderson-type fluctuation of site energy represented by $W$. In Figure 1 we demonstrate the $d$-electron density of states for such site energy fluctuations up to $W = 0.2$ eV. Expectedly, one finds only negligible effects near the gap edge in the resulting density of states. That is, the gap is extremely robust against such weak disorder. This means that even an underestimated resistivity (by assuming all the states are itinerant), one would still obtain a large insulating-like resistivity at low temperature, without saturation. Thus, the puzzle remains. It turns out that the resolution of the above issues lies in a novel characteristic of Kondo insulators in general (topological or not), in contrast to typical band insulators, namely a extreme sensitivity of local gap features against disorder. To illustrate this generic characteristic of all Kondo insulators, we use a minimal model known as the periodic Anderson model (PAM), consisting of itinerant non-interacting $d$ orbitals with on-site energy $\epsilon_{d}$ and highly localised interacting $f$ orbitals with on-site Coulomb repulsion $U$ and on-site energy $\epsilon_{f}$. Additionally, the $d$ and $f$ orbitals hybridize via a local coupling $V$, such that, the Hamiltonian is given in
standard notation by, $H = H_d + H_f + H_{hyb}$, where

$$H_d = -t \sum_{\langle ij \rangle \sigma}^{} \left[ d^\dagger_{i \sigma} d_{j \sigma} + H.c. \right] + \sum_{j \sigma}^{} (\epsilon_{dj} - \mu) d^\dagger_{j \sigma} d_{j \sigma}, \quad (1)$$

$$H_f = + \sum_{j \sigma} \epsilon_f f^\dagger_{j \sigma} f_{j \sigma} + U \sum_{j}^{} n_{fj \uparrow} n_{fj \downarrow}, \quad (2)$$

$$H_{hyb} = V \sum_{j \sigma}^{} \left[ d^\dagger_{j \sigma} f_{j \sigma} + H.c. \right]. \quad (3)$$

This model is known to capture the non-trivial local physics of Kondo screening at very low temperature in the regime when $Ut \gg V^2$, where the very low-energy physics is controlled by the emergence of bound singlet states. These entangled spin-singlet states, also known as the Kondo singlets, are composed of anti-ferromagnetically coupled $d$ and $f$ electrons via an spin exchange coupling $J \sim V^2/U$ and a binding energy, so-called Kondo scale $\omega_K$. The most dramatic characteristic of the Kondo screening is the exponential (many orders of magnitude) suppression of its energy scale from that of the Hamiltonian ($t$, $V$, and $U$), $\omega_K \propto e^{-1/(\rho_0 J)}$, where $\rho_0$ represents the “bare” density of states of the $d$ electrons at the chemical potential. Consequently, near half-filling (number of $d$ electrons $n_d$ and $f$ electron $n_f$ sums to 2 per atom), the coherent charge gap opening related to the periodic occurrence of the Kondo singlets in a lattice is also very small, of the order of the Kondo scale, $\Delta_g \sim \omega_K$. A Kondo insulator is thus formed at exactly half-filling, when the chemical potential falls inside the charge gap.

Now we will show that unlike the typical charge gap in band insulators, such a dramatically suppressed emerged gap (and the local Kondo scale) is extremely sensitive to disorder. This fragility of the Kondo insulating gap against disorder provides a natural explanation of the above puzzles. We simulate the weak disorder in real materials by adding to this model Anderson-type disorder in the $d$-electron site energies, with fluctuations $\sim 0.2eV$, similar to that used for the non-interacting case demonstrated in Fig. [1]. For the current calculations, we choose the parameters such that this gap is around $0.01eV$ in the clean case, similar to the real Kondo insulator materials. Furthermore, the band-filling constraint now translates as, $\langle n_f \rangle + \langle n_d \rangle = 2$, where $\langle ... \rangle$ denotes disorder averaged values. We respect this constraint by fixing $n_f = 1$ uniformly on all sites, while varying $n_d$ locally via a spatially variable ($\epsilon_{di}$, drawn from a distribution $P(\epsilon_{di}) = \frac{1}{\sqrt{2\pi W^2}} \exp\{-\frac{1}{2}(\epsilon_{di}/W)^2\}$, such that $\langle n_d \rangle = 1$ on average.
FIG. 2. Effect of disorder on the Kondo insulator density of states: The zero temperature density of states (DOS) of the $d$ electrons of a Kondo insulator is plotted as a function of energy, for different values of $d$ site energy fluctuation. The magnitude of fluctuation is represented by $W$. In contrast to the $U = 0$ case (Fig. 1), the Kondo insulating gap of a clean Kondo insulator ($W = 0$) starts filling up at minimal disorder strengths ($W = 0.1$) rapidly evolving into a pseudogap ($W = 0.2, 0.25$) eV, with a non-zero density of states at the chemical potential. The parameters used for this figure are $U = 1.9$, $V = 0.44$ eV to generate a clean Kondo insulating gap of full width $\Delta_g \approx 0.01$ eV.

Thus, within this model, $W$ would signify the local fluctuations in the $d$-levels additionally implying fluctuations in the local density of states (LDOS) of the conduction electrons.

Instead of delving into the detailed low energy dynamics that would dictate this physical situation, a straight look at the resulting density of states illustrated in Figure 2 immediately reveals the ‘fragility’ of the Kondo gap in great contrast to its non-interacting counterpart (Figure 1). With the incorporation of disorder, the prominent charge gap rapidly fills out representing a ‘soft’ gap at $W = 0.1$ eV and evolving into a ‘pseudogap’ with finite spectral weight at the chemical potential, with a meagre increase of $W$ to $0.2$ eV.

The occurrence of such ‘pseudogap’ feature in the ground-state, bulk spectral function would not only induce a plateau in low $T$, D.C. resistivity ($\rho(T)$) of such a system, but also result in a high temperature insulator like activated transport as we now demonstrate. In main panel of Fig. 3 we plot $\rho(T)$ on a linear-log scale for $W = 0.25$. The saturation knee occurs at a $T \sim 2$ K in close agreement to experimental reports on SmB$_6$. In the inset we plot $\rho(T)$ on a linear scale to highlight the activated transport regime at higher $T$'s, characteristic of insulators. Our model of a disordered Kondo insulator produces an activated transport for $T \gtrsim 20$ K with a transport gap, $\Delta \sim 0.003$ eV which is of the same order as that reported in experiments on SmB$_6$. In the following discussion we show how
FIG. 3. D.C. resistivity and electronic specific heat: (a) (Main) The temperature \(T\) dependent D.C. resistivity \(\rho(T)\) is plotted, for \(W = 0.25\) eV, with \(T\) being plotted on a log scale. In agreement with experimental observations, a resistivity plateau sets in for temperatures, \(T \lesssim 2\) K, crossing over to a regime of activated transport characteristic of Kondo insulators. (a) (Inset) In the inset we plot \(\rho(T)\) on a linear scale to highlight the activated transport for \(T \gtrsim 20\) K with a transport gap, \(\Delta \sim 0.003\) eV. (b) (Main) The specific heat \(C\) in units of the universal gas constant \(R\), is plotted as a function of temperature \(T\), for a fixed disorder strength, \(W = 0.25\) eV. Clearly, the low \(T\) specific heat has an appreciable linear component as also observed in experiments. We observe two regimes with a dominant linear coefficient \(\gamma = 0.1, 0.05\) K\(^{-1}\), respectively, the change of slope being accompanied by a knee at \(\sim 2\) K. The lowest temperature reported in the available experimental data for the specific heat of SmB\(_6\) is \(\sim 2\) K. As demonstrated in the figure, our model predicts a \(\gamma \approx 0.05R \sim 100\) mJ K\(^{-2}\) mol\(^{-1}\) in the regime \(2 \sim 8\) K. (b) (Inset) The linear coefficient, \(\gamma\), is plotted as a function of \(T\) on a linear-log scale. While the specific heat is purely linear as also seen in the experiments, it certainly comprises of a dominant linear term.

Our model for disordered Kondo insulators not only gives rise to such (weakly) metallic behavior, with finite conductivity at \(T = 0\), but also a modified thermodynamic response, in consistence with the ‘puzzling’ experimental observations in several Kondo insulators.

Among the several puzzling observations in KI’s SmB\(_6\) and Ce\(_3\)Pt\(_3\)Bi\(_4\), is the large low \(T\) specific heat contribution with a dominant \(T\)-linear contribution, shown to be predominantly a bulk property. We thus turn our focus on to the thermodynamic response due to the electronic specific heat, \(C(T)\), and demonstrate how our microscopic model reproduces such an experimental observation. Figure 3(b) shows the computed specific heat \(C(T)\) in units of the universal gas constant, \(R \approx 8.3\) J K\(^{-1}\) mol\(^{-1}\), for a fixed parameters of the model used. The specific heat clearly depicts a low \(T\) linear behavior, behaving as \(C(T) = \gamma RT\).
exhibiting an enhancement in $\gamma$ for $T \lesssim 2K$. It should be noted that the most recent $C(T)$ measurements exhibit a significant sample dependence with $\gamma \sim 10 - 50\ \text{mJ K}^{-2}\text{mol}^{-1}$. As shown, our calculations successfully bring out the general trends observed in the experiments concerning candidate TKI’s, namely SmB$_6$ and Ce$_3$Pt$_3$Bi$_4$, in regards to the bulk thermodynamic response. The thermodynamic response is also in consistence with the observed transport in these systems. Nevertheless, the $\gamma$ value predicted by our calculations is $\sim 100\ \text{mJ K}^{-2}\text{mol}^{-1}$ (for $2\ K < T < 10\ K$) is slightly overestimated than experimental reports.

![Distribution of Kondo scales](image)

**FIG. 4.** Distribution($P$) of Kondo scales($\omega_K$): $P(\omega_K)$ The distribution of local Kondo scales ($P(\omega_K)$) computed for different strengths of fluctuation in the Anderson-type quenched disorder, viz, $W = 0.2, 0.25, 0.3\text{eV}$. The solid lines are a guide to the eye. The bare Hamiltonian parameters used are $U = 1.9, V = 0.44\text{eV}$.

The microscopic mechanism behind the fragile nature of a Kondo insulator against disorder (and the related pseudogap formation) can be understood as the following. The randomness introduced by site energy fluctuations induce a spatially non-uniform screening of the localised $f$-electrons. More precisely, the strength of this local screening depends on the local hybridization function or quantum-mechanical coupling ($\Delta(\epsilon_d)$) between the $f$-electrons and the $d$-electrons. The local Kondo scale ($\omega_K$) quantifying this process of Kondo screening is thereby given by $\omega_K \propto \exp(-1/\Delta(\epsilon_d))$. The $f$-electrons thus become extremely sensitive to this microscopic fluctuation in the $d$-electron local density of states induced by the local disorder. Consequently, a broad distribution of ‘exponentially’ small local Kondo scales emerge as illustrated in Figure 4 where we demonstrate $P(\omega_K)$ for three such closely spaced disorder values, namely, $W = 0.2, 0.25, 0.3\text{eV}$. As shown in Figure 4 these emerged scales (spanning from $10^{-4}$ to $10^{-2}\text{eV}$) are orders of magnitude smaller than the clean lattice coherence scale.
Such a broad distribution of Kondo scales provides a broad avenue of extremely low energy scales over which the underlying Kondo insulator density of states is dramatically influenced. The Kondo gap that would straddle the Fermi level in the clean Kondo insulator would now move above or below the Fermi level depending on the \( \{\epsilon_{d_i}\} \), and the amount of spectral weight acquired around the Fermi level, would depend on the underlying local Kondo scale which could be exponentially small as seen from Figure 4. In fact, the local depletion or accumulation of local \( d \)-orbital charge, \( n_d \), may also reflect as many body quasi-particle or low energy resonances in the \( f \) and \( c \) spectral functions, in the vicinity of the Fermi level (for details see Figure (1) of the supplementary information), on energy scales of the order of the underlying Kondo scale. Thus in great contrast to a non-interacting band insulator the Kondo insulating charge gap is extremely fragile in the presence of such quenched disorder, producing dramatically large effects on the low energy density of states with nominal site energy fluctuations.

2. DISCUSSION

The above fragility of Kondo insulators originates from the sensitivity of local Kondo physics against disorder, and should apply to all Kondo insulators. Specifically for topological Kondo insulators, while the global topological features should remain robust against disorder, the destruction of the local gap scale, however, would ruin the compact manifold on which a topology can be defined. This generic consideration suggests that other strongly interacting systems like the good Slater insulators, in which the non-local interaction induced insulating gap scale is comparable to that of the Hamiltonian without significant suppression, would be much more robust playgrounds for exploring the interplay between many-body correlation and topology. In summary, we demonstrate the extreme fragility of Kondo insulating gap against even modest amount of disorder, in great contrast to typical band insulators. Consequently, Kondo insulators generically develop a pseudo-gap that naturally accounts for the seemingly contradictory observations (metallic vs. insulating characteristics) in several topological Kondo insulators. In essence, the emergent local Kondo scale fluctuates dramatically, in ducing modifications in the low-energy many-body electronic structure. The original clean gap is thereby filled with finite density of states. This dominant local physics compromises the building block (a truly insulating bulk) of topologi-
cal Kondo insulators, and suggests strongly that systems like the Slater insulators would be a more promising direction to extend the realm of topology to strongly correlated systems.

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SUPPLEMENTARY INFORMATION FOR FRAGILITY OF THE KONDO INSULATING GAP AGAINST DISORDER: A RESOLUTION TO RECENT PUZZLES IN TOPOLOGICAL KONDO INSULATORS

1. HAMILTONIAN:

The periodic Anderson model, that we describe below, is considered to be minimal model for describing heavy fermion systems. The Hamiltonian for the periodic Anderson model is given by,

\[
H = H_d + H_f + H_{hybridization},
\]

\[
H_d = -t \sum_{\langle ij \rangle \sigma} [d_{i\sigma}^\dagger d_{j\sigma} + H.c.] + \sum_{j\sigma} (\epsilon_{d_j} - \mu)d_{j\sigma}^\dagger d_{j\sigma},
\]

\[
H_f = +\sum_{j\sigma} \epsilon_{f_j} f_{j\sigma}^\dagger f_{j\sigma} + U \sum_j n_{f_j\uparrow} n_{f_j\downarrow},
\]

\[
H_{hybridization} = V \sum_{j\sigma} [d_{j\sigma}^\dagger f_{j\sigma} + H.c.].
\]

These are modeled by two sets of bands, which in the case of SmB\textsubscript{6} would correspond to the highly localised Sm-4f orbital with strong electron-electron repulsive interactions, \(U\), and the extended, Sm-5d. The \(f - d\) orbitals hybridize via a local matrix, \(V\). While the presence of \(U\) in the \(f\)-orbital leads to Kondo scattering in the system, \(V\) is responsible for the formation of a hybridization gap, \(\Delta_g\). In Equation (7) \(c\) represents the conduction band orbital and \(d_{i\sigma}^\dagger (d_{i\sigma})\) represents creation (annihilation) of an electron with spin \(\sigma\) in the \(d\)-orbital at site \(i\) with \(t\) being the kinetic energy of the electrons residing in the conduction band and \(\mu\) being the chemical potential; \(n_{f_j\uparrow (\downarrow)}\) represents the local occupancy in the \(f\)-orbital. Note that this gap, \(\Delta_g\), would be present at the Fermi level in a 1/2-filled lattice of the above model. The 1/2-filling condition in a clean Kondo insulator is respected when the \(f\)-orbital occupancy, \(n_f\) and the \(d\)-orbital occupancy, \(n_d\) together sum to, \(n_f + n_d = 2\). In a disordered system, these occupancies are replaced by their disorder averaged values, such that for a disordered Kondo insulator, the former relation should read as, \(\langle n_f \rangle + \langle n_d \rangle = 1\), where \(\langle ... \rangle\) denotes disorder averaged values. \(\Delta_g\) would be present even in the non-interacting, half-filled lattice, representing a band insulator. Thus the \(U = 0\) limit of Equation (7) represents the model used in Fig. 1 of the main text. Disorder is introduced as as standard Anderson-type
fluctuations in on-site energies $\epsilon_{di}$ of the $d$-electrons and is mathematically introduced from a gaussian distribution given by,

$$P(\epsilon_{di}) = \frac{1}{\sqrt{2\pi W^2}} \exp\left(-\frac{1}{2} \frac{\epsilon_{di}^2}{W^2}\right),$$  

such that on an average the on-site energy, $\langle \epsilon_{di} - \mu \rangle = 0$, to respect the half-filling condition. In the calculations presented here, we respect the $1/2$-filling constraint by fixing $n_f = 0.5$ uniformly on all sites, while $n_d$ varies locally depending on the $\epsilon_{di} - \mu$ of the disorder realization, with $\langle n_d \rangle = 0.5$ for the disorder averaged system, guaranteed by setting $\langle \epsilon_d - \mu \rangle = 0$.

2. **CALCULATION OF THE SPECTRAL FUNCTION**

In the main text we reported the analysis of the electronic structure, d.c. resistivity and the specific heat of disordered Kondo insulators. In this section we describe the theoretical framework that we use to compute the electronic spectral functions. We utilize the dynamical mean field theory (DMFT) framework\textsuperscript{30} for tackling the many-body effects due to the strongly correlated $f$-electrons present in these systems and the coherent potential approximation (CPA) to understand the effects due to disorder. For a clean system, the DMFT framework maps a strongly correlated lattice to an auxiliary strongly interacting impurity problem, that in this particular case, is a single impurity Anderson model (SIAM). In the SIAM we have an strongly interacting impurity, with local repulsive interactions embedded in a non-interacting host, that is determined self-consistently within a computational framework. In the presence of disorder this scheme maps the disordered lattice on to an ensemble of impurity problems each of which is embedded in a disorder averaged effective medium. In the following we outline the self-consistency equations that constitute the above scheme.

The physical quantity that describes the single particle excitations in a many body system is the Green function or the ‘propagator’. For a clean Kondo insulator or heavy fermion metallic system within the framework of DMFT, the $d(f)$- electron Green’s func-
The quasiparticle spectra (or density of states) for a respective Kondo insulator described by Equation (7) could thus be derived to be,

\[ D^d(\omega) \sim \rho_0 \left( \omega - \epsilon_c - \frac{ZV^2}{\omega - Z\epsilon_f^*} \right), \]  

\[ D^f(\omega) \sim \frac{Z^2V^2}{\omega - Z\epsilon_f^*} \rho_0 \left( \omega - \epsilon_d - \frac{ZV^2}{\omega - Z\epsilon_f^*} \right), \]

where, \( \epsilon_f^* \) is a renormalization incurred by the bare \( f \)-level due to the underlying many-body dynamics. The low energy behavior embodied in Equations (11) and (12) would be extremely important in understanding why the Kondo gap is so fragile against minute amount of disorder.

Subsequently for a clean Kondo insulator, \( G^d(\omega) = \left( \frac{\omega^+ - \frac{V^2}{\omega^+ - \Sigma_f(\omega)} - \Delta(\omega)}{\omega^+ - \Sigma_f(\omega) - E_f} \right)^{-1} \) and \( G^f(\omega) = \left( \frac{\omega^+ - \Sigma_f(\omega) - \frac{V^2}{\omega^+ - \Delta(\omega)}}{\omega^+ - \Delta(\omega)} \right)^{-1} \). \( \Sigma_f(\omega) \) is the conventional Hartree corrected conventional self-energy of the correlated \( f \) electrons, \( \Sigma_f \) being purely local or momentum independent within DMFT. The \( d \)-electrons being itinerant hybridize with the non-interacting (DMFT) host via the true hybridization function, \( \Delta(\omega) \), while the quantity, \( \frac{V^2}{\omega^+ - \Delta(\omega)} = \Delta_f(\omega) \), may be thought of as an effective hybridization function for the otherwise localized \( f \)-electrons. Subsequently, the quantity, \( \Sigma_d(\omega) = \frac{V^2}{\omega^+ - \Delta(\omega)} \) may be thought of as an effective \( d \)-electron self energy.

In the presence of disorder, the above Greens functions are replaced by their disorder
FIG. 5. **Density of states in presence of particle hole asymmetry** The f-electron (top panel) and the d-electron (bottom panel) density of states for various $\epsilon_d$ is plotted to demonstrate how a variation of $\epsilon_d$ may not only introduce low-lying electronic states but also induce low lying sharp features on the order of the respective Kondo scale.

averages as the following:

$$G_{d \text{ave}}^d(\omega) = \langle G_j^c(\omega) \rangle$$

$$=-\left( \frac{V^2}{\omega^+ - \Sigma_f(\omega) - \Delta_{\text{ave}}(\omega) - \epsilon_{dj}} \right)^{-1},$$

(13)

$$G_{f \text{ave}}^f(\omega) = \langle G_j^f(\omega) \rangle$$

$$=-\left( \frac{V^2}{\omega^+ - \Sigma_f(\omega) - \omega^+ - \Delta_{\text{ave}}(\omega) - \epsilon_{dj}} \right)^{-1},$$

(14)

where $j$ represents the disorder realization and correspondingly, $\epsilon_{dj}$ represents the random c-electron energy drawn from some disorder distribution, $P(\epsilon_{dj})$, that in the current case is represented by a Gaussian function with a mean at $\langle \epsilon_{dj} \rangle = \epsilon_d^d = 0$, and the variance given by the disorder strength, $W$. Notice that in the above equations, the CPA is constituted in an arithmetic sum of the $G_j^d(\omega)$’s, embodied within the definition of $\langle \ldots \rangle$, and also in approximating $\Delta_j(\omega) = \Delta_{\text{ave}}(\omega)$ to be the same for all the disorder realizations. The disorder averaged c- and f- electron spectral functions may then be evaluated as, $D_{\text{ave}}^d(\omega) = -\frac{1}{\pi} \text{Im} G_{\text{ave}}^d(\omega)$ and $D_{\text{ave}}^f(\omega) = -\frac{1}{\pi} \text{Im} G_{\text{ave}}^f(\omega)$, respectively.
The underlying lattice information is built in the equation:

\[
G_{\text{latt}}(\omega) = \int_{-\infty}^{\infty} \frac{\rho_0(e)de}{\omega + e - \Sigma_{\text{ave}}(\omega)} = H[\gamma_{\text{ave}}],
\]

where, a disorder averaged \(c\)-electron self-energy, \(\Sigma_{\text{ave}}^{d}(\omega)\) can be extracted from Equation (13), and \(H[\gamma_{\text{ave}}]\) is the Hilbert transform of \(\gamma_{\text{ave}} = \omega + e - \Sigma_{\text{ave}}\). Equation (15) helps us construct a new hybridization function,

\[
\Delta_{\text{ave}}(\omega) = \gamma_{\text{ave}} - 1/H[\gamma_{\text{ave}}]
\]

In the present calculations we use a semi-circular density of states, corresponding to a Bethe lattice, that is represented by \(\rho_0(e) = \frac{2}{\pi t}[1 - (e/t)^2]^{1/2}\). This reduces, \(\Delta_{\text{ave}}(\omega) = \frac{t^2}{\pi} G_{\text{latt}}^{d}(\omega)\). Equations (13), (15), and (16) constitute the DMFT self-consistency equations and determine the disorder averaged effective medium. At DMFT convergence, \(G_{\text{latt}}^{d}(\omega) = G_{\text{ave}}^{d}(\omega)\) within some tolerance. Nonetheless, it is worth mentioning that the qualitative features of results present is independent of the specific choice of the lattice.

The possible manifestations of site dilution in the form of Kondo holes in a Kondo insulator or heavy fermion metal had been the focus of several theoretical studies. While some of these early studies fail to capture the relevant energy scales determining the underlying physical observations in these systems, others emphasize on the necessity of introducing a concentration dependence on the bare Hamiltonian parameters for capturing the respective experimental observations. In contrast, our theory captures several experimental features in these Kondo insulators without having to rely on any disorder induced doping effects or artificial tuning of the average orbital energy based on the amount of dilution.

Finally, we now comment on the calculation of the interacting self-energy, \(\Sigma_{f}(\omega)\). We use the local moment approach to compute the \(f\)-electron self-energy. The LMA is a diagrammatic perturbation theory based approach, built around the two broken-symmetry, local moment solutions \((\mu = \pm|\mu_0|)\) of an unrestricted Hartree-Fock mean field approximation. Subsequently, the physics due to Kondo effect embodied in spin-flip dynamics are built in through an infinite-order resummation of a specific class of diagrams that quantify the transverse spin-flip processes. A low energy spin flip scale, \(\omega_m\) is thereby generated and is identified through the position of the peak of the imaginary part of the transverse spin
polarization propagator within this approach. Physically and quantitatively, this low energy scale is of the same order as the Kondo scale, \( T_K \) (or more precisely, \( k_B T_K \)) as mentioned in this this work. For more details about the local moment approach as used in impurity or clean and disordered lattice systems, we urge the readers to refer to several previous works carried out with this approach as outlined in References 35–37 and the references therein.

3. TRANSPORT: D.C. CONDUCTIVITY

Within the large dimensional framework of the DMFT, a knowledge of the one particle excitations represented by the Greens functions and their \((\omega, T)\) dependencies are sufficient to determine the transport properties. In particular, the absence of any momentum dependence in the electronic self-energy leads to the strict absence of any vertex corrections in the current-current correlation function. Thus within DMFT, the conductivity, for a Bethe lattice is given by,

\[
\sigma(\omega; T) = \sigma_0 \frac{\omega}{\omega} \int_{-\infty}^{\infty} d\omega_1 \frac{f(\omega_1) - f(\omega + \omega_1)}{\omega} \langle D^d_{\text{ave}}(\epsilon, \omega; T) \rangle_{\epsilon} \langle D^d_{\text{ave}}(\epsilon, \omega + \omega_1; T) \rangle_{\epsilon}
\]

where, \( \langle D^d_{\text{ave}}(\epsilon, \omega; T) \rangle_{\epsilon} = \int_{-\infty}^{\infty} d\epsilon \rho_0(\epsilon) D^d_{\text{ave}}(\epsilon, \omega_1; T) \), with \( \sigma_0 \sim 10^4 - 10^5 \Omega^{-1} cm^{-1} \), \( D^d_{\text{ave}}(\epsilon, \omega; T) = -\frac{1}{\pi} \text{Im} G^d_{\text{ave}}(\epsilon, \omega; T) \) and \( f(\omega) \) is the Fermi distribution function. The d.c. resistivity can then be evaluated as, \( \rho(\omega = 0; T) \propto \left[ \int_{-\infty}^{\infty} \frac{-\partial f(\omega)}{\partial \omega} \langle D^d_{\text{ave}}(\epsilon, \omega; T) \rangle_{\epsilon} \right]^2 d\omega \]^{-1}. For the hypercubic lattice,

\[
\sigma(\omega; T) \propto \frac{1}{\omega} \int_{-\infty}^{\infty} d\omega_1 \frac{f(\omega_1) - f(\omega + \omega_1)}{\omega} \langle D^d_{\text{ave}}(\epsilon, \omega; T) D^d_{\text{ave}}(\epsilon, \omega + \omega_1; T) \rangle_{\epsilon}
\]

4. SPECIFIC HEAT

In the following we outline the method and assumptions underlying the calculation of specific heat for the system studied. Our basic assumption underlying the treatment of the disordered system, lies in mapping the interacting disordered system onto an ensemble of independent, Anderson impurities, each of which is embedded into a bath via a hybridization
function, that in turn depends on $\Delta_{\text{ave}}(\omega)$ and the local potentials, $\epsilon_{cj}$’s, as outlined in Appendix 2 by equations 13, 14, 15 and 16. The specific heat for the original system is then calculated by taking the average over the single-impurity results with the appropriate distribution function, which in the current case is a Gaussian. The calculation of specific heat would thus involve the computation of the total energies of the ensemble of Anderson impurities, such that $C_v(T) = \frac{\partial E_{\text{ave}}}{\partial T}$, where $E_{\text{ave}}$ is the disorder averaged energy of the system. In the following, we outline the equations determining the total energy calculation of a single impurity Anderson model.

The single impurity Anderson model is represented as,

$$
H_{SIAM} = \sum_{k \sigma} \epsilon_{ck} c_k^{\dagger} c_k + \epsilon_d \sum_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + U n_{d\uparrow} n_{d\downarrow} + \\
\sum_{k \sigma} V_k c_{k\sigma}^{\dagger} d_{\sigma} + \text{h.c.},
$$

(19)

where, $\epsilon_{ck}$ represents the energy dispersion of the underlying host of $c$-electrons in which a correlated impurity site represented by $d$ electrons is embedded via the hybridization energy denoted by $V_k$, such that the hybridization function is given by, $\sum_k \frac{|V_k|^2}{\omega - \epsilon_{ck}} = \Delta(\omega)$; $n_{d\sigma}$ denoted the occupancy of the $d$-electron with spin $\sigma$ on the impurity site and $U$ is the Coulomb energy cost to be paid when two electrons of opposite spin sit on the impurity site; $\epsilon_d$ is the on site potential energy of the impurity site.

$$
E_{\text{imp}} = \epsilon_d \sum_{\sigma}(n_{d\sigma}) + UD + \frac{1}{2} E_{\text{hyb}} + \\
\frac{1}{\pi} \sum_{\sigma} \int d\omega n_F(\omega) \text{Im} \left[ G_{d\sigma}(\omega) \omega \frac{\partial \Delta(\omega)}{\partial \omega} \right],
$$

(20)

where, $D$, is the double occupancy on the impurity site and can be represented in terms of the single particle spectral function, $D_G = -\text{Im}G_{\sigma}(\omega)/\pi$ and the imaginary part of the
single particle self energy, \( D^\sigma \Sigma = -\text{Im} \Sigma_\sigma(\omega)/\pi \), as the following:

\[
\langle n_{d\uparrow} n_{d\downarrow} \rangle = \frac{\Sigma^{\uparrow}_{\text{Hartree}}}{U} \int d\omega_1 D^{\uparrow}_{G}(\omega_1)n_F(\omega_1)
+ \frac{1}{U} \int d\omega_1 d\omega_2 D^{\uparrow}_{G}(\omega_1)D^{\uparrow}_{\Sigma}(\omega_2)\frac{n_F(\omega_1) - n_F(\omega_2)}{\omega_1 - \omega_2}
= n_{\text{occ}}\Sigma^{\uparrow} + \frac{1}{U} \int d\omega_1 d\omega_2 D^{\uparrow}_{G}(\omega_1)D^{\uparrow}_{\Sigma}(\omega_2)\frac{n_F(\omega_1) - n_F(\omega_2)}{\omega_1 - \omega_2},
\]

where \( n_F \) is the Fermi distribution function. The term \( E_{\text{hyb}} \) represents the energy of the impurity due to its hybridization with the \( c \)-electrons and is given by,

\[
E_{\text{hyb}} = -\frac{2}{\pi} \sum_{\sigma} \int d\omega n_F(\omega)\text{Im}[\Delta(\omega)G_{\sigma\sigma}(\omega)]
\]

As mentioned earlier, we use the local moment approach to compute the impurity self-energy and the impurity properties within the DMFT framework. While this approach comes with its limitations it’s single particle properties have been extensively benchmarked with the numerically exact, numerical renormalization group calculations. For the current case of total energy calculation, and thereby the specific heat, we ensured that it reproduces

FIG. 6. I(Main panel)The specific heat of a Kondo insulator is plotted as \( C_v \) v/s \( T \) on a linear scale for \( U = 1.3, \ 1.9, \ 2.3 \). (Inset) \( \ln(C_vT) \) v/s \( 1/T \) is plotted to demonstrate the gradual crossover to a low \( T \) activated behavior of \( C_v \). The solid black line depicts a straight line fit. The expected trend, of a decreasing magnitude of the slope with an increasing \( U \) is also successfully captured within the simulation.
the basic features in some known limits of the system under consideration. In Figure 6 we therefore plot the computed $C_v(T)$ for a clean Kondo insulator. As seen from Figure 6 where we plot $\ln(T C_v)$ vs $1/T$, the method clearly depicts the expected trends for that of a clean Kondo insulator, namely, a low $T$ activated behavior. It also correctly depicts a decreasing magnitude of the slope with increasing $U$; this slope is also a measure of the hybridization gap.

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* corresponding email: weiku@mailaps.org

1 M. Dzero, J. Xia, V. Galitski, and P. Coleman, Annual Review of Condensed Matter Physics 7, 249 (2016).

2 J. C. Nickerson, R. M. White, K. N. Lee, R. Bachmann, T. H. Geballe, and G. W. Hull, Phys. Rev. B 3, 2030 (1971).

3 W. A. Phelan, S. M. Koolpayeh, P. Cottingham, J. W. Freeland, J. C. Leiner, C. L. Broholm, and T. M. McQueen, Phys. Rev. X 4, 031012 (2014).

4 N. Wakeham, P. F. S. Rosa, Y. Q. Wang, M. Kang, Z. Fisk, F. Ronning, and J. D. Thompson, Phys. Rev. B 94, 035127 (2016).

5 J. W. Allen, B. Batlogg, and P. Wachter, Phys. Rev. B 20, 4807 (1979).

6 J. W. Allen, Philosophical Magazine 96, 3227 (2016).

7 B. Gorshunov, N. Sluchanko, A. Volkov, M. Dressel, G. Knebel, A. Loidl, and S. Kunii, Phys. Rev. B 59, 1808 (1999).

8 P. Syers, D. Kim, M. S. Fuhrer, and J. Paglione, Phys. Rev. Lett. 114, 096601 (2015).

9 D. Kim, S. Thomas, T. Grant, J. Botimer, Z. Fisk, and J. Xia, Scientific reports 3, 3150 (2013).

10 N. Wakeham, Y. Q. Wang, Z. Fisk, F. Ronning, and J. D. Thompson, Phys. Rev. B 91, 085107 (2015).

11 W. K. Park, L. Sun, A. Noddings, D.-J. Kim, Z. Fisk, and L. H. Greene, Proceedings of the National Academy of Sciences 113, 6599 (2016).

12 N. Xu, P. K. Biswas, J. H. Dil, R. S. Dhaka, G. Landolt, S. Muff, C. E. Matt, X. Shi, N. C. Plumb, M. Radović, E. Pomjakushina, K. Conder, A. Amato, S. V. Borisenko, R. Yu, H.-M. Weng, Z. Fang, X. Dai, J. Mesot, H. Ding, and M. Shi, Nature Communications 5, 4566 (2014).

13 M. Neupane, N. Alidoust, S.-Y. Xu, T. Kondo, Y. Ishida, D. J. Kim, C. Liu, I. Belopolski, Y. J.
Jo, T.-R. Chang, H.-T. Jeng, T. Durakiewicz, L. Balicas, H. Lin, A. Bansil, S. Shin, Z. Fisk, and M. Z. Hasan, *Nature Communications* **4**, 2991 (2013).

14 D. J. Kim, J. Xia, and Z. Fisk, *Nature Materials* **13**, 466 (2014).

15 Y. S. Eo, A. Rakoski, J. Lucien, D. Mihaliov, C. Kurdak, P. Ferrari Silveira Rosa, D.-J. Kim, and Z. Fisk, ArXiv e-prints (2018), arXiv:1803.00959 [cond-mat.str-el].

16 Y. Li, Q. Ma, S. X. Huang, and C. L. Chien, *Science Advances* **4** (2018), 10.1126/sciadv.aap8294.

17 N. J. Laurita, C. M. Morris, S. M. Koohpayeh, P. F. S. Rosa, W. A. Phelan, Z. Fisk, T. M. McQueen, and N. P. Armitage, *Phys. Rev. B* **94**, 165154 (2016).

18 S. Gabáni, G. Prístáš, I. Takáčová, N. Sluchanko, K. Siemensmeyer, N. Shitsevalova, V. Filipov, and K. Flachbart, *Solid State Sciences* **47**, 17 (2015), special Issue: International Symposium on Boron, Borides and Related Materials, ISBB 2014, Honolulu, Hawaii.

19 M. Boulanger, F. Laliberté, S. Badoux, N. Doiron-Leyraud, W. A. Phelan, S. M. Koohpayeh, T. M. McQueen, X. Wang, Y. Nakajima, T. Metz, J. Paglione, and L. Taillefer, ArXiv e-prints (2017), arXiv:1709.10456 [cond-mat.str-el].

20 B. S. Tan, Y.-T. Hsu, B. Zeng, M. C. Hatnean, N. Harrison, Z. Zhu, M. Hartstein, M. Kiourlapou, A. Srivastava, M. D. Johannes, T. P. Murphy, J.-H. Park, L. Balicas, G. G. Lonzarich, G. Balakrishnan, and S. E. Sebastian, *Science* **349**, 287 (2015).

21 J. J. van den Broeke, S. N. Kempkes, A. Quelle, X. F. Wang, J. Paglione, and C. Morais Smith, ArXiv e-prints (2018), arXiv:1803.03553 [cond-mat.str-el].

22 J. Knolle and N. R. Cooper, *Physical Review Letters* **118**, 096604 (2017), arXiv:1608.02453 [cond-mat.str-el].

23 D. Chowdhury, I. Sodemann, and T. Senthil, ArXiv e-prints (2017), arXiv:1706.00418 [cond-mat.str-el].

24 I. Sodemann, D. Chowdhury, and T. Senthil, *Phys. Rev. B* **97**, 045152 (2018), arXiv:1708.06354 [cond-mat.str-el].

25 G. Baskaran, ArXiv e-prints (2015), arXiv:1507.03477 [cond-mat.str-el].

26 R. Yu, H. Weng, X. Hu, Z. Fang, and X. Dai, *New Journal of Physics* **17**, 023012 (2015).

27 D. Kim, J. Xia, Z. Fisk, et al., *Nature Materials* **13**, 466 (2014).

28 M. E. Valentine, S. Koohpayeh, W. A. Phelan, T. M. McQueen, P. F. Rosa, Z. Fisk, and N. Drichko, *Physical Review B* **94**, 075102 (2016).

29 W. T. Fuhrman, J. R. Chamorro, P. A. Alekseev, J.-M. Mignot, T. Keller, P. Nikolic, T. M.
McQueen, and C. L. Broholm, ArXiv e-prints (2017), arXiv:1707.03834 [cond-mat.str-el]

30 A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996)

31 P. Schlottmann, Phys. Rev. B 46, 998 (1992)

32 P. S. Riseborough, Phys. Rev. B 68, 235213 (2003).

33 C. Grenzebach, F. B. Anders, G. Czycholl, and T. Pruschke, Phys. Rev. B 77, 115125 (2008)

34 P. Kumar and N. S. Vidhyadhiraja, Phys. Rev. B 90, 235133 (2014)

35 D. E. Logan, M. P. Eastwood, and M. A. Tusch, Journal of Physics Condensed Matter 10, 2673 (1998)

36 N. S. Vidhyadhiraja and D. E. Logan, Journal of Physics: Condensed Matter 17, 2959 (2005).

37 S. Sen, H. Terletska, J. Moreno, N. S. Vidhyadhiraja, and M. Jarrell, Phys. Rev. B 94, 235104 (2016)