Kondo Impurities in the Kitaev Spin Liquid: Numerical Renormalization Group Solution and Gauge-Flux-Driven Screening

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Kitaev's honeycomb-lattice compass model describes a spin liquid with emergent fractionalized excitations. Here, we study the physics of isolated magnetic impurities coupled to the Kitaev spin-liquid host. We reformulate this Kondo-type problem in terms of a many-state quantum impurity coupled to a multichannel bath of Majorana fermions and present the numerically exact solution using Wilson's numerical renormalization group technique. Quantum phase transitions occur as a function of Kondo coupling and locally applied field. At zero field, the impurity moment is partially screened only when it binds an emergent gauge flux, while otherwise it becomes free at low temperatures. We show how Majorana degrees of freedom determine the fixed-point properties, make contact with Kondo screening in pseudogap Fermi systems, and discuss effects away from the dilute limit.

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Spin liquids constitute a fascinating class of states of local-moment magnets, characterized by the absence of symmetry-breaking order at low temperatures [1]. Very often, these states are topologically nontrivial, displaying an emergent gauge structure and fractionalized excitations. Given that the exotic properties of spin liquids are difficult to detect directly in local observables, much additional information can be obtained by studying the distinctive response to local perturbations. In particular, impurities or defects can act as *in situ* probes. This general concept of characterizing nontrivial magnetic states via their response to isolated impurities has been successfully applied in the past, with prominent examples being vacancy-induced moments in confined spin-gap magnets [2], universal fractional moments near quantum critical points [3], the fractionalization of orphan spins in strongly frustrated magnets [4], and the pinning of emergent magnetic monopoles in spin ice [5].

In this Letter, we present a detailed study of the physics of a magnetic (Kondo) impurity coupled to the gapless spin-liquid phase of Kitaev's honeycomb-lattice compass model [6]. This Kitaev model is a rare example of an exactly solvable model for a fractionalized spin liquid in two dimensions. Its solution can be cast into itinerant Majorana fermions coupled to a static $\mathbb{Z}_2$ gauge field. These properties enable an exact reformulation of the Kondo problem in terms of a complex quantum impurity coupled to noninteracting fermions, suitable for treatment using Wilson's numerical renormalization group (NRG) [7,8]. NRG is a nonperturbative method that yields essentially exact numerical results down to lowest temperatures for any coupling strength.

Our main results for an isolated Kondo impurity in the Kitaev spin liquid, Fig. 1, can be summarized as follows: As a function of the Kondo coupling K, the model displays a single first-order quantum phase transition (QPT) at $K = K_c > 0$: There is partial screening for large antiferromagnetic couplings, $K_c < K < \infty$, whereas the impurity spin is unscreened, otherwise, $-\infty < K < K_c$. The transition is accompanied by the binding of a gauge flux to the impurity. The renormalization-group (RG) flow in the individual flux sectors is nontrivial, see Fig. 2. Importantly, there is no screening—and no QPT—in the flux-free sector of the Hilbert space due to an emergent particle-hole symmetry. A magnetic field applied to the impurity can drive multiple transitions; it also induces flux binding for ferromagnetic K. We are able to characterize all fixed points in terms of their magnetic response and residual entropy, in part arising from localized Majorana zero modes, and we provide analytical expressions for the relevant crossover scales. Our results connect to those

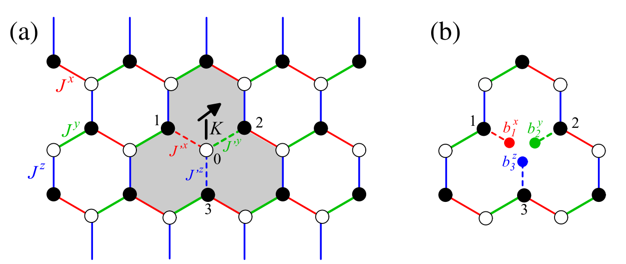

FIG. 1. (a) Setup for the Kitaev Kondo problem: an extra spin (black arrow) and the bulk spin at site 0 are coupled by the Kondo coupling $K \equiv K^x = K^y = K^z$. The bulk exchange couplings are denoted by $J^{x,y,z}$, and we allow for different couplings $J'^{x,y,z}$ next to the impurity. The large shaded plaquette will be dubbed "impurity plaquette." (b) Illustration of dangling gauge Majorana modes relevant for the vacancy fixed points ($K \to \pm\infty$).

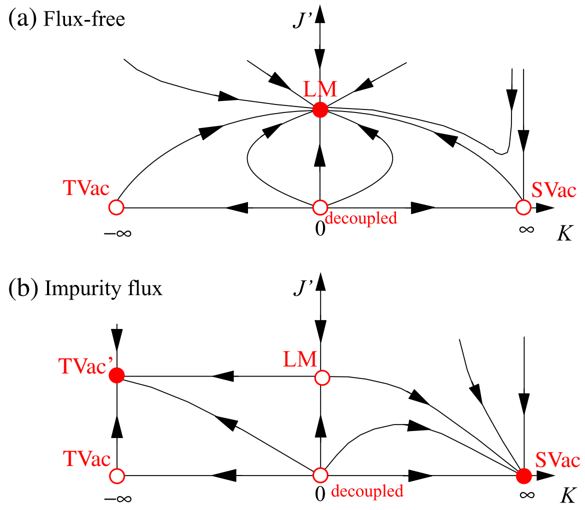

FIG. 2. Schematic RG flow for the isotropic Kitaev Kondo model in a plane spanned by the Kondo coupling K and the coupling J' between site 0 and sites 1,2,3. (a) Flux-free sector of the Hilbert space. (b) Sector with a $\mathbb{Z}_2$ flux through the impurity plaquette, $W_I = -1$. Full (open) dots denote stable (unstable) fixed points.

obtained for isolated vacancies [9,10] and encompass the case of substitutional spin-1 impurities.

Our work goes far beyond previous approximate treatments of Kondo impurities in spin liquids [11–16]. For the Kitaev Kondo (KK) model, the full solution with NRG reveals a far richer range of physics, controlled by nonperturbative effects related to the pseudogap Kondo problem and not captured within weak-coupling RG schemes. Our analysis corrects aspects of earlier work [15,16] on the same model as detailed in Section IV of Ref. [17].

Model.—The Kitaev model [6] describes spins 1/2 at sites i of a honeycomb lattice, with sublattices A and B. The Ising-like nearest-neighbor interactions J^α, $\alpha = x, y, z$, are tied to the real-space bond direction, reflecting strong spin-orbit coupling. The bulk Hamiltonian reads

$$\mathcal{H}_{\rm Kit} = -J^x \sum_{\langle ij\rangle_x} \hat\sigma_i^x \hat\sigma_j^x - J^y \sum_{\langle ij\rangle_y} \hat\sigma_i^y \hat\sigma_j^y - J^z \sum_{\langle ij\rangle_z} \hat\sigma_i^z \hat\sigma_j^z, \qquad (1)$$

where $\hat\sigma_j^\alpha$ are Pauli matrices, and $\langle ij\rangle_\alpha$ denotes an α bond as in Fig. 1. We focus on the isotropic case $J \equiv J^x = J^y = J^z$.

We consider a Kondo problem with a spin-1/2 impurity, $\vec{S}$, coupled to the Kitaev spin on site 0 of sublattice A. The full Hamiltonian is $\mathcal{H}_{\rm KK} = \mathcal{H}_{\rm Kit} + \mathcal{H}_{\rm Kon}$ with

$$\mathcal{H}_{\rm Kon} = \sum_\alpha K^\alpha \hat S^\alpha \hat\sigma_0^\alpha + \sum_\alpha h^\alpha \hat S^\alpha, \qquad (2)$$

where $\vec{K}$ is the Kondo coupling and $\vec{h}$ a local field applied to the impurity [22]. For the purpose of analysis we will allow the exchange couplings connecting site 0 to its neighbors 1,2,3 to take values $J'^\alpha \neq J^\alpha$, see Fig. 1.

NRG formulation.—Application of NRG to the Kitaev Kondo problem is made possible because the bulk Kitaev model has an infinite number of conserved $\mathbb{Z}_2$ fluxes: For every elementary plaquette with spins $1, \ldots, 6$, the operator $\hat W_p = \hat\sigma_1^x \hat\sigma_2^y \hat\sigma_3^z \hat\sigma_4^x \hat\sigma_5^y \hat\sigma_6^z$ is conserved, with eigenvalues $W_p = \pm 1$. Consequently, the Hilbert space decomposes into flux sectors, defined by the set of $\{W_p\}$. Using the representation $\hat\sigma_i^\alpha = \imath \hat b_i^\alpha \hat c_i$ of each bulk spin in terms of four Majorana fermions, $\hat c_i$ and $\hat b_i^\alpha$ [6], the operators $\hat u_{ij} = \imath \hat b_i^{\alpha_{ij}} \hat b_j^{\alpha_{ij}}$, defined on each lattice bond, are separately conserved. Their eigenvalues $u_{ij} = \pm 1$ relate to the plaquette fluxes via $W_p = u_{21} u_{23} u_{43} u_{45} u_{65} u_{61}$. For a given set $\{u_{ij}\}$, the original bulk Hamiltonian (1) reduces to a tight-binding model for the c ("matter") Majorana fermions,

$$\mathcal{H}_u = \imath \sum_{\langle ij\rangle_\alpha} J^\alpha u_{ij} \hat c_i \hat c_j, \qquad (3)$$

with hopping energies $J^\alpha u_{ij}$ encoding the coupling to the static $\mathbb{Z}_2$ gauge field. The ground state of $\mathcal{H}_u$ is located in the flux-free sector, with $u_{ij} = 1$, where the spectrum can be found by Fourier transformation [6,17].

In the presence of the Kondo term, $K \neq 0$, the fluxes in the three plaquettes adjacent to site 0 are no longer individually conserved. However, their product W_I (the flux in the impurity plaquette, Fig. 1), as well as all outer fluxes, remain conserved. This implies that the bulk system, with site 0 removed, forms a bath of free fermions with Hamiltonian $\mathcal{H}_{\rm bath}$ in any given flux sector. This bath is coupled to a generalized "impurity" which now consists of the Kondo spin and the Kitaev spin at site 0, also including the surrounding flux degrees of freedom. The impurity Hamiltonian $\mathcal{H}_{\rm imp}$ acts in a Hilbert space of 16 states. The coupling between impurity and bath, $\mathcal{H}_{\rm hyb}$, arises from the Kitaev exchanges J'^α between site 0 and sites 1,2,3, such that the bath is characterized by a 3×3 matrix propagator. For isotropic couplings and flux configurations preserving the $\mathbb{Z}_3$ lattice rotation symmetry, the bath can be decomposed into angular-momentum modes, such that $\mathcal{H}_{\rm bath}$ eventually consists of three channels of spinless fermions. The explicit forms of $\mathcal{H}_{\rm bath}$, $\mathcal{H}_{\rm imp}$, and $\mathcal{H}_{\rm hyb}$ are specified in the Supplemental Material [17].

With fluxes fixed, the Hamiltonian $\mathcal{H}_{\rm bath} + \mathcal{H}_{\rm imp} + \mathcal{H}_{\rm hyb}$ is equivalent to $\mathcal{H}_{\rm KK}$ and can be solved via NRG [7,8]. Iterative diagonalization of a semi-infinite-chain Hamiltonian yields the many-particle level flow as well as physical observables as a function of temperature. Since separate NRG runs are performed in each flux sector, NRG thermodynamics are representative of the full Kitaev model at temperatures below the flux gap. Based on the results in Refs. [6,9] we expect the ground state of $\mathcal{H}_{\rm KK}$ to have a flux-free bath, and W_I either $+1$ or -1.

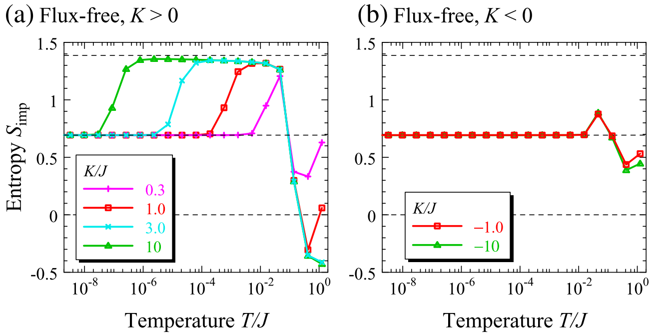

FIG. 3. NRG results for the impurity contribution to the total entropy, $S_{imp}(T)$, vs T/J in the no-flux case for $J' = J$ and various K. The horizontal dashed lines indicate $S_{imp} = 0$, $\ln 2$, and $\ln 4$. The crossover behavior for $T/J > 10^{-1}$ is a band-edge effect.

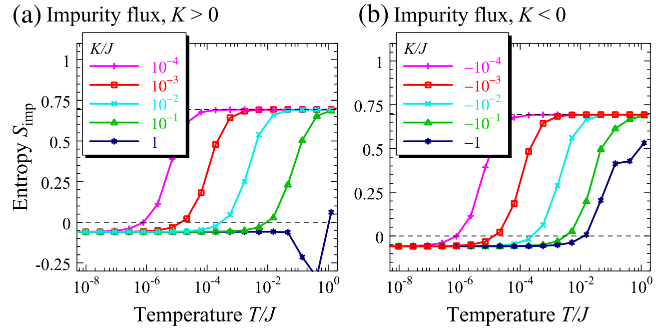

FIG. 4. Impurity entropy as in Fig. 3, but for the vacancy-flux case, with $J' = J$ and various K.

Fixed points.—We start by enumerating the trivial RG fixed points—this is most efficiently done using the couplings K and J' as (renormalized) parameters. $K = J' = 0$ describes the fully decoupled situation, while $K = 0$ and $J' = J$ is the local-moment (LM) fixed point, where the unscreened Kondo spin is decoupled from the Kitaev bulk. Further, $K = +\infty$ causes singlet formation between the Kondo spin and the Kitaev spin 0, i.e., Kondo screening—this induces a singlet vacancy (SVac) in the host (therefore, $J' = 0$). Similarly, $K = -\infty$ and $J' = 0$ corresponds to a triplet vacancy (TVac). We also find a fixed point at $K = -\infty$ but with finite J', denoted TVac′. Note that all fixed points are separately defined in each flux sector.

NRG results: Flux-free case.—We have extensively studied the Kitaev Kondo model using NRG. We start with results for the flux-free sector, i.e., $W_p = +1$ on all outer plaquettes and $W_I = +1$ on the impurity plaquette.

The impurity entropy $S_{imp}(T)$, obtained as the entropy difference between the systems with and without Kondo spin (with fluxes fixed), is shown in Fig. 3 for various values of K/J, keeping $J' = J$. We find that the impurity entropy reaches $\ln 2$ in the low-T limit for all couplings K; the NRG level structure of this fixed point is identical to that at $K = 0$, $J' = J$ [17]. We conclude that, in the flux-free case, there is a *single* stable phase controlled by the LM fixed point, Fig. 2, without Kondo screening.

For $K \gtrsim J$, we find an intermediate crossover from $S_{imp} \approx \ln 4$ to $\ln 2$ upon lowering T. As explained below, the fixed point associated with $\ln 4$ entropy is identified as SVac, corresponding to a strong coupling Kondo-screened state. However, this fixed point is unstable: below a scale T^*, well fit by $T^* \propto J'^3 J^2/K^4$ [17], the system evolves toward the LM fixed point and the impurity moment becomes free.

For ferromagnetic $K < 0$ [Fig. 3(b)], the LM fixed point is again stable. For $J' = J$, no intermediate RG flow is observed. Only for small J' do we see incipient flow via TVac, with $S_{imp} \approx \ln 12$; the LM crossover scale in this case is extracted as $T^* \propto J'$ [17].

NRG results: Impurity-flux case.—Now, we turn to the case where the impurity plaquette is threaded by a $\mathbb{Z}_2$ flux, $W_I = -1$, while $W_p = +1$ otherwise. NRG results for the impurity entropy are shown in Fig. 4. We find that $S_{imp} \approx -0.06$ at low T for all K.

For $J' = J$, there is a single crossover upon cooling, here, from $S_{imp} = \ln 2$ to -0.06, with a crossover scale $T^* \propto |K|$ for both signs of K. The NRG levels identify the intermediate $\ln 2$ fixed point as LM, whereas the low-T fixed points correspond to $K \to \infty$ and $K \to -\infty$, i.e., SVac and TVac′, respectively. Notably, we also observe a clear TVac → TVac′ crossover for small J' and large negative K [17]: On lowering the temperature through $T^* \propto J'^2/J$, the entropy decreases from $S_{imp} \approx 1.04$ to -0.06.

Analytics: Flux-free case.—Analytical considerations essentially enable a full understanding of the numerical findings. We start analyzing the vicinity of LM in the flux-free sector. Here, the Kondo spin is coupled to a Majorana bath at site 0 with a power-law density of states (DOS), $\rho(\omega) = |\omega|^r$ with $r = 1$. This problem is related to the extensively studied pseudogap Kondo model [23–26] at particle–hole (p-h) symmetry; recall that on-site potentials are forbidden for Majorana fermions. Importantly, the p-h symmetric pseudogap Kondo model exhibits no screening, even for strong antiferromagnetic Kondo coupling, because the relevant resonant-level fixed point is unstable for $r > 1/2$ [24–26]. This argument carries over to the present case, implying that SVac must be unstable in the flux-free case. In fact, the relevant perturbation to SVac has scaling dimension unity and initial value $J'^3/(JK^2)$; SVac is destabilized once this perturbation reaches the scale K^2/J^2 [17], explaining the numerically identified T^*.

References [15,16] argued that the flux-free sector displays a QPT between unscreened and screened phases. However, this is not the case—the QPT is an artifact of weak-coupling RG [17,25], not observed in the NRG solution.

It is instructive to analyze S_{imp} at the unstable SVac fixed point, where the Kondo spin and the host spin at site 0 form a tightly bound singlet complex. Since site 0 is then effectively cut out from the host [9], the three dangling gauge Majorana fermions $\hat{b}_1^x$, $\hat{b}_2^y$, $\hat{b}_3^z$, give a residual entropy $\frac{3}{2}\ln 2$. But $S_{\rm imp}$ is the entropy *relative* to that of the Kitaev host with no impurity (and therefore, no vacancy), and so, we must subtract the contribution of the Kitaev site 0 to the host entropy to obtain $S_{\rm imp}$. Site 0 is coupled to three spinless electron channels and can itself be viewed as a Majorana resonant-level model. The s-wave channel responsible for screening site 0 has a power-law diverging DOS $1/(\omega \ln^2 \omega)$, and so, its residual entropy [24,27,28] is $(-\frac{1}{2}\ln 2)$ (the factor of $\frac{1}{2}$ arising here because we are dealing with Majoranas). Overall, $S_{\rm imp}^{\rm SVac} = (\frac{3}{2}\ln 2) - (-\frac{1}{2}\ln 2) = \ln 4$ as found from NRG.

At TVac, the Kondo impurity and spin 0 form an $S = 1$ triplet which contributes an additional $\ln 3$ entropy, giving overall $S_{\rm imp}^{\rm TVac} = S_{\rm imp}^{\rm SVac} + \ln 3 = \ln 12$, again confirmed by NRG [17].

Analytics: Impurity-flux case.—It is important to realize that the condition $W_I = -1$ induces a finite DOS at site 0 when $J' \neq 0$ [9], and it imposes a threefold bath degeneracy because $W_I = -1$ can be achieved with a flux in any of the three plaquettes next to site 0 (the fourth configuration with fluxes through all three plaquettes is higher in energy). This degeneracy is lifted by the Kondo impurity; hence, K couples two degenerate subsystems—the Kondo spin and the bath—resulting in an entropy quench and concomitant partial screening. In contrast to standard Kondo problems [25,29], the Kondo temperature is, therefore, $T^* \propto |K|$.

The $S_{\rm imp}$ values arise as follows: Because of the subtraction of the impurity-free reference system, $S_{\rm imp}^{\rm LM} = \ln 2$ despite the threefold degeneracy of the Kitaev host. However, $S_{\rm imp}$ is lower by $\ln 3$ at the $K \neq 0$ fixed points, due to the lifted flux degeneracy. As before, SVac and TVac ($K = \pm\infty$) contain three dangling gauge Majoranas. Since there is no bath divergence in the impurity-flux case, we have $S_{\rm imp}^{\rm SVac} = \frac{3}{2}\ln 2 - \ln 3 \approx -0.06$ and $S_{\rm imp}^{\rm TVac} = S_{\rm imp}^{\rm SVac} + \ln 3 = \frac{3}{2}\ln 2$. For ferromagnetic K, broken spin symmetry drives the flow to TVac′: the spin-triplet degeneracy is lifted such that $S_{\rm imp}^{\rm TVac'} = S_{\rm imp}^{\rm SVac}$.

Field response.—The response to a local magnetic field h characterizes the fate of the Kondo spin. In the stable LM phase of the flux-free case, the Kondo spin is unscreened and the local susceptibility displays a low-T Curie law, $\chi_{\rm loc}(T) = C_{\rm loc}/T$, arising from the residual magnetic moment on the Kondo site, with $C_{\rm loc} \leq 1$ (and $C_{\rm loc} = 1$ only at $K = 0$) [22].

For the impurity-flux case we first note that the $K = \infty$ model is known to display a weakly singular response arising from the three dangling gauge Majorana fermions, $\chi \propto 1/\ln T$ [9]. Rather surprisingly, we find that the SVac phase displays a low-T Curie law for any $K < \infty$, but with a much reduced $C_{\rm loc}$. This Curie response arises from a

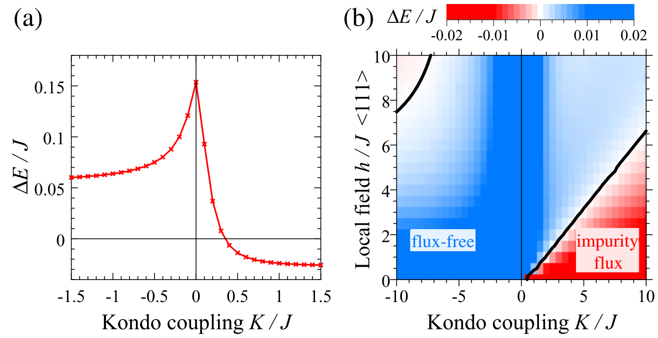

FIG. 5. Energy difference between impurity-flux and no-flux ground states, $\Delta E = E_{\rm flux} - E_{\rm noflux}$, as function of K/J (a) at $h = 0$ and (b) as a function of h, with the lines denoting phase boundaries.

subtle interplay of Majorana zero modes and the tightly bound singlet: Virtual triplet excitations couple pairs of zero modes; e.g., $\hat{b}_1^x$ and $\hat{b}_2^y$ acquire a coupling, producing an effective free moment along z [17]. Together, this results in partial screening. A similar Curie law is found in the TVac′ phase, but with $C_{\rm loc}$ of order unity because virtual excitations are less costly.

Beyond linear response, h quenches the entropy contributions both from the residual moment and the localized Majorana zero modes [17].

Flux transition.—Given that NRG calculations are performed in each flux sector, the global ground state is determined by comparing NRG ground-state energies. The energy difference ΔE between the impurity-flux and flux-free sectors is shown in Fig. 5(a). We conclude that, at zero field, a first-order quantum phase transition occurs at $K_c \approx 0.35J$ between a flux-free unscreened LM phase and a partially screened SVac phase with impurity flux. A local field h drives multiple first-order transitions; for h along the $\langle 111 \rangle$ direction, flux binding can also occur for ferromagnetic K, Fig. 5(b).

Finally, we note that, for elevated temperatures, $T \gtrsim |\Delta E|$, the behavior is given by a thermal mixture of different flux sectors, as demonstrated for the plain Kitaev model in Ref. [30].

Finite impurity concentration.—The physics at small but finite defect concentration is a rich subject. Because of the absence of extended spin correlations in the Kitaev model, residual moments do not mutually interact [10]. Defect-induced magnetic order will, therefore, only emerge on taking into account bulk interactions beyond Kitaev [31–33]—this is beyond the scope of the present work. However, the flux binding is a robust feature: The disordered flux arrangement for substitutional $S = 0$ impurities (effectively realized for $K > K_c$) will strongly scatter matter Majoranas and dramatically decrease the magnetic low-T thermal conductivity; this does not apply to $S = 1$ impurities which do not bind fluxes.

Conclusions.—We have solved the Kondo problem for the gapless Kitaev model using NRG—this represents the first numerically exact solution for a quantum impurity coupled to a spin liquid. We have determined the phase diagram and characterized the RG fixed points in terms of localized Majorana zero modes. The case of an $S = 1$ substitutional spin is encompassed by our solution at large ferromagnetic K; it behaves like a free moment with Curie susceptibility. Our approach can be extended to Kitaev models on other lattices [34–37] and more complicated impurity problems. Experimental realizations using magnetic adatoms on layers of α-$RuCl_3$ [38] or related materials appear possible.

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