Breakdown of heavy quasiparticles in a honeycomb Kondo lattice: A quantum Monte Carlo study

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We show that for the half-filled Kondo lattice model on the honeycomb lattice a Kondo breakdown occurs at small Kondo couplings $J_k$ within the magnetically ordered phase. Our conclusions are based on auxiliary field quantum Monte Carlo simulations of the so-called composite fermion spectral function. Within a U(1) gauge theory formulation of the Kondo model, it becomes apparent that a Higgs mechanism dictates the weight of the resonance in the spectral function. For the honeycomb lattice we observe that for small $J_k$ the quasiparticle pole gives way to incoherent spectral weight but it remains well defined for the square lattice. Our result provides an explicit example where the magnetic transition and the breakdown of heavy quasiparticles are detached as observed in Yb(Rh$_{0.93}$CO$_{0.07}$)$_2$Si$_2$ [Friedemann et al., Nat. Phys. 5, 465 (2009)].

Strongly correlated many body systems are characterized by the emergence of new elementary excitations. This can occur through the fractionalization of the electron within a parton type construction – fractional quantum Hall effect [1] or Luttinger liquids [2] – or through the formation of a composite object. Examples of the latter range from the understanding of single-hole dynamics in quantum antiferromagnets [3, 4] to the emergence of the electron in $Z_2$ lattice gauge theories in which the electron is a bound state of an orthogonal fermion and $Z_2$ matter [5–7].

The Kondo effect is yet another example of the emergence of a composite fermion carrying the quantum numbers of the electron. Consider a spin-1/2 magnetic impurity embedded in Fermi liquid with finite density of states at the Fermi energy. In the presence of time reversal symmetry the Kondo coupling between the impurity and Fermi liquid is always relevant and leads to the emergence of a composite fermion. It consists of the spin-1/2 and conduction electrons and becomes itinerant thereby releasing the $\ln(2)$ entropy. If one replaces the metal by a Dirac liquid with vanishing density of states at the Fermi energy, the Kondo coupling is irrelevant and one will generically observe a transition from an unscreened to screened moment at finite value of the Kondo coupling [9, 10]. This transition corresponds to the breakdown of the aforementioned composite fermion [11, 12]. Such phenomena are not limited to the realm of impurity physics [13]. Neutron scattering experiments of metallic Yb$_2$Pt$_2$Pb [14] suggest a Kondo breakdown phase of a one-dimensional spin chain embedded in a three-dimensional metal. Furthermore, numerical evidence of this state of matter has been observed in models of spin chains on semimetals [15]. In dense systems such as in YbRh$_2$Si$_2$ [16–18] or CeCoIn$_5$ [19], the notion of Kondo breakdown or orbital Mott selective transitions [20] has deep implications since the composite fermions drop out from the Luttinger count. For systems with an odd number of localized spins per unit cell and no further spontaneous symmetry breaking, this implies a violation of the Luttinger sum rule. Owing to Oshikawa’s [21] work such a violation can be understood if the spin system shows topological degeneracy akin of a spin liquid [22, 23]. For an even number of spins per unit cell, such topological constraints do not hold. In this case, Kondo breakdown

\[ Z_k = \begin{cases} 0, & \langle S \rangle \neq 0, \langle b \rangle \neq 0, \langle S \rangle \neq 0, \langle b \rangle \neq 0, \langle S \rangle = 0 \end{cases} \]

FIG. 1. Ground-state phase diagram of the half-filled Kondo lattice model on the honeycomb and square lattices. On both lattices we observe a magnetic order-disorder transition denoted by a red circle and order parameter corresponding to $\langle S \rangle$. For the honeycomb lattice (a) we observe a breakdown of the heavy quasiparticle in the spin-density-wave (SDW) phase as indicated by the vanishing residue $Z_k^0$ of the pole at the $\Gamma$ point in the composite fermion Green’s function. For the square lattice (b) we observe only the order-disorder transition since, down to our lowest value $J_k/W = 0.025$, $Z_k^0$ at the $M = (\pi, \pi)$ point remains finite. All the values of $Z_k^0$ are extrapolated to the thermodynamic limit [8]. We use the mean-field notation, $\langle b \rangle$, to track the magnitude of the residue.
does not imply a violation of Luttinger’s theorem.

Since the tight binding model on the honeycomb lattice provides a realization of Dirac electrons, one may ask the question if and how the aforementioned Kondo breakdown transition in the impurity limit [9, 10] is carried over to the dense case described by the half-filled Kondo lattice model. In Ref. [24] it is argued that the Kondo coupling is marginal in the weak coupling limit thereby opening the possibility of Kondo breakdown transitions in magnetically ordered metallic states. The central result of this Letter is summarized in Fig. 1: Kondo breakdown proceeds to the dense case described by the half-filled Kondo lattice model. In Ref. [24] it is argued that the Kondo term $H_{\text{KLM}}$ on the honeycomb lattice. In contrast no breakdown is observed on the square lattice.

$U(1)$ gauge theory approach. Since the Kondo effect and concomitant emergence of the composite fermion is not related to spontaneous symmetry breaking, some care has to be taken in defining the onset of these phenomena. They become particularly transparent within a $U(1)$ gauge theory approach to the Kondo lattice model [25–27]. The Kondo lattice model (KLM) on the honeycomb lattice reads:

$$
\hat{H}_{\text{KLM}} = \sum_{i,j} T_{i,j} \hat{c}_i^\dagger \hat{c}_j + \frac{J_k}{2} \sum_i \hat{c}_i^\dagger \sigma \cdot \hat{S}_i, \quad (1)
$$

where $\hat{c}_i^\dagger = (\hat{c}_{i,\uparrow}^\dagger, \hat{c}_{i,\downarrow}^\dagger)$ is a spinor where $\hat{c}_{i,\sigma}^\dagger$ creates an electron in Wannier state centered around lattice site $i$ and $z$ component of spin $\sigma = \uparrow, \downarrow$. $J_k$ is the Kondo exchange coupling between conduction electrons and spins s=1/2, $\hat{S}_i$, with $\sigma$ being a vector of Pauli spin matrices. The matrix $T_{i,j}$ accounts for nearest neighbor hopping with amplitude $-t$. We adopt an Abrikosov representation of the spin operator, $\hat{S}_i = \frac{1}{2} f_i^\dagger \sigma f_i$ with $\hat{f}_i = (\hat{f}_{i,\uparrow}, \hat{f}_{i,\downarrow})$ and constraint $\hat{f}_i^\dagger \hat{f}_i = 1$. To proceed we use the following rewriting of the Kondo term $-\frac{4k}{\pi} (\hat{V}_i^\dagger \hat{V}_i + \hat{V}_i \hat{V}_i^\dagger)$ with $\hat{V}_i^\dagger = \hat{c}_i^\dagger f_i$. In the constrained Hilbert space, this rewriting is exact. To formulate the path integral, we will work in an unconstrained Hilbert space and impose it energetically with a Hubbard-U term: $H_U = U \sum_i (f_i^\dagger f_i - 1)^2$. Importantly the fermion parity on the $f$-orbitals is a constant of motion such that it is very efficient to implement in numerical simulations. We can decouple the Kondo (Hubbard) term with a complex (real) field, $b_i(\tau), a_{0,i}(\tau)$ to obtain the following action in terms of Grassmann variables $\hat{f}_i(\tau)$ and $\hat{c}_i(\tau)$

$$
S = S_0 + \int_0^\beta d\tau \left\{ \sum_i \left[ \frac{\partial^2}{\partial \tau} \right] b_i(\tau)^2 + i a_{0,i}(\tau) + f_i^\dagger(\tau) \left[ \partial_\tau - i a_{0,i}(\tau) \right] f_i(\tau) + b_i(\tau) \hat{c}_i^\dagger f_i + \bar{b}_i(\tau) f_i^\dagger \hat{c}_i \right\} \quad (2)
$$

with $S_0 = \int_0^\beta d\tau \sum_{i,j} \hat{c}_i^\dagger(\tau) \left[ \partial_\tau \delta_{i,j} + T_{i,j} \right] \hat{c}_j(\tau)$. The above corresponds to the action in the limit $U \to \infty$ where local $U(1)$ gauge invariance is apparent. In particular the canonical transformation, $\hat{f}_i(\tau) \to f_i(\tau) e^{i \chi_i(\tau)}$ amounts to redefining the fields $a_{0,i}(\tau) \to a_{0,i}(\tau) + \partial_\tau \chi_i(\tau)$ and $b_i(\tau) \to b_i(\tau) e^{-i \chi_i(\tau)}$, such that the partition function remains invariant. We are now in a position to probe for various phases with gauge invariant quantities. Magnetism, triggered by the RKKY interaction, corresponds to a spontaneous global SU(2) spin symmetry breaking and long ranged correlations of the order parameter $\hat{\delta}_i = \frac{1}{2} f_i^\dagger \sigma f_i$. Clearly $\hat{\delta}_i$ carries no U(1) charge. To define the Kondo effect we consider the fermion field

$$
\tilde{\hat{f}}_i(\tau) = e^{i \varphi_i(\tau)} \hat{f}_i(\tau), \quad \text{with} \quad e^{i \varphi_i(\tau)} = \frac{b_i(\tau)}{\bar{b}_i(\tau)} \quad (3)
$$

As argued in the Supplemental Material [8], $\tilde{\hat{f}}_i(\tau)$ has the quantum numbers of a physical fermion: it carries no gauge charge, has an electron charge $e$, and spin 1/2. The Kondo effect corresponds to the emergence of this fermion at low energies as signaled by a pole (resonance) in the dense case (single impurity limit) in the corresponding spectral function [28, 29]. There is no symmetry that imposes $\langle \tilde{\hat{f}}_i(\tau) \tilde{\hat{f}}_j(\tau) \rangle$ to vanish between two space-time points and the pole in the corresponding spectral function reflects this fact. Furthermore, if the ground state turns out to be a Fermi liquid, the Luttinger volume will have to account for the composite fermion.

The above can be understood in terms of a Higgs [30] mechanism in which the phase fluctuations of $\varphi_i(\tau)$ become very slow such that $\varphi_i(\tau)$ can be set to a constant. In this case there is no distinction between $\tilde{\hat{f}}_i(\tau)$ and $\hat{f}_i(\tau)$ or, in other words, $\tilde{\hat{f}}_i(\tau)$ has lost its gauge charge and has acquired a unit electric charge. This Higgs mechanism is captured in mean-field large-$N$ approaches of the Kondo lattice where Kondo screening corresponds to $\langle b_i(\tau) \rangle \neq 0$ [31, 32].

The above definition of the fermion field, $\tilde{\hat{f}}$, depends explicitly on the gauge field that is not accessible in generic numerical simulations (e.g. exact diagonalization). However, reintroducing amplitude fluctuations of the $b$-field, we have $\tilde{\hat{f}}_i \propto b_i(\tau) f_i(\tau) \propto \left[ f_i^\dagger(\tau) c_i(\tau) \right] f_i(\tau)$. As shown in Ref. [33] and in the large-$N$ limit, the right hand side of the latter equation is nothing but the composite fermion field:

$$
\tilde{\hat{f}}_i \propto \psi_i = S_i \cdot \sigma c_i. \quad (4)
$$
We also note that $\langle b_i b_i^\dagger \rangle \propto \langle \bar{V}_i^\dagger \bar{V}_i \rangle \propto (\hat{c}_i^\dagger \hat{\sigma}_i \cdot \hat{S}_i)$ such that the local spin correlations between the conduction electrons and impurity spins correspond to the modulus of the boson field. If this quantity remains finite in the considered parameter regime, we will conclude that an adequate gauge field independent representation of the local spin correlations between the conduction electrons and impurity spins correspond to the modulus of the boson field.

FIG. 2. Composite fermion spectral function $A_\psi(k, \omega)$ along the $\Gamma$-$K$-$M$-$\Gamma$ path in momentum space with $\Gamma = (0,0)$, $K = (4\pi, 0)$, and $M = (\pi, \frac{\pi}{3})$ on the $L = 18$ honeycomb KLM for representative values of $J_b/W$ corresponding to: (a) Kondo; (b) and (c) Kondo+SDW, and (d) SDW phases.

FIG. 3. (a) Composite fermion Green’s function $G_\psi(k = \Gamma, \tau)$ at $J_b/W = 0.067$, and (b)-(d) the corresponding spectral function $A_\psi(k, \omega)$ on the honeycomb KLM with different sizes $L$.

Upon crossing over to the magnetically ordered phase, see Figs. 2(b) and 2(c), while some incoherent spectral weight sets in at high energies. In contrast, the spectrum in Fig. 2(d) with $J_b/W = 0.067$ deep inside the magnetic phase, looks different: the composite fermion bands have disappeared indicative of the breakdown of Kondo screening. If Kondo screening is not present in the magnetically ordered phase, one can adopt a large-$S$ approximation. In leading order in $S$, the spectral function $A_\psi(k, \omega)$ will follow the conduction electron spectral function $A_c(k, \omega)$, i.e., $A_\psi(k, \omega) \approx S^2 A_c(k, \omega)$ [33]. A comparison of $A_\psi(k, \omega)$ in Fig. 2(d) with the corresponding spectrum $A_c(k, \omega)$ included in Ref. [8], confirms this expectation and allows one to recognize in $A_\psi(k, \omega)$ a pronounced image of the conduction electron band consistent with the large-$S$ limit.

In order to get further insight into the observed re-arrangement of spectral weight in $A_\psi(k, \omega)$, we plot in Fig. 3(a) raw data of $G_\psi(k, \tau)$ at the $\Gamma$ point at our smallest Kondo coupling $J_b/W = 0.067$ for different system sizes $L$. Generically, the existence of long lived quasiparticles requires that the Green’s function displays a free particle behavior at long imaginary times,

$$G(k, \tau) \approx \frac{1}{2\pi} \int_0^\infty d\omega \frac{Z_k \omega e^{-\Delta_{qp}(\omega)\tau}}{\omega^2 + \Delta_{qp}(\omega)^2},$$

where $Z_k$ is the quasiparticle residue of the doped hole at momentum $k$ and frequency $\omega = -\Delta_{qp}$. As is apparent, the $L = 6$ data quickly converge to the exponential decay, which as shown in Fig. 3(b), deceptively generates a low energy pole, and consequently a well defined composite fermion band, in the corresponding spectral function $A_\psi(k, \omega)$. On the other hand, upon increasing system size it becomes more difficult to track the exponential form of $G_\psi(k = \Gamma, \tau)$ whose long time tail systematically flattens. As a consequence, while a faint signature of the composite fermion band can still be spotted in $A_\psi(k, \omega)$ for $L = 9$, see Fig. 3(c), the band has essentially disappeared from the $L = 12$
spectrum in Fig. 3(d). At the same time, the overall spectrum around the Γ point broadens substantially and may plausibly be thought of as a continuum that stems from decay of the composite quasiparticle. Thus, the data are suggestive of the absence of Kondo screening in the thermodynamic limit.

It is striking to compare the results in Fig. 3 with those on the square lattice obtained at even smaller value of \( J_0/W = 0.025 \), see Fig. 4. Irrespective of the system size \( L \), the composite fermion Green’s function \( G_\psi(k, \tau) \) at the \( M = (\pi, \pi) \) point shows the same asymptotic behavior in the long time limit which implies the continued existence of the pole in the corresponding spectrum \( A_\psi(k, \omega) \), see Figs. 4(b)-4(d). As can be seen, \( A_\psi(k, \omega) \) shares aspects of both the large-\( N \) approach (flat composite fermion bands) and large-\( S \) limit, i.e., the image of the conduction electron band shifted by the antiferromagnetic wavevector \( Q = (\pi, \pi) \). Taken together, these spectral features imply coexistence of coherent Kondo screening and long range magnetic order.

To substantiate the vanishing of the composite fermion band as a function of \( J_0/W \), we extract the quasiparticle residue \( Z^\psi_k \) at the Γ point by fitting the long time tail of \( G_\psi(k = \Gamma, \tau) \) to the exponential form followed by the finite-size scaling analysis [8]. For comparison, we have equally analyzed the asymptotic behavior of \( G_\psi(k, \tau) \) at the \( M \) point on the square lattice and constructed the respective phase diagrams compiled in Fig. 1.

Since increasing \( J_0 \) promotes the Kondo effect, it ultimately drives the magnetic order-disorder transition that occurs at \( J_0/W \approx 0.223 \) (honeycomb) and \( J_0/W \approx 0.181 \) (square) [43–45]. Thus, the strong coupling region in Fig. 1 is lattice independent and hosts a Kondo screened phase. In contrast, a weak coupling part of the phase diagram turns out to be non-generic: While pinning down the precise scaling of \( Z^\psi_k \) at the Γ point on the honeycomb lattice is a challenge, our data show that it is a monotonically decreasing function of \( J_0/W \) and vanishes slightly below \( J_0/W = 0.1 \). The vanishing quasiparticle residue indicates that composite quasiparticles lose their integrity. We interpret this as the destruction of Kondo screening. This is in stark contrast to the square lattice where composite fermions are found down to our smallest value \( J_0/W = 0.025 \) as signaled by a finite quasiparticle residue \( Z^\psi_k \) at the M point.

We also track the location and the size of the quasiparticle gap. Given that at large \( J_0/W \) the quasiparticle gap is located at the Γ point while the noninteracting model features gapless Dirac excitations at the K point, one shall resolve a change in the position of the minimal gap as a function of \( J_0/W \). The data in Fig. 5(a) extracted from the long time behavior of \( G_\psi(k, \tau) \) at the both \( k \) points confirm this expectation. As is apparent, the change takes place on the magnetically ordered side of \( J_0^c \) but far away from Kondo breakdown. Further, the comparison of Figs. 5(a) and 5(c), the latter showing the evolution of the quasiparticle gap at the M point on the square lattice, reveals two common features: (i) the development of the cusp preceding the magnetic order-disorder transition, and (ii) a linear in \( J_0/W \) scaling of the gap in the weak coupling limit. It is a direct consequence of the Fermi surface nesting-driven magnetic order and can be captured within a mean-field SDW framework [46, 47].

Finally, as shown in Fig. 5(b) we do not resolve any signs of the breakdown of Kondo screening in the local spin-spin correlation function \( S^{ij} = \frac{1}{2N} \sum_i \langle \hat{S}_i^j \sigma \hat{S}_{i+1}^j \rangle \).
\( \hat{S}_i \) which remains finite down to our lowest value of \( J_b/W \), just like that measured on the square lattice, see Fig. 5(d). This seemingly counterintuitive result becomes clear by noting that \( S^{\text{cf}} \) measures the amplitude of the boson field, \( |b|^2 \). Hence, Fig. 5(b) implies that the modulus of the boson field remains constant for all values of the Kondo coupling and that Kondo breakdown occurs due to phase fluctuations. The latter explains the failure of the mean-field approaches to provide consistent results for both lattices [8].

**Summary and conclusions.** We have investigated a Kondo breakdown defined by the destruction of the composite fermion in Eq. (3). In the realm of the Kondo lattice considered here, this amounts to the loss of a pole in the composite fermion Green’s function. Our main result, is that Kondo breakdown occurs in the magnetic phase of the half-filled KLM on the honeycomb lattice. This stands in stark contrast to our results on the square lattice where down to the lowest values of the Kondo coupling, we observe no breakdown of the composite fermion.

Our results show that the magnetic transition and Kondo breakdown are detached as observed in Yb(\( \text{Rh}_{0.93}\text{Co}_{0.07})_2\text{Si}_2 \) [48]. The observed Kondo breakdown corresponds to a modification of the excitation spectra, and does not necessarily translate into a thermodynamic transition. This stands in agreement with the Fradkin-Shenker phase diagram where confined and Higgs phases are adiabatically connected. It would be of great interest to modify the KLM so as to allow for a deconfined phase and probe the full richness of the Fradkin-Shenker phase diagram as suggested in Ref. [27]. On the experimental side, we hope that our results will have an impact on the studies aimed at exploring quantum impurity problems in graphene in a dense situation [49–51].

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Supplemental Material for:
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AUXILIARY FIELD QMC AND U(1) GAUGE THEORY OF THE KONDO LATTICE MODEL

To at best understand the phases of the Kondo lattice model,

$$\hat{H}_{KLM} = \sum_{i,j} T_{i,j} \hat{c}_i^\dagger \hat{c}_j + \frac{J_k}{2} \sum_i \hat{c}_i^\dagger \sigma \cdot \hat{S}_i,$$  \hspace{1cm} (S1)

where $\hat{c}_i^\dagger = \left( \hat{c}_{i,\uparrow}^\dagger, \hat{c}_{i,\downarrow}^\dagger \right)$ is a Wannier-state spinor, we adopt an Abrikosov representation of the spin operator, $\hat{S}_i = \frac{i}{2} \hat{f}_i^\dagger \sigma \cdot \hat{f}_i$ with $\hat{f}_i^\dagger = \left( \hat{f}_{i,\uparrow}^\dagger, \hat{f}_{i,\downarrow}^\dagger \right)$ and constraint $\hat{f}_i^\dagger \hat{f}_i = 1$. In the constrained Hilbert space, the identity:

$$\frac{J_k}{4} \hat{c}_i^\dagger \sigma \cdot \hat{S}_i = - \frac{J_k}{4} \left( \hat{v}_i^\dagger \hat{v}_i + \hat{\bar{v}}_i^\dagger \hat{\bar{v}}_i \right)$$  \hspace{1cm} (S2)

with $\hat{v}_i^\dagger = \hat{c}_i^\dagger \hat{f}_i$ holds. To proceed we relax the constraint and consider the Hamiltonian

$$\hat{H}_{KLM} = \lim_{U \to \infty} \left\{ \sum_{i,j} T_{i,j} \hat{c}_i^\dagger \hat{c}_j - \frac{J_k}{8} \sum_i \left[ \left( \hat{v}_i^\dagger + \hat{\bar{v}}_i \right)^2 + \left[ i \hat{v}_i^\dagger - i \hat{\bar{v}}_i \right]^2 \right] + \frac{U}{2} \sum_i \left( \hat{f}_i^\dagger \hat{f}_i - 1 \right)^2 \right\}.$$  \hspace{1cm} (S3)

Since the Hubbard term commutes with the Hamiltonian, the projection onto the physical Hilbert space occurs at a rate set by $\left\langle \left( \hat{f}_i^\dagger \hat{f}_i - 1 \right)^2 \right\rangle \propto e^{-\beta U/2}$, where $\beta$ corresponds to the inverse temperature. Using the Trotter decomposition, and Hubbard Stratonovich transformation to decouple the perfect square terms we obtain the following form for the grand-canonical partition function [53]:

$$Z = \text{Tr} e^{-\beta \hat{H}_{KLM}} \propto \int D \left\{ \hat{f}_i^\dagger(\tau), \hat{f}_i(\tau), c_i^\dagger(\tau), c_i(\tau), b_i(\tau), a_{0,i}(\tau) \right\} e^{-S}$$  \hspace{1cm} (S4)

with

$$S = \int_0^\beta d\tau \left\{ \sum_i \left[ \frac{N}{J_k} |b_i(\tau)|^2 + \frac{N}{U} |a_{0,i}(\tau)|^2 + \frac{i N}{2} a_{0,i}(\tau) \right] + \frac{N}{2} a_{0,i}(\tau) \right\} e^{\hat{i} \sum_{i,j} [\partial_\tau - i \alpha_{0,i}(\tau)] \hat{f}_i^\dagger(\tau) \hat{f}_i(\tau) + b_i(\tau) c_i^\dagger(\tau) c_i(\tau) + \bar{b}_i(\tau) \hat{f}_i^\dagger(\tau) \hat{f}_i(\tau)}$$

$$+ \sum_{i,j} \left[ c_i^\dagger(\tau) \partial_\tau \delta_{i,j} + T_{i,j} \right] c_j(\tau) \right\}.$$  \hspace{1cm} (S5)

In the above, $a_{0,i}(\tau)$ is a real field used to impose the constraint, $b_i(\tau)$ a complex field for the Kondo term, and $c_i^\dagger$ as well as $\hat{f}_i^\dagger$ are spinors of Grassmann variables. We have also taken the liberty of enhancing the spin index from $N = 2$ to a general $N$ with constraint $\hat{f}_i^\dagger \hat{f}_i = N/2$ [45, 54]. The above action is the starting point for auxiliary field QMC simulations [37] as well as for the classification of phases. For the QMC simulations we use the Gauss-Hermite quadrature to replace continuous fields by discrete ones. The integration over the Grassmann variables yields the fermion determinant, that for particle-hole symmetric conduction electrons and even values of $N$ is positive semi-definite. The integration over the Hubbard-Stratonovich fields is then carried out with Monte Carlo importance sampling. For details of the implementation, we refer the reader to Ref. [37]. In particular for the calculation presented here, we have used the implementation of the Kondo lattice model of the ALF-2.0 library.

The constraint leads to a U(1) local gauge invariance. In particular, and only in the $U \to \infty$ limit, the canonical transformation

$$\hat{f}_i(\tau) \rightarrow \hat{f}_i(\tau) e^{i \chi_i(\tau)}$$  \hspace{1cm} (S6)

amounts to redefining the fields

$$a_{0,i}(\tau) \rightarrow a_{0,i}(\tau) + \partial_\tau \chi_i(\tau) \quad \text{and} \quad b_i(\tau) \rightarrow b_i(\tau) e^{-i \chi_i(\tau)}$$  \hspace{1cm} (S7)

in the action.
PHASES OF THE KONDO LATTICE MODEL

The above action allows us to define precisely the two phases of the Kondo lattice model that are of importance to us in the present article. The spin-density-wave (SDW) phase is characterized by long ranged order in

\[ \langle \frac{1}{2} f_i^\dagger \sigma f_i - \frac{1}{2} f_j^\dagger \sigma f_j \rangle \] (S8)

and is hence characterized by a non-vanishing vacuum expectation value of \( \langle \frac{1}{2} f_i^\dagger \sigma f_i \rangle \) in the thermodynamic limit characteristic of spontaneous symmetry breaking of the global SU(2) spin symmetry. Note that the above expectation value is taken with respect to the action of Eq. (S5).

The Kondo phase is more subtle to define since it is not characterized by a broken symmetry. Let \( b_i(\tau) = |b_i(\tau)| e^{i\varphi_i(\tau)} \) and

\[ \hat{f}_i(\tau) = e^{i\varphi_i(\tau)} f_i(\tau). \] (S9)

\( \hat{f}_i \) is a physical fermion operator. As mentioned above, under a local U(1) gauge transformation, \( f_i \to f_i e^{i\chi_i(\tau)}, \varphi_i(\tau) \to \varphi_i(\tau) - \chi_i(\tau) \) such that \( \hat{f}_i \) remains invariant. It hence carries no gauge charge. \( \hat{f}_i \) carries electric charge. Consider the global U(1) charge transformation, \( \hat{T}(\alpha) = e^{i\alpha} \Sigma_i \hat{c}_i. \) Since \( \hat{T}(\alpha) \) is a conserved quantity, and the physical electron transforms as \( \hat{T}(\alpha)^{-1} \hat{c}_i \hat{T}(\alpha) = e^{i\alpha} \hat{c}_i \), the phase \( \varphi_i(\tau) \) transforms as \( \varphi_i(\tau) \to \varphi_i(\tau) + \alpha \). Hence \( \hat{f}_i \) transforms as the electron: \( \hat{f}_i \to \hat{f}_i e^{i\alpha} \). In the heavy fermion phase, the electron operator \( \hat{f}_i \) emerges as a new particle excitation that acquires coherence. This is what is meant in colloquial terms by the spins delocalize and participate in the Luttinger volume.

Since in the heavy fermions phase \( \hat{f}_i \) is the emergent quasiparticle, it is natural to write the action for this degree of freedom. From Eq. (S5) and in the limit \( U \to \infty \), one readily obtains:

\[
S = \int_0^\beta d\tau \left\{ \sum_i \left[ \frac{N}{T_h} |b_i(\tau)|^2 + i \frac{N}{2} a_{0,i}(\tau) + \hat{f}_i^\dagger(\tau) \left[ \partial_\tau - i a_{0,i}(\tau) - i \partial_\tau \varphi_i(\tau) \right] \hat{f}_i(\tau) + |b_i(\tau)| \left( c_i^\dagger \hat{f}_i + \hat{f}_i^\dagger c_i \right) \right] \\
+ \sum_{i,j} c_i^\dagger(\tau) \left[ \partial_\tau \delta_{i,j} + T_{i,j} \right] c_j(\tau) \right\}. \] (S10)

Importantly, \( \hat{f}_i(\tau) \) does not possess a local U(1) gauge charge such that \( \langle \hat{f}_i^\dagger(\tau) \hat{f}_j(\tau') \rangle \) does not vanish by symmetry for \( (i, \tau) \neq (j, \tau') \). In contrast, owing to the local U(1) symmetry, \( \langle \hat{f}_i^\dagger(\tau) \hat{f}_j(\tau') \rangle = 0 \) if \( (i, \tau) \neq (j, \tau') \).

Since in the Kondo phase \( \hat{f}_i \) is the emergent low lying quasiparticle, we expect the phase \( \varphi_i(\tau) \) to vary slowly in time. This freezing out of the dynamics of the gauge field corresponds to the Higgs mechanism. Here \( \varphi \) drops out from the action and the relevant theory is that of interacting \( c \) and \( f \) electrons which is very reminiscent of the physics of the periodic Anderson model. This formalizes the accepted notion that the Kondo lattice model shares the very same physics as the periodic Anderson model in the local moment regime. If the ground state turns out to be a Fermi liquid, then Luttinger theorem should apply and both electron species should be included in the Luttinger count. In the Higgs phase, \( \varphi \), is stuck in a gauge choice, say \( \varphi = 0 \). Hence there is no distinction between the \( \hat{f}_i(\tau) \) and \( f_i(\tau) \). In other words, the Abrikosov fermion looses its gauge charge and acquires an physical electric one. In this sense we have for the Kondo phase

\[ \langle b_i(\tau) \rangle \propto \langle f_i^\dagger(\tau) c_i(\tau) \rangle \neq 0. \] (S11)

Let us note that in any exact evaluation of the partition function — as carried out in our Monte Carlo simulations — \( \langle f_i^\dagger(\tau) c_i(\tau) \rangle \) vanishes identically. However, the measurement of \( \langle e^{-i\varphi_i(\tau)} f_i^\dagger(\tau) c_i(\tau) \rangle \) is finite and captures the hybridization matrix element characteristic of large-N mean-field theories.

We now argue that, at least in the large-N limit, \( \hat{f}_i \) corresponds to the composite fermion operator. Including amplitude fluctuations we have:

\[ \hat{f}_i \propto b_i(\tau) f_i(\tau) \propto \left[ f_i^\dagger(\tau) c_i(\tau) \right] f_i(\tau). \] (S12)

The above is precisely the form of the composite fermion operator, considered in this article, in the large-N limit [33].

We are now in a position to define precisely the relevant phases of the KLM that we encounter in this article. They are summarized in Table I.
Phases \( \langle f^\dagger \sigma f_i \rangle \langle b_i(\tau) \rangle \)

| Phases           | SDW | Kondo | Kondo+SDW |
|------------------|-----|-------|-----------|
|                  | ✓   | ×     | ✓ ✓        |

TABLE I. SDW, Kondo and Kondo+SDW phases of the Kondo lattice model. ✓ (×) refers to a non-vanishing (vanishing) value of the order parameter.

SUPPLEMENTAL QMC RESULTS

QMC setup

The approach relies on the U(1) gauge formulation of the KLM described above. The integration over the Grassmann variables yields the fermion determinant. For the particle-hole symmetric conduction band, one will readily show, that it is positive semi-definite \([55, 56]\). To formulate the algorithm, we discretize the imaginary time and choose \( \Delta \tau_t = 0 \) on the honeycomb (square) lattice and use the Gauss-Hermite quadrature to discretize the fields.

We have used a projective version of the QMC algorithm based on the imaginary time evolution of a trial wave function \( |\Psi_T\rangle \), with \( \langle \Psi_T|\Psi_0\rangle \neq 0 \), to the ground state \( |\Psi_0\rangle \):

\[
\frac{\langle \Psi_0|\hat{O}|\Psi_0\rangle}{\langle \Psi_0|\Psi_0\rangle} = \lim_{\Theta \to \infty} \frac{\langle \Psi_T|e^{-\Theta \hat{H}}\hat{O}e^{-\Theta \hat{H}}|\Psi_T\rangle}{\langle \Psi_T|e^{-2\Theta \hat{H}}|\Psi_T\rangle}. \tag{S13}
\]

Since the energy scale of the RKKY interaction scales as \( J_k^2 \), convergence to the magnetically ordered ground state in the weak coupling requires adequately increased projection parameters, i.e., \( \Theta t = 40 \) at \( J_k/t = 0.8 \) and \( \Theta t = 160 \) at \( J_k/t = 0.4 \) on the honeycomb lattice. On the other hand, on the square lattice \( \Theta t = 80 \) was found to be already sufficient down to \( J_k/t = 0.2 \).

For the analytical continuation, we have made use of the stochastic Maximum Entropy method \([57]\) implemented in the ALF-library.

Magnetic order-disorder transition

In order to determine the precise location of the magnetic order-disorder transition, we calculate the spin structure factor for the \( f \) spins

\[
S^f(k) = \frac{4}{L^2} \sum_{\delta=A,B} \sum_r e^{ik \cdot r} \langle \hat{S}_\delta(r) \cdot \hat{S}_\delta \rangle, \tag{S14}
\]

from which we construct the renormalization group invariant correlation ratio

\[
R_f = 1 - \frac{S^f(Q + \delta k)}{S^f(Q)}, \tag{S15}
\]

where \( Q = (0,0) \) is the ordering wavevector and \( \delta k \) is the smallest wavevector on the \( L \times L \) honeycomb lattice. As can be seen in Fig. S1, \( R_f \) scales to unity (zero) for ordered (disordered) states and shows a crossing point as a function of system size at the critical point \( J_k^c \). Given that the charge degrees of freedom are gapped across the transition, we expect that it belongs to the universality class of the 3D classical Heisenberg (O(3)) model. Indeed, assuming the correlation length exponent \( 1/\nu = 1.40511(6) \) \([58]\) of the latter and using the scaling assumption

\[
R_f = f[(J_k/J_k^c - 1) L^{1/\nu}], \tag{S16}
\]
FIG. S1. Correlation ratio $R_f$ defined in Eq. (S15) as a function of $J_k/W$. Left inset shows the scaling collapse of $R_f$ for $L \geq 12$ assuming the critical exponent $1/\nu = 1.40511(6)$ of the 3D classical Heisenberg (O(3)) model [58]. Right inset shows the staggered magnetic moment $m_{\alpha = \{c,f\}}$ in the thermodynamic limit.

we obtain for $L \geq 12$ a good quality data collapse of $R_f$ shown in the left inset of Fig. S1. It allows us to estimate $J^c_k/W = 0.2227(3)$.

As shown in Fig. S2, we have equally performed finite-size scaling of both $S^f(Q)$ and the spin structure factor for the conduction electron spins

$$S^c(Q) = \frac{1}{L^2} \sum_{\delta=A,B} \sum_r e^{iQ \cdot r} \langle \hat{c}^\dagger_{\delta}(r) \sigma \hat{c}_{\delta}(r) \cdot \hat{c}^\dagger_{\delta}(r) \sigma \hat{c}_{\delta}(r) \rangle.$$  \hspace{1cm} (S17)

We have used linear [Fig. S2(a)] and second-order [Fig. S2(b)] polynomial forms in $1/L$. The resultant orbital $\alpha = \{c,f\}$ resolved staggered magnetic moments

$$m_{\alpha} = \sqrt{\lim_{L \to \infty} \frac{S^\alpha(Q)}{2L^2}}$$  \hspace{1cm} (S18)

both scale continuously to zero at $J^c_k/W = 0.223(1)$ (see the right inset of Fig. S1) which matches perfectly the previously extracted critical point $J^c_k/W = 0.2227(3)$. We note that the good agreement between the extrapolation with an analytical form in $1/L$ and the data collapse based on the correlation ratio $R_f$ can be ascribed to the very small anomalous dimension of 3D O(3) criticality.

FIG. S2. Finite-size extrapolation of the antiferromagnetic spin structure factor at $Q = (0,0)$ on the honeycomb KLM for the (a) $f$- and (b) $c$-electrons on approaching the magnetic order-disorder transition point; solid lines are linear and second-order polynomial fits to the QMC data.
Conduction electron spectral function

Figure S3 plots the conduction electron spectral function, \( A_c(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} \, G_c^{\text{ret}}(\mathbf{k}, \omega) \), where

\[
G_c^{\text{ret}}(\mathbf{k}, \omega) = -i \int_0^\infty dt e^{i\omega t} \sum_\sigma \langle \{ \hat{c}_{\mathbf{k},\sigma}(t), \hat{c}_{\mathbf{k},\sigma}^\dagger(0) \} \rangle \tag{S19}
\]

from the stochastic analytical continuation of the QMC data generated on the \( L = 18 \) honeycomb KLM.

In the region of the phase diagram with active Kondo screening, the composite fermion and conduction electron operators share the same quantum numbers. Thus their single particle spectral functions shall have identical supports both revealing the low energy composite fermion bands. However, the corresponding quasiparticle poles of the conduction electron Green’s function carry much less spectral weight such that \( A_c(\mathbf{k}, \omega) \) exhibits relatively faint bands, see Figs. S3(a) and S3(b). Moreover, since the quasiparticle residue in the small \( J_k/W \) limit tracks the Kondo scale \( Z_k \approx e^{-W/J_k} \), resolving composite quasiparticles in Fig. S3(c) requires a logarithmic scale as the spectral weight is nearly fully exhausted by two bands separated by a small gap at the Dirac point \( K \) but otherwise closely reminiscent of the tight binding band structure of the honeycomb lattice.

![Figure S3](image)

FIG. S3. Same as in Fig. 2 in the main text but for the conduction electrons.

Quasiparticle residue \( Z_k^{\psi} \) and single particle gap \( \Delta_{qp}(\mathbf{k}) \)

The behavior of the imaginary time composite fermion Green’s function \( G_{\psi}(\mathbf{k}, \tau) \) at large times, \( G(\mathbf{k}, \tau) \overset{\tau \to \infty}{\to} Z_K e^{-\Delta_{qp}(\mathbf{k})\tau} \), allows one to extract the quasiparticle residue \( Z_K^{\psi} \) and the corresponding single particle gap \( \Delta_{qp}(\mathbf{k}) \) without the need of analytical continuation. Figure S4 shows the finite-size scaling analysis of the resultant QMC data which led us to the \( J_k/W \)-dependence of the quasiparticle residue \( Z_k^{\psi} \) and the corresponding single particle gap \( \Delta_{qp}(\mathbf{k}) \) at the \( \Gamma \) and Dirac \( K \) points (honeycomb lattice) as well as at the \( M \) point (square lattice) presented in the main text.

Figure S5(a) illustrates the behavior of the composite fermion spectral function \( A_{\psi}(\mathbf{k}, \omega) \) at the \( \Gamma \) and Dirac \( K \) points for different values of Kondo coupling \( J_k/W \). The corresponding density of states \( A_{\psi}(\omega) = \frac{1}{T} \sum_k A_{\psi}(\mathbf{k}, \omega) \) is shown in Fig. S5(b).

As can be seen, in the Kondo insulating phase at \( J_k/W = 0.233 \), coherent Kondo screening results in a well-defined peak at the \( \Gamma \) momentum which determines the minimal gap. The latter is also seen in \( A_{\psi}(\omega) \) since the flat band of composite fermion quasiparticles generates a sharp peak that flanks the gap. The low energy part of \( A_{\psi}(\mathbf{k}, \omega) \) evolves smoothly across the magnetic order-disorder transition at \( J_k/W = 0.2227(3) \) with a gradual shift of the minimal gap from the \( \Gamma \) point to the Dirac \( K \) point. As is apparent, the change in the position of the minimal gap takes place away from \( J_k^c \). Assuming a rigid band shift, the switch of Fermi wavevector in the metallic state at small dopings would lead to a change in the Fermi surface topology (Lifshitz transition). Note however that this change in topology of the Fermi surface is unrelated to the breakdown of Kondo screening \([59]\).
FIG. S4. Finite-size extrapolation of the quasiparticle residue \( Z^\psi_k \) (top) and the corresponding single particle gap \( \Delta_{qp}(k) \) (bottom) extracted from the imaginary-time composite fermion Green’s function \( G_\psi(k,\tau) \) at the (a,b) \( \Gamma = (0,0) \) and (c,d) Dirac \( K = (\frac{\sqrt{3}}{2}a,0) \) points on the honeycomb KLM and at the (e,f) \( M = (\pi,\pi) \) point on the square KLM. Solid lines are linear in \( 1/L \) fits to the QMC data.

FIG. S5. (a) Composite fermion spectral function \( A_\psi(k,\omega) \) at the \( \Gamma \) and Dirac \( K \) points and (b) the corresponding density of states \( A_\psi(\omega) = \frac{1}{2\pi} \sum_k A_\psi(k,\omega) \) with decreasing (from bottom to top) Kondo coupling \( J_k \) obtained on the \( L = 18 \) honeycomb KLM.

As long as the magnetic order and low energy composite fermion band coexist (Kondo+SDW phase), one can track the signature of the quasiparticle band in \( A_\psi(\omega) \). This should be contrasted with the SDW phase where in the absence of Kondo screening, signaled by a broad featureless spectrum at the \( \Gamma \) point, an appropriate approach is the large-\( S \) picture. It accounts for the observed rearrangement of \( A_\psi(\omega) \) such that a dominant contribution occurs at \( \omega/W \simeq 1/6 \). It reflects the van Hove singularity in the conduction electron density of states.

**Local spin-spin correlation function \( S^{cf} \)**

Figure S6 shows finite-size scaling of the local spin-spin correlation function

\[
S^{cf} = \frac{2}{3N} \sum_i \langle \hat{c}_i^\dagger \sigma \hat{c}_i \cdot \hat{S}_i \rangle
\]  

which led us to the \( J_k/W \)-dependence of this quantity presented in the main text.
In this section, we review mean-field approximations in the aim of providing an account of our results. We will see that both the large-\(N\) as well as the bond fermion mean-field approximations fail at providing consistent results for the square and honeycomb lattices.

In the large-\(N\) mean-field approximation we neglect the fluctuations of the boson field \(b_i(\tau)\) and take into account the constraint on average. The field \(b_i(\tau)\) possesses phase as well as amplitude fluctuations. Phase fluctuations will not be taken into account at the mean-field level and the only manner in which Kondo breakdown can occur is through the vanishing of the amplitude of the boson field. This actually stands at odds with our QMC data that suggest that the amplitude of the field remains constant for all values of the Kondo coupling and that Kondo breakdown occurs due to phase fluctuations. In the single impurity limit, or equivalently in the absence of magnetic ordering, this approach does capture the differences between the honeycomb and square lattices, see Fig. S7. However, when magnetic ordering, alongside Kondo screening is included, the approximation yields Kondo breakdown in the magnetic phase for both the honeycomb (see Fig. S8 and also Ref. [46]) and square [44, 47] lattices.

An approximation that captures the coexistence of Kondo screening and magnetism on the square lattice, is the bond fermion mean-field approximation [60, 61]. In this strong coupling approach, the Kondo effect is accounted for by a vacuum expectation value of the singlet correlator, \(\langle \hat{S}^\dagger_i \hat{S}_i \rangle = \frac{1}{\sqrt{2}} \left( \hat{c}_{i,\uparrow}^\dagger \hat{f}_{\uparrow,i}^\dagger \hat{c}_{i,\downarrow}^\dagger \hat{f}_{\downarrow,i}^\dagger \right)\). Since \(\langle |b_i|^2 \rangle \propto \langle \hat{V}_i \hat{V}_i^\dagger \rangle \propto \langle \frac{1}{2} \hat{b}_i^\dagger \hat{b}_i \rangle \), a non-vanishing vacuum expectation value of \(\hat{S}^\dagger_i \hat{S}_i\), \(s\), corresponds to the Kondo effect. By virtue of completeness, we have included this approximation in subsection , and the reader will convince oneself that only solutions with a finite value of \(s\) will occur, see Fig. S9. As such this approximation invariably predicts coexistence of magnetism and the Kondo effect, for both the square and honeycomb lattices. This again stands at odds with our QMC results of the main text.

**Large-\(N\) mean-field approach**

The Kondo lattice Hamiltonian given in Eq. (S1) in terms of the fermionic representation of spin operator \(\hat{S}_i = \frac{1}{2} \sum_{\sigma,\sigma'} \hat{f}_{\sigma,i}^\dagger \hat{f}_{\sigma,i} + \hat{f}_{\sigma,i} \hat{f}_{\sigma,i}^\dagger\) with the constraint \(\hat{f}_{\uparrow,i}^\dagger \hat{f}_{\downarrow,i}^\dagger + \hat{f}_{\downarrow,i} \hat{f}_{\uparrow,i} = 1\) can be written as,

\[
\hat{H} = \sum_{k,\sigma} c_k \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\sigma} + \frac{J_k}{4} \sum_i \left( \hat{f}_{\uparrow,i}^\dagger \hat{c}_{i,\downarrow} + \hat{c}_{i,\downarrow}^\dagger \hat{f}_{\uparrow,i} + \hat{f}_{\downarrow,i}^\dagger \hat{c}_{i,\uparrow} + \hat{c}_{i,\uparrow}^\dagger \hat{f}_{\downarrow,i} \right)^2 - \frac{J}{4} \sum_i \left[ \left( \hat{f}_{\uparrow,i}^\dagger \hat{f}_{\downarrow,i} + \hat{f}_{\downarrow,i}^\dagger \hat{f}_{\uparrow,i} \right)^2 + \left( \hat{f}_{\uparrow,i}^\dagger \hat{c}_{i,\downarrow} + \hat{c}_{i,\downarrow}^\dagger \hat{f}_{\uparrow,i} \right)^2 \right].
\]  

(S21)

In the large-\(N\) approach we allow for Kondo screening as well as antiferromagnetic ordering with the following mean-field decouplings,

\[
(\hat{f}_{\uparrow,i}^\dagger \hat{f}_{\downarrow,i}^\dagger - \hat{f}_{\downarrow,i}^\dagger \hat{f}_{\uparrow,i}^\dagger) = m_f e^{iQ \cdot \hat{r}_i}, \quad (\hat{c}_{i,\uparrow}^\dagger \hat{c}_{i,\downarrow} + \hat{c}_{i,\downarrow}^\dagger \hat{c}_{i,\uparrow}) = -m_c e^{iQ \cdot \hat{r}_i}, \quad (\hat{f}_{\uparrow,i}^\dagger \hat{f}_{\downarrow,i}^\dagger + \hat{f}_{\downarrow,i}^\dagger \hat{f}_{\uparrow,i}^\dagger) = (\hat{f}_{\uparrow,i}^\dagger \hat{c}_{i,\downarrow} + \hat{c}_{i,\downarrow}^\dagger \hat{f}_{\uparrow,i}^\dagger) = V.
\]  

(S22)

Here, \(m_f\) denotes the staggered magnetization on localized spins, \(m_c\) denotes the staggered magnetization of conduction electrons, \(V\) denotes the hybridization parameter between \(\hat{c}\) and \(\hat{f}\) electrons and \(Q\) is the antiferromagnetic ordering wavevector.
For a honeycomb KLM the mean-field Hamiltonian in the momentum space can be written as follows,

$$\hat{H}_{mf} = \sum_{k, \sigma} \phi_{k, \sigma}^\dagger \begin{pmatrix} \frac{J_{mf} \sigma}{4} & Z(k) & -\frac{J_V}{2} & 0 \\ Z(k) & -\frac{J_{mf} \sigma}{4} & 0 & -\frac{J_V}{2} \\ -\frac{J_V}{2} & 0 & -\frac{J_{mc} \sigma}{4} & 0 \\ 0 & -\frac{J_V}{2} & 0 & \frac{J_{mc} \sigma}{4} \end{pmatrix} \phi_{k, \sigma} + e_0 N_u. \quad (S23)$$

Here, \( \phi_{k, \sigma}^\dagger = \{ \phi_{k, a, \sigma}^\dagger, \phi_{k, b, \sigma}^\dagger, \phi_{k, \sigma}^\dagger \} \), \( e_0 = \left( \frac{J_V^2}{2} + \frac{J_{mc} m_c}{4} \right) \), \( Z(k) = -t \left( 1 + e^{-ik \cdot a_2} + e^{-ik \cdot (a_2 - a_1)} \right) \) with \( a_1 = (1, 0) \) and \( a_2 = \left( \frac{1}{2}, \frac{\sqrt{3}}{2} \right) \) and \( N_u \) is the number of unit cells.

Diagonalization of the mean-field Hamiltonian gives the following dispersion relations,

$$E_{k, n} = \pm \frac{1}{4} \sqrt{P_k + \frac{1}{2} \sqrt{Q_k - 4R_k}} \quad (S24)$$

with,

$$P_k = 8 |Z(k)|^2 + \left( m_c^2 J_f^2 \right) / 2 + \left( m_f^2 J_f^2 \right) / 2 + 4 J_f^2 V^2,$$

$$Q_k = \left( -16 |Z(k)|^2 - m_c^2 J_f^2 - m_f^2 J_f^2 - 8 J_f^2 V^2 \right)^2,$$

$$R_k = \left( 16 m_c^4 |Z(k)|^2 J_f^2 + m_c^2 m_f^2 J_f^4 + 8 m_c m_f J_f^2 V^2 + 16 J_f^4 V^4 \right).$$

The ground state energy per unit cell can be computed as,

$$e_g = e_0 + \frac{2}{N_u} \sum_{k, n, E_{k, n} < 0} E_{k, n}. \quad (S25)$$

The self consistent equations of mean-field parameters can obtained from the saddle point approximation,

$$\frac{de_g}{dV} = 0, \quad \frac{de_g}{dm_f} = 0, \quad \frac{de_g}{dm_c} = 0. \quad (S26)$$

FIG. S7. Hybridization parameter \( V \) as a function of \( J_k / W \) in the absence of magnetic order computed within the large-\( N \) mean-field approach. (a) For a square KLM. (b) For a honeycomb KLM.

Figures S7(a) and S7(b) plot the hybridization order parameter as a function of \( J_k / W \) on the square and honeycomb lattices in the absence of magnetic order. Figure S8 was obtained by taking into account both Kondo screening and magnetic order and plots the mean-field order parameters \( m_f, m_c, \) and \( V \) as a function of \( J_k / W \) for the honeycomb KLM.
FIG. S8. Mean-field order parameters as a function of $J_k/W$ for the honeycomb KLM within the large-$N$ mean-field approach.

Bond fermion mean-field theory

To formulate the bond fermion mean-field theory we consider the states:

$$\hat{s}^\dagger_i |0\rangle = \frac{1}{\sqrt{2}} \left( \hat{c}^\dagger_{i,\uparrow} \hat{f}^\dagger_{i,\downarrow} - \hat{c}^\dagger_{i,\downarrow} \hat{f}^\dagger_{i,\uparrow} \right) |0\rangle$$

$$\hat{f}^\dagger_{i,\sigma} |0\rangle = \frac{1}{\sqrt{2}} \left( \hat{c}^\dagger_{i,\sigma} \hat{f}^\dagger_{i,\sigma} + \hat{c}^\dagger_{i,\sigma} \hat{f}^\dagger_{i,\sigma} \right) |0\rangle$$

$$\hat{d}^\dagger_{i,\sigma} |0\rangle = \hat{c}^\dagger_{i,\sigma} \hat{f}^\dagger_{i,\sigma} |0\rangle$$

(S27)

Here, $\hat{s}^\dagger$ and $\hat{f}^\dagger_{i,1,0,-1}$ denote a singlet and three triplet states with one conduction electron per site and $\hat{h}^\dagger$ and $\hat{d}^\dagger$ denote holons and doublons of the conduction electrons. In this representation, the constraint

$$\hat{s}^\dagger_i \hat{s}_i + \sum_{m=1,0,-1} \hat{f}^\dagger_{i,m} \hat{f}_i,m + \sum_{\sigma=\uparrow,\downarrow} (\hat{h}^\dagger_{i,\sigma} \hat{h}_{i,\sigma} + \hat{d}^\dagger_{i,\sigma} \hat{d}_{i,\sigma}) = 1$$

(S28)

suppresses the unphysical states.

The conduction electron operator and the spin operators on $\hat{f}$ and $\hat{c}$ electrons in the above representation take the following forms,

$$\hat{c}^\dagger_{i,\sigma} = \frac{\sigma}{\sqrt{2}} (\hat{s}^\dagger_i + \sigma \hat{t}^\dagger_{i,0}) \hat{h}_{i,-\sigma} + \hat{t}^\dagger_{i,\sigma} \hat{h}_{i,-\sigma} - \frac{\hat{d}^\dagger_{i,\sigma}}{\sqrt{2}} (\hat{s}_i - \sigma \hat{t}_{i,0}) + \sigma \hat{d}^\dagger_{i,-\sigma} \hat{t}_{i,-\sigma}$$

(S29)

$$\hat{S}_{i,\alpha} = \frac{1}{2} (\hat{t}^\dagger_{i,\alpha} \hat{s}_i + \hat{t}^\dagger_{i,\alpha} \hat{s}_i - i \epsilon_{\alpha\beta\gamma} \hat{t}^\dagger_{i,\beta} \hat{f}_{i,\gamma}) + \hat{h}_i \hat{h}_{i,\alpha} + \hat{d}^\dagger_{i,\alpha} \hat{d}_{i,\alpha}$$

(S30)

$$\hat{S}_{i,\alpha}^\dagger = \frac{1}{2} (- \hat{t}^\dagger_{i,\alpha} \hat{s}_i - i \epsilon_{\alpha\beta\gamma} \hat{t}^\dagger_{i,\beta} \hat{f}_{i,\gamma})$$

(S31)

where $\epsilon_{\alpha\beta\gamma}$ is the totally antisymmetric tensor, the holon and doublon spin operators read $\hat{S}_{i,\alpha}^h = \frac{1}{2} \sum_{\sigma,\sigma'} \hat{h}^\dagger_{i,\sigma} \hat{h}_{i,\sigma'}$ and $\hat{S}_{i,\alpha}^d = \frac{1}{2} \sum_{\sigma,\sigma'} \hat{d}^\dagger_{i,\sigma} \hat{d}_{i,\sigma'}$ and the triplon operators are defined as follows,

$$\hat{t}^\dagger_{i,z} |0\rangle = \hat{t}^\dagger_{i,0} |0\rangle, \quad \hat{t}^\dagger_{i,x} |0\rangle = \frac{1}{\sqrt{2}} \left( \hat{t}^\dagger_{i,1} + \hat{t}^\dagger_{i,-1} \right) |0\rangle, \quad \hat{t}^\dagger_{i,y} |0\rangle = - \frac{i}{\sqrt{2}} \left( \hat{t}^\dagger_{i,1} - \hat{t}^\dagger_{i,-1} \right) |0\rangle.$$  

(S32)

In the bond fermion mean-field approach to the KLM, the Kondo phase corresponds to condensation of singlets $\langle \hat{s} \rangle$ and the SDW phase corresponds to condensation of $z$ component of triplets $\langle \hat{t}_{i,z} \rangle$ in the singlet background. Hence, we consider the following mean-field approximation [60]:
where $\phi$ is a function of both the transverse and longitudinal spin fluctuations.

Using the saddle point approximation, the mean-field Hamiltonian in momentum space can be written as follows:

$$
\hat{H}_{mf} = \epsilon_0 N_u + \mu \sum_{\mathbf{k},\mathbf{\sigma}} \left( \hat{h}_{\mathbf{k},\mathbf{\sigma}} \hat{\phi}_{\mathbf{k},\mathbf{\sigma}} + \hat{\phi}_{\mathbf{k},\mathbf{\sigma}} \right) + \frac{1}{2} \left( s^2 - m^2 \right) \sum_{\mathbf{k},\mathbf{\sigma}} \left( \hat{h}_{\mathbf{k},\mathbf{\sigma}}^a \hat{\phi}_{\mathbf{k},\mathbf{\sigma}}^a + \hat{\phi}_{\mathbf{k},\mathbf{\sigma}}^a \hat{h}_{\mathbf{k},\mathbf{\sigma}}^a + H.c \right) + \frac{1}{2} (s + m)^2 \sum_{\mathbf{k},\mathbf{\sigma}} \left( \hat{h}_{\mathbf{k},\mathbf{\sigma}}^b \hat{\phi}_{\mathbf{k},\mathbf{\sigma}}^b + \hat{\phi}_{\mathbf{k},\mathbf{\sigma}}^b \hat{h}_{\mathbf{k},\mathbf{\sigma}}^b + H.c \right)
$$

Here, $\epsilon_0 = \left( -\frac{3\alpha}{2} s^2 + \frac{3\alpha}{4} m^2 + \mu(s^2 + m^2 + 1) \right)$ and $N_u$ is the number of unit cells. We use the global Lagrange multiplier $\mu_i = \mu$ to impose the constraint $\mu(s^2 + m^2 - 1)$. Note that in the above we have ignored all the terms corresponding to the transverse and longitudinal spin fluctuations.

The mean-field Hamiltonian in momentum space can be written as follows,

$$
\hat{H}_{mf} = \epsilon_0 N_u + \sum_{\mathbf{k},\mathbf{\sigma}} \phi_{\mathbf{k},\mathbf{\sigma}}^* M(\mathbf{k}) \phi_{\mathbf{k},\mathbf{\sigma}}
$$

where $\phi_{\mathbf{k},\mathbf{\sigma}} = \{ \hat{h}_{\mathbf{k},\mathbf{\sigma}}^a, \hat{h}_{\mathbf{k},\mathbf{\sigma}}^b, \hat{\phi}_{\mathbf{k},\mathbf{\sigma}}^a, \hat{\phi}_{\mathbf{k},\mathbf{\sigma}}^b \}$ and the matrix $M(\mathbf{k})$

$$
M(\mathbf{k}) = \\
\begin{pmatrix}
\mu & \alpha_k & 0 & 0 & 0 & 0 & 0 & \beta_k \\
\alpha_k^* & \mu & 0 & 0 & 0 & 0 & \gamma_k & 0 \\
0 & 0 & \mu & \alpha_k & 0 & -\gamma_k & 0 & 0 \\
0 & 0 & \alpha_k^* & \mu & -\beta_k & 0 & 0 & 0 \\
0 & 0 & 0 & -\beta_k & \mu & \alpha_k & 0 & 0 \\
0 & 0 & -\gamma_k & 0 & \alpha_k & -\mu & 0 & 0 \\
0 & 0 & 0 & 0 & -\mu & \alpha_k^* & 0 & 0 \\
\beta_k^* & 0 & 0 & 0 & 0 & \alpha_k & -\mu & 0
\end{pmatrix}
$$

with

$$
\alpha_k = -\frac{1}{2} (s^2 - m^2) Z(\mathbf{k}), \quad \beta_k = -\frac{1}{2} (s + m)^2 Z(\mathbf{k}), \quad \gamma_k = -\frac{1}{2} (s - m)^2 Z(\mathbf{k}), \quad Z(\mathbf{k}) = -t(1 + e^{-i k \cdot a_2} + e^{-i k \cdot (a_2 - a_1)}).
$$

The matrix $M(\mathbf{k})$ can be diagonalized via unitary transformation which gives the following dispersion relations for $z$ component of spin $\sigma = \uparrow (\downarrow)$,

$$
E_{k,n} = \pm \sqrt{\frac{1}{2} (m^2 + s^2)^2 |Z(\mathbf{k})|^2 + \mu^2 + 2 \sqrt{\frac{1}{4} |Z(\mathbf{k})|^4 (m^2 - s^2)^2 + \frac{1}{16} |Z(\mathbf{k})|^4 (m^2 + s^2)^4}}.
$$

The mean-field ground state energy per unit cell can be computed as follows,

$$
e_g = \epsilon_0 + \frac{2}{N_u} \sum_{\mathbf{k},n,E_{k,n}<0} E_{k,n}.
$$

Next, using the saddle point approximation,

$$
\frac{de_g}{ds} = 0, \quad \frac{de_g}{d\mu} = 0, \quad \frac{de_g}{dm} = 0
$$
we obtain the following self consistent equations for mean-field parameters $\mu$, $m^2$, and $s^2$,

$$\mu = \frac{J_k}{4} - \frac{1}{2N_u} \sum_{k} |Z(k)|^2 (m^2 + s^2) \left( \frac{1}{E_{k,1}} + \frac{1}{E_{k,2}} \right) - \frac{1}{4N_u} \sum_{k} |Z(k)|^4 (m^2 + s^2)^3 \left( \frac{1}{E_{k,1}} - 1 + \frac{1}{E_{k,2}} \right)$$  (S40)

$$m^2 = \frac{1}{2N_u} \sum_{k} |Z(k)|^2 m^2 (s^2 - m^2) \left( \frac{1}{E_{k,1}} - 1 + \frac{1}{E_{k,2}} \right)$$  (S41)

$$s^2 = -1 - \frac{1}{N_u} \sum_{k} \mu \left( \frac{1}{E_{k,1}} + \frac{1}{E_{k,2}} \right) - \frac{1}{N_u} \sum_{k} |Z(k)|^2 (s^2 - m^2)^2 \mu \left( \frac{1}{E_{k,1}} - 1 + \frac{1}{E_{k,2}} \right)$$  (S42)

where $E_{k,1}$ and $E_{k,2}$ are the two lowest quasiparticle bands and $A_k$ has the following form,

$$A_k = \sqrt{\frac{1}{4} \mu^2 |Z(k)|^2 (m^2 - s^2)^2 + \frac{1}{16} |Z(k)|^4 (m^2 + s^2)^4}.$$

The magnetization of $c$ and $f$ electrons can be computed as follows,

$$m_c = \frac{2}{N_u} \sum_{i} (-1)^i \langle \hat{S}_{z,i}^c \rangle = 2ms$$  (S43)

$$m_f = \frac{2}{N_u} \sum_{i} (-1)^i \langle \hat{S}_{z,i}^f \rangle = 2ms + \frac{1}{N_u} \sum_{k} 2|Z(k)|^2 \mu ms (s^2 + m^2)$$  (S44)

Figure S9 plots the mean-field order parameters obtained within the bond fermion mean-field approach as a function of $J_k/W$ for the honeycomb KLM.

![Graph showing mean-field order parameters as a function of $J_k/W$ for the honeycomb KLM within the bond fermion mean-field approach.](image)