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Global phase diagram of a spin-orbital Kondo impurity model and the suppression of Fermi-liquid scale

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Many correlated metallic materials are described by Landau Fermi-liquid theory at low energies, but for Hund metals the Fermi-liquid coherence scale $T_{\text{FL}}$ is found to be surprisingly small. In this Letter, we study the simplest impurity model relevant for Hund metals, the three-channel spin-orbital Kondo model, using the numerical renormalization group (NRG) method and compute its global phase diagram. In this framework, $T_{\text{FL}}$ becomes arbitrarily small close to two new quantum critical points (QCPs) which we identify by tuning the spin or spin-orbital Kondo couplings into the ferromagnetic regimes. We find quantum phase transitions to a singular Fermi-liquid or a novel non-Fermi-liquid phase. The new non-Fermi-liquid phase shows frustrated behavior involving alternating overscreenings in spin and orbital sectors, with universal power laws in the spin ($\omega^{-1/5}$), orbital ($\omega^{1/5}$) and spin-orbital ($\omega^1$) dynamical susceptibilities. These power laws, and the NRG eigenlevel spectra, can be fully understood using conformal field theory arguments, which also clarify the nature of the non-Fermi-liquid phase.

Introduction.—A very large number of correlated metallic materials, are “bad metals”, namely in a broad regimes of temperature $T$ characterized by deviations from the Landau Fermi-liquid (FL) $T^2$ law [1] and their values of resistivity exceeding the Mott-Ioffe-Regel limit [2]. One class of bad metals are the Hund metals, i.e. 3$d$ and 4$d$ multiorbital systems where correlations derive from the Hund’s coupling $J_H$ [3–7]. They include ruthenates [8–13], iron pnictides and chalcogenides [14–20]. The Landau FL quasiparticles emerge only below a coherence scale $T_{\text{FL}}$ which is much smaller than the natural energy scales of the problem, set by the electronic bandwidth. Why is $T_{\text{FL}}$ so small in units of the bandwidth? This “naturalness problem” is a central problem of condensed matter physics which has attracted considerable attention in the community. Its solution should also provide a clue as to what reference system should be used to describe the anomalous behavior observed in a broad energy regime above $T_{\text{FL}}$, when no other instabilities such as magnetism or superconductivity intervene.

Two different directions have been followed to address this puzzle. The first invokes the proximity to quantum critical points (QCPs) [21–23], signaling the transition to an ordered phase, or to an unconventional one such as fractionalized Mott insulators [24, 25]. An alternative starting point has been provided by the development of the combination of ab-initio electronic structure and dynamical mean field theory (LDA+DMFT) [26–29]. Here, the excitations of a solid are understood in terms of atomic multiplets embedded in an effective medium, and the evolution of the electronic structure from atomic multiplet excitations into quasiparticles arises naturally as temperature is lowered. This approach has provided quantitative predictions in many materials of interest [3, 19, 28, 30–36], where the ab-initio LDA+DMFT calculations are in surprisingly good agreement with experiments. However, the solution of the LDA+DMFT equations is a complex problem, which generically yields a non-zero FL scale. Hence no connection with the ideas of QCPs was made. The question of how to reduce the FL scale to exactly zero and how to characterize the ensuing anomalous behavior above $T_{\text{FL}}$ has remained open.

In this Letter, we provide an answer to this question by computing a global phase diagram of the simplest three-channel spin-orbital Kondo model which captures the essential physics of Hund metals, using the exact numerical renormalization group (NRG) method [37]. By tuning the spin or spin-orbital Kondo couplings into the ferromagnetic regimes, we push $T_{\text{FL}}$ to be exactly zero and identify QCPs. We find quantum phase transitions to a singular-Fermi-liquid (SFL) phase and to a novel non-Fermi-liquid (NFL) phase showing frustrated behavior of alternating overscreenings in spin and orbital sectors, with universal power laws in dynamical susceptibilities. We use conformal field theory (CFT) arguments [38–43] to identify the nature of the NFL phase, analytically reproduce the NRG eigenlevel spectra and explain the power laws. Our global phase diagram provides a clear picture for understanding the suppression of coherence in Hund metals in terms of proximity to QCPs.

Model and Methods.—We study the three-channel spin-orbital Kondo (3soK) model derived from a realistic Anderson impurity model in [20, 44] for the studies of Hund metals. $H_{\text{bath}} = \sum_{p \sigma} \varepsilon_p \psi^\dagger_{p \sigma} \psi_{p \sigma}$ describes a symmetric, flat-band bath with half-bandwidth $D = 1$, where $\psi^\dagger_{p \sigma}$ creates an electron with momentum $p$ and...
spin $\sigma$ in orbital $m \in \{1, 2, 3\}$. The bath couples to the impurity spin $S$ and orbital isospin $T$ via

$$H_{\text{int}} = J_0 S \cdot J_{\text{sp}} + K_0 T \cdot J_{\text{orb}} + I_0 S \cdot J_{\text{sp-orb}} \cdot T.$$  

(1)

Here $S$ are SU(2) generators in the $S = 1$ representation, normalized as $\text{Tr}(S^a S^b) = \frac{1}{2} \delta_{a,b}$, and $T$ are SU(3) generators in the $3$, i.e. $\text{(01)}$ representation [45] (orbital angular momentum takes $L = 1$ in this representation), and $\text{Tr}(T^a T^b) = \frac{1}{2} \delta_{a,b}$, $J_{\text{sp}}$, $J_{\text{orb}}$ and $J_{\text{sp-orb}}$ are the bath spin, orbital and spin-orbital densities at the impurity site, with $J_{\text{sp}}^\dagger = \psi^\dagger_m \frac{1}{2} \sigma^a \sigma \psi_m \sigma$, $J_{\text{orb}}^\dagger = \psi^\dagger_m \frac{1}{2} \tau^a_m \psi_m \sigma$, $J_{\text{sp-orb}}^\dagger = \frac{1}{2} \psi^\dagger_m \sigma^a \sigma^b \psi_m \sigma$ (summation over repeated indices is implied) and normalized $\psi^\dagger_m = \frac{1}{\sqrt{N}} \sum_p \psi^\dagger_p \sigma_p$.

Here $\delta$ are Pauli [Gell-Mann] matrices, with normalization $\text{Tr}(\sigma^a \sigma^b) = 2 \delta_{a,b}$ [Tr($\tau^a \tau^b$) = $2 \delta_{a,b}$]. $J_0$, $K_0$ and $I_0$ are bare spin, orbital and spin-orbital Kondo exchange couplings, and we treat them as independent parameters with positive and negative values describing antiferromagnetic (AFM) and ferromagnetic (FM) couplings, respectively. We take $K_0 = 0.3$ throughout.

We use the full-density-matrix NRG [46] method to solve this model, exploiting its full $U(1)_{\text{ch}} \times SU(2)_{\text{sp}} \times SU(3)_{\text{orb}}$ symmetry using QSpace [45]. Symmetry labels $Q \equiv [q, S, (\lambda_1, \lambda_2)]$ are used to label multiplets, where $q$ is the bath particle number relative to half-filling of the bath (we choose $q_{\text{imp}} = 0$ because the impurity site has no charge dynamics), $S$ is the total spin, and $(\lambda_1, \lambda_2)$ labels a SU(3) representation described by a Young diagram with $\lambda_1 + \lambda_2$ boxes in its first (second) row. The impurity multiplet has $Q_{\text{imp}} = [0, 1, (01)]$. The bath is discretized logarithmically and mapped to a semi-infinite "Wilson chain" with exponentially decaying hoppings, and the impurity coupled to chain site $k = 0$. The chain is diagonalized iteratively while discarding high-energy states, thereby zooming in on low-energy properties: the finite-size level spacing of a chain ending at site $k \geq 0$ is of order $\omega_k \propto \Lambda^{-k/2}$. Here $\Lambda > 1$ is a discretization parameter, chosen to be 4 in this work. The RG flow can be visualized by combining the rescaled low-lying NRG eigenvalue spectra, $E = (E - E_{\text{ref}})/\omega_k$ vs. $\omega_k$, with increasing even or odd $k$. The imaginary part of the impurity dynamical susceptibilities $\chi^\text{imp}_{\lambda, \lambda'}$ and $\chi^\text{imp}_{\lambda', \lambda}$ were calculated at temperature $T = 10^{-16}$. Computational details are presented in the Supplemental Material [47].

**Fixed points.**—The calculated global phase diagram as a function of $J_0$ and $I_0$ is shown in Fig. 1(a). We first describe the low-energy fixed points found in the phase diagram. Throughout the entire regions where all three Kondo couplings are AFM, and for part of regions where $J_0$ or $I_0$ takes FM values (orange region), the system flows to a low-energy FL fixed point. This is seen in the NRG flow diagram and dynamical impurity susceptibilities $\chi^\text{imp}$ at $J_0 = I_0 = 0.01$ in Figs. 2(a,d). The ground state is a spin and orbital singlet, with impurity entropy $S^\text{imp} = \ln 1$ (orange curve in Fig. 1(d)). For small $\omega$, all
When $I_0$ takes strong FM and $J_0$ strong AFM couplings (pink region), we find a novel NFL fixed point, showing very interesting frustrated behavior of alternating overscreenings in spin and orbital sectors. Figure 3 analyzes the transition from FL to NFL at $J_0 = 0.3$. Figs. 3(c,f) and 4(c,f) show the NRG flow and $\chi^{\text{imp}}$ towards the NFL fixed point. The two lowest multiplets with either orbital singlet, $[+1, \frac{1}{2}, (00)]$, or spin singlet, $[0, 0, (01)]$, are very close in energy. The dynamical susceptibilities follow perfect and universal power laws for the spin ($\omega^{-1/5}$), orbital ($\omega^{1/5}$) and spin-orbital ($\omega^{1/2}$) operators. The impurity entropy $S_{\text{imp}}$ evaluates to $\ln \frac{1 + \sqrt{5}}{2}$ [pink curve in Fig. 1(d)]. This value can be obtained from Eq.(6) in [51] for a general SU($N$)$_K$ Kondo model ($K$ is the number of channels) with $N = 3, K = 2, Q = 2$ indicating SU(3)$_2$ orbital overscreening, or with $N = 2, K = 3, Q = 1$ indicating SU(2)$_3$ spin overscreening. Motivated by this, we follow the recently developed SU(2)$_2 \times$SU(3)$_3$ CFT approach [43] to identify the nature of this fixed point. Its NRG eigenstate spectra $Q'=[q', S', (\lambda'_1 \lambda'_2)]$ can be reproduced by applying either a SU(2)$_3$ fusion procedure in the spin sector or a SU(3)$_2$ fusion procedure in the orbital sector, i.e. fusing a spectrum of free fermion $Q=[q, S, (\lambda_1 \lambda_2)]$, with an effective impurity multiplet labeling either $Q_{\text{imp}}^{\text{eff}}=[+1, \frac{1}{2}, (00)]$, or $Q_{\text{imp}}^{\text{eff}}=[0, 0, (01)]$. Double fusion of the spectrum $Q'$ with the conjugate representation of the impurity multiplet, $Q_{\text{imp}}^{\text{eff}}=[-1, \frac{1}{2}, (00)]$, or $Q_{\text{imp}}^{\text{eff}}=[0, 0, (10)]$, yields the quantum numbers $Q''=[q'', S'', (\lambda''_1 \lambda''_2)]$ to characterize the CFT boundary operators, with scaling dimensions $\Delta$, determining the behavior of dynamical susceptibilities.

Tables S1–S2 in the Supplemental Material [47] show the CFT results of the fixed point spectra and compare them with the NRG spectra at $J_0 = 0.3, I_0 = -0.01$. Both fusion procedures yield the same results, which reproduce the NRG spectra very well. The scaling dimension of the leading boundary operator in the spin, orbital and spin-orbital sectors are found to be
\(\Delta_{\text{sp}} = \frac{2}{3}, \Delta_{\text{orb}} = \frac{3}{2}\) and \(\Delta_{\text{sp-orb}} = 1\), respectively. They are also consistent with the CFT results in [51] for either a spin SU(2)\(_3\)-Kondo model \((\Delta_{\text{sp}} = \frac{2}{\sqrt{3}}, \Delta_{\text{orb}} = \frac{3}{2+\sqrt{2}})\), or an orbital SU(3)\(_2\)-Kondo model \((\Delta_{\text{sp}} = \frac{2}{3+\sqrt{2}}, \Delta_{\text{orb}} = \frac{3}{2+\sqrt{2}})\). The power laws of dynamical susceptibilities can then be understood by the CFT procedure [43] \(\chi_{\text{imp}}^{\text{sp}} \sim \omega^{2\Delta_{\text{sp}}-1} = \omega^{-1/5}\), \(\chi_{\text{imp}}^{\text{orb}} \sim \omega^{2\Delta_{\text{orb}}-1} = \omega^{1/5}\) and \(\chi_{\text{sp-orb}}^{\text{imp}} \sim \omega^{2\Delta_{\text{sp-orb}}-1} = \omega^1\), respectively.

The impurity entropy and the CFT analysis both suggest that the spin SU(2)\(_3\) and orbital SU(3)\(_2\) Kondo models with overscreened fixed points are actually equivalent and complementary descriptions of this NFL fixed point. It indicates an alternating spin SU(2)\(_3\) and orbital SU(3)\(_2\) overscreening process by successively binding one electron or one hole, as illustrated by the cartoon picture at the bottom right of Fig. 1(a), similar in spirit to that of Nozières and Blandin [52]. To be specific, the strong AFM orbital coupling binds the bare impurity \(Q_{\text{imp}} = [0, 1, (01)]\) and one bath electron \([+1, \frac{1}{2}, (10)]\) into a fully screened orbital singlet with either spin \(\frac{3}{2}\) or \(\frac{1}{2}\): \([0, 1, (01)] \otimes [+1, \frac{1}{2}, (10)] \rightarrow [+1, \frac{1}{2}, (00)] \oplus [+1, \frac{1}{2}, (00)].\) In the FL phase, the spin \(\frac{1}{2}\) multiplet has the lower energy; it can then bind three holes to form a fully screened orbital singlet \([0, 0, (00)] \rightarrow [0, 0, (00)]\), with a very small energy difference. As functions of \(I_J\) and \(I_0\), \(J_0 - J_0^{(c)}\) and \(\mid 0 - I_0^{(c)}\), to approach exactly zero at the critical values \(J_0^c\) and \(I_0^c\), signalling the existence of QCPs [21, 22]. The exponents found are \(\alpha = 1.8\) in the FL-SFL transition, and \(\alpha = 1\) for FL-NFL. We show \(T_{\text{FL/SFL}}\) as functions of \(I_J\) at \(I_0 = 0.01\) in Fig. 1(b), and \(T_{\text{FL/NFL}}\) as functions of \(I_J\) at \(I_0 = 0.3\) in Fig. 1(c). More data are shown in Fig. S5 [47].

When approaching the QCP in the FL-SFL transition, as in Fig. 2 by decreasing \(I_J\), the spin-orbital separation window [7, 53] increases a lot, as seen in Figs. 2(b,e) for \(J_0 = -0.3643\), and a wide crossover regime, SFL', forms at intermediate energies. There the impurity entropy \(S_{\text{imp}}\) evaluates to \(\ln(1+\sqrt{2}) + \ln 3\) [green curve in Fig. 1(d)], corresponding to an orbital overscreened SU(3)\(_2\) fixed point, coupled to a fluctuating spin-1 moment. This is consistent with the recent findings in the region \(I_0 = 0\) and \(J_0 \rightarrow 0^+\) in [54]. \(\chi_{\text{imp}}\) follows a universal power-law of \(\omega^{1/5}\), showing similarity with the NFL phase due to the same orbital SU(3)\(_2\) overscreening, while \(\chi_{\text{orb}}\) follows an approximate power law (with some non-power-law corrections, see [47]). Across the phase transition, the multiplet \([+1, \frac{1}{2}, (00)]\) is pushed down to be the new ground state, while the original ground state \([-2, 0, (00)]\) of the FL phase is pushed up to very high energy.

When approaching the QCP in the FL-NFL transition as illustrated in Fig. 3, fine-tuning of \(I_J\) generates a large crossover regime NFL' at intermediate energies [Figs. 3(b,e)], where the set of low-lying states is simply the union of those of the FL and NFL spectra (see Table S4 in [47]). NFL' thus represents a “level-crossing” scenario [47, 55, 56], involving two orthogonal low-energy subspaces whose levels cross when \(I_J\) is tuned. When sufficiently close, both subspaces contribute to thermodynamic and dynamical properties. Here, the FL and NFL compete in the intermediate-energy regime, and \(I_J\) determines either FL [Fig. 3(a,d)] or NFL [Fig. 3(c,f)] to be the low-energy fixed point. The impurity entropy \(S_{\text{NFL}}^{\text{imp}}\) evaluates to \(\ln(c_{\text{NFL}}^{\text{imp}} + c_{\text{NFL}}^{\text{imp}}) = \ln(1+\sqrt{2})\) [red curve in Fig. 1(d)], not \(\ln 1+\ln 1+\sqrt{2}\), because the FL and NFL subspaces do not overlap. Hence the total effective impurity degrees of freedom is the sum of the contributions of those two sectors [47]. \(\chi_{\text{imp}}\) of NFL' follow the same power laws as NFL because the NFL part dominates in this regime. For more details on NFL', see [47].

The transition from SFL to NFL shown in Fig. 4 confirms the picture of alternating overscreenings. Tuning \(J_0\) to be more AFM, the state \([0, 0, (01)]\) is pushed down to be nearly degenerate with the ground state \([+1, \frac{1}{2}, (00)]\) [Fig. 4(b)], signalling the start of the alternating overscreening process. \(\chi_{\text{sp}}\) bends downward away from the \(\omega^{-1}\) behavior towards a \(\omega^{-1/5}\) dependence, while \(\chi_{\text{orb}}\) bends upward away from the \(\omega\)-linear behavior towards a \(\omega^{1/5}\) dependence, \(\chi_{\text{sp-orb}}\) still follows \(\omega^1\).

**Conclusion.—**To summarize, we have presented a global phase diagram of the 3soK model. This allows us to follow the suppression of the coherence scale in Hund
metals down to zero energy. The new NFL phase contains the essential ingredients needed to understand the actual incoherent behavior seen above $T_{FL}$. Recent advances in the physics of cold atoms might actually offer a concrete realization of the phase diagram of the model studied. Indeed it has been recently demonstrated that it is possible to simulate SU($N$) impurity models with tunable exchange interactions reaching both FM and AFM regimes [57, 58].

The iron pnictides display an intriguing QCP, as for example in Ba$_2$(As$_{1-x}$P$_x$)$_2$ [18, 59–61], where a divergent electron mass and concomitant destruction of the FL state was observed. This QCP has motivated several theoretical studies [62–64]. Further progress from the perspective of this work would require the DMFT self-consistency condition and more realistic band structures. In the DMFT treatment of a lattice model, the SFL and the NFL phases are expected to turn into magnetically ordered states, but the impurity model studied here with its power-law singularities would describe the behavior above $T_{FL}$.

The approach presented here, which takes into account the Hund’s coupling and the multiorbital nature, is in the same spirit as the ideas of local quantum criticality used to describe Kondo breakdown using impurity models [65], so it would then be also useful for unconventional quantum phase transitions observed in other heavy-fermion materials [66–69]. The global phase diagram of this $3\sigma$K model will also have potential impact on the studies of real multichannel spin and (or) orbital Kondo systems or quantum dots systems, for instance, generalize the studies in [70–74] to three-channel cases.

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[47] See Supplemental Material at [url] for: computational details, more NRG flow diagrams and dynamical susceptibilities in Sec. S-I, more data of $T_{FL}$, $T_{SFL}$ and $T_{NFL}$ as functions of $J_0$ and $I_0$ in Sec. S-II, CFT analysis in Sec. S-III, the detailed interpretation the “level-crossing” scenario and a proof of the impurity entropy $S_{imp}$ of NFL in Sec. S-IV, the impurity spectral functions $A_\gamma(\omega)$ in Sec. S-V, the coefficients of specific heat $\gamma(T)$ in Sec. S-VI, the impurity static susceptibilities for NFL and SFL phases in Sec. S-VII, the energy difference of multiplets $|+1, \frac{1}{2}, 0 \rangle$ and $|+1, \frac{3}{2}, 0 \rangle$ along the phase boundary in Sec. S-VIII, the justification of the 3soK model in Sec. S-IX, the dependence on the discretization parameter $\Lambda$ in Sec. S-X, and the irreducible representations of SU(3) in Sec. S-XI. The Supplemental Material includes Refs. [7, 43, 50, 51, 53, 55, 56, 75–79].

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