

From itinerant to local-moment antiferromagnetism in Kondo lattices: Adiabatic continuity versus quantum phase transitions

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Motivated by both experimental and theoretical activities, we discuss the fate of Kondo screening and possible quantum phase transitions in antiferromagnetically ordered phases of Kondo lattices. While transitions with topological changes of the Fermi surface may occur, we demonstrate that an entirely continuous evolution from itinerant to local-moment antiferromagnetism (i.e., from strong to negligible Kondo screening) is possible as well. This situation is in contrast to that in a nonsymmetry-broken situation where a quantum phase transition toward an exotic metallic spin-liquid state necessarily accompanies the disappearance of Kondo screening. We discuss criteria for the existence of topological transitions in the antiferromagnetic phase as well as implications for theoretical scenarios and for current experiments.

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I. INTRODUCTION

Quantum criticality in heavy-fermion metals is an active topic in current condensed-matter research. Much work has focused on the nature of the quantum phase transition (QPT) between a paramagnetic heavy Fermi liquid (FL) and an antiferromagnetic (AF) metal.^{1,2} Various experimental data appear to be inconsistent with the theoretical predictions for a spin-density wave (SDW) transition in a metal.^{3–5} This has prompted proposals about a different transition scenario where the Kondo effect breaks down at the antiferromagnetic quantum critical point (QCP). Then the heavy quasiparticles of FL, formed from conduction (c) and local-moment (f) electrons, disintegrate at the QCP.

Such a Kondo-breakdown transition involves degrees of freedom other than the antiferromagnetic fluctuations at the ordering wave vector \vec{Q} , and different theoretical descriptions have been proposed.^{6–8} Si *et al.*⁷ have employed an extension of dynamical mean-field theory (DMFT) to argue that magnetic fluctuations in two space dimensions render the Kondo effect critical at the AF QCP. In contrast, the scenario of Senthil *et al.*^{8–11} is centered around a Kondo-breakdown transition between two *paramagnetic* states: a heavy Fermi liquid with Kondo screening and a so-called fractionalized Fermi liquid (FL^{*}) without Kondo screening. In FL^{*}, frustration and/or strong quantum fluctuations preclude magnetic long-range order of the f moments, which instead form an exotic spin liquid,¹² decoupled from the conduction electrons. A sharp distinction between FL and FL^{*} is in the Fermi volume (assuming one f electron per unit cell in the paramagnet): FL has a “large” Fermi volume including the f electrons, whereas the Fermi volume of FL^{*} is “small,” i.e., only determined by the c electrons. Loosely speaking, the f electrons may be called “itinerant” in FL and “localized” in FL^{*}. In this scenario, antiferromagnetism may occur as a secondary instability of FL^{*} such that a conventional AF phase is reached via the Kondo-breakdown transition.^{10,11}

The possibility of having distinct quantum critical points between FL and AF raises the question whether distinct AF phases (i.e., with “itinerant” or “localized” f electrons) may be discriminated. Consider commensurate order with an even

number N of sites in the unit cell (other cases will be discussed briefly toward the end of the paper). Then, the size of the Brillouin zone (BZ) in the AF phase is reduced by a factor N compared to the paramagnetic phase and as a result “large” and “small” Fermi volume are no longer distinct. However, it has been proposed that the situations differ with respect to their Fermi-surface topology.^{9,13–15} Two phases, AF_L and AF_S, corresponding to itinerant and local-moment antiferromagnetism, respectively, have been introduced^{13,14} with the notion that they are separated by one or more quantum phase transitions. In this context, it has been suggested that in AF_S Kondo screening is absent.

In this paper, we argue that such a sharp distinction between AF_L and AF_S does not exist. To this end, we invoke continuity arguments between Kondo and weakly interacting electron models and demonstrate the possibility of a continuous Fermi-surface (FS) evolution between the situations of itinerant and local-moment antiferromagnetism. Kondo screening hence disappears smoothly in the AF phase: Technically, a line of renormalization-group fixed points emerges describing AF-polarized Fermi liquids. This finding does not contradict microscopic calculations,^{15,16} which find a topological Lifshitz transition inside the antiferromagnetic phase, but shows that such a transition is not connected to a breakdown of the Kondo effect. We also discuss conditions for the occurrence of FS-topology-changing transitions.

We note that many experimental criteria for Kondo screening, e.g., the existence of a maximum in the resistivity $\rho(T)$ at the coherence temperature, do not provide a sharp distinction between itinerant and local-moment AF. This means, e.g., that the maximum in $\rho(T)$ will be gradually washed out and disappear when tuning from itinerant to local-moment AF.

The remainder of this paper is organized as follows: In Sec. II we start by characterizing ground states of Kondo lattices, and we discuss the adiabatic continuity to phases of weakly interacting electrons. In Sec. III we give an explicit example for a continuous Fermi-surface evolution in a mean-field Kondo-lattice model smoothly connecting the situations of “itinerant” and “localized” f electrons in the presence of commensurate antiferromagnetism. We then reformulate our

findings in the languages of renormalization group (Sec. IV) and slave-particle theory coupled to gauge fields (Sec. V), establishing connections to earlier work. We close with remarks on recent theoretical and experimental results. The detailed discussion of band structures, of criteria for topological transitions, and of the interesting case of incommensurate magnetic order are relegated to the Appendixes A–D.

II. GENERAL CONSIDERATIONS

Consider a Kondo-lattice model in d spatial dimensions with a unit cell containing one c and f orbital each,

$$\mathcal{H}_{\text{KLM}} = \sum_{\vec{k}\sigma} (\epsilon_{\vec{k}} - \mu) c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} + J \sum_i \vec{S}_i \cdot \vec{s}_i, \quad (1)$$

where the chemical potential μ controls the filling n_c of the conduction (c) band with dispersion $\epsilon_{\vec{k}}$, and $\vec{s}_i = \sum_{\sigma\sigma'} c_{i\sigma}^\dagger \vec{\tau}_{\sigma\sigma'} c_{i\sigma} / 2$ is the conduction electron-spin density on site i . Sometimes it is useful to explicitly include a Heisenberg-type exchange interaction between the f electron local moments \vec{S}_i , $\mathcal{H}_I = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$, which may originate from superexchange [or Ruderman-Kittel-Kasuya-Yosida (RKKY)] interactions.¹⁷

A. Phases

If Kondo screening of the local moments \vec{S}_i dominates over intermoment interactions then a heavy FL results. The Fermi volume is “large,” i.e., includes the local-moment electrons, $\mathcal{V}_{\text{FL}} = K_d (n_{\text{tot}} \bmod 2)$ with $n_{\text{tot}} = n_c + n_f = n_c + 1$, in agreement with Luttinger’s theorem.¹⁸ Here, the factor of 2 accounts for the spin degeneracy of the bands, and $K_d = (2\pi)^d / (2v_0)$ is a phase-space factor with v_0 as the unit-cell volume.

Kondo screening may break down due to competing exchange interactions among the local f moments. If the local-moment magnetism is dominated by geometric frustration or strong quantum fluctuations,¹² the f moment subsystem may form a paramagnetic spin liquid without broken symmetries, only weakly interacting with the c electrons.⁸ The resulting FL* phase is necessarily exotic as it features a “small” Fermi volume $\mathcal{V}_{\text{FL}^*} = K_d (n_c \bmod 2)$ violating Luttinger’s theorem. As discussed in Ref. 8, the low-energy excitations of the fractionalized spin liquid account for the Luttinger violation. Thus, the Fermi volume provides a sharp distinction between FL and FL*.

If the heavy FL phase undergoes a standard SDW transition, we obtain a conventional metallic AF phase—often denoted as “itinerant” antiferromagnet—with Fermi-liquid properties. For the simplest case of collinear commensurate antiferromagnetism with an even number N of sites in the AF unit cell, the spin degeneracy of the bands is preserved (see Appendix A), and the onset of AF order simply implies a “backfolding” of the bands into the AF Brillouin zone. This results in a Fermi volume $\mathcal{V}_{\text{AF}} = K'_d (N n_{\text{tot}} \bmod 2)$ with $K'_d = K_d / N$. This value of \mathcal{V}_{AF} equals $K'_d (N n_c \bmod 2)$, i.e., the distinction between “large” and “small” Fermi volume is lost.

On the other hand, one may consider a “local-moment” AF phase. In the language of the Kondo model, this is obtained by forming a local-moment antiferromagnet from the f spins and then switching on a weak Kondo coupling to the c electrons. Importantly, this phase has Fermi-liquid properties as well.

Parenthetically, we note that a distinct magnetic phase is obtained by the onset of magnetic order in the fractionalized FL* phase.⁹ This exotic AF* phase characterized by topological order is not of interest for the body of the paper but will be briefly discussed in Sec. V.

B. Adiabatic continuity and weakly interacting electron states

The FL phase of a Kondo lattice is adiabatically connected to the noninteracting limit of the corresponding Anderson lattice model,

$$\mathcal{H}_{\text{ALM}} = \sum_{\vec{k}\sigma} (\epsilon_{\vec{k}} - \mu) c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} + \sum_{\vec{k}\sigma} (\epsilon_f - \mu) f_{\vec{k}\sigma}^\dagger f_{\vec{k}\sigma} + V \sum_{\vec{k}\sigma} (f_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} + c_{\vec{k}\sigma}^\dagger f_{\vec{k}\sigma}) + U \sum_i n_{f,i\uparrow} n_{f,i\downarrow} \quad (2)$$

in standard notation. While this Anderson model can be mapped to the Kondo model in the Kondo limit $V \rightarrow \infty$, $U \rightarrow \infty$, and $\epsilon_f \rightarrow -\infty$ with V^2 / ϵ_f finite, the properties of the heavy FL phase of both models can in principle be obtained perturbatively in U starting from two hybridized noninteracting bands.¹⁹ In other words, no phase transition occurs between the free-fermion situation $U=0$ and the large- U Fermi-liquid phase in the Anderson model.²⁰

As the itinerant AF phase is obtained from FL by the onset of SDW order, it is adiabatically connected to a noninteracting electron system of two hybridized bands in the presence of a staggered magnetic mean field.^{21,22}

Now we turn to the local-moment AF phase. Consider first the system of f moments alone: This is an AF Mott insulator. In the band picture, the f band is half-filled; after backfolding this translates into integer band filling for an even number N of sites in the AF unit cell. (The same applies to odd N , but here the spin degeneracy is lifted, see Appendix A.) As large band gaps are induced by the AF order parameter, noninteracting f electrons in the presence of an antiferromagnetic exchange (mean) field are insulating as well, i.e., there is no distinction here between band and Mott insulator. This fact is well known, e.g., for a half-filled one-band Hubbard model, where itinerant and local-moment antiferromagnet are continuously connected upon variation of U .²³ Consequently, for *vanishing* Kondo coupling, the local-moment AF phase of the Kondo lattice is adiabatically connected to a noninteracting Anderson model with vanishing hybridization and mean-field antiferromagnetism. Further, in such a two-band model of noninteracting electrons with f band gap, a small c - f hybridization is a marginal perturbation as it shifts the bands but leaves the topology of the Fermi surface unchanged.

C. Evolution of phases

Recent theory works^{13–15} suggested that local-moment and itinerant antiferromagnetism in Kondo lattices are dis-

tinct phases, which are separated by (at least) one quantum phase transition. There are, in fact, two issues here, related to (A) possibly different Fermi-surface topologies, and (B) a possible breakdown of Kondo screening within the AF phase, to be discussed in turn.

(A) The local-moment AF phase (dubbed AF_S) displays a Fermi surface with a topology inherited from the bare c band, while the itinerant AF phase (dubbed AF_L) was argued to display a different FS topology.¹⁴ (In the simplest models, AF_L has a holelike FS whereas AF_S has an electronlike FS.) If this difference in topology indeed exists, it necessitates one or more topology-changing transitions inside the AF phase. Such a transition can be of Lifshitz or van Hove type where a local band extremum or a saddle point crosses the Fermi level, respectively—both cases cause (weak) thermodynamic singularities and lead to abrupt changes in the electron orbits as measured, e.g., in the de-Haas-van-Alphen effect. The variational Kondo-lattice-model calculations of Ref. 15 indeed showed two AF phases with different FS topology; however, in a large parameter regime, a direct first-order transition from FL to AF_S was found.

(B) In Ref. 14, the AF_S phase was argued to be stable against a small Kondo coupling. The authors concluded that this situation is qualitatively different from AF_L , and consequently AF_L and AF_S have to be separated by a quantum phase transition associated with the breakdown of Kondo screening (which may coincide with the transition in FS topology).

In the following, we argue that (A') a continuous FS evolution between itinerant and local-moment AF phases is possible (using an explicit example, Sec. III), and (B') Kondo screening disappears smoothly in the AF phase (Sec. IV). Consequently, a sharp distinction between two *phases* AF_S and AF_L is not meaningful.

III. WEAKLY INTERACTING ELECTRONS: FERMISURFACE EVOLUTION

We now give an explicit example for a continuous evolution from itinerant to local-moment AF in a model of effectively noninteracting electrons. This approach can be justified by invoking either the equivalence of the relevant Fermi-liquid phases to phases of noninteracting electrons (Sec. II B) or the well-known mean-field treatments of the Kondo or Anderson lattice models. For instance, for the Kondo lattice the Kondo interaction is decoupled using a slave-boson field b . At the saddle-point level, one obtains a two-band model of noninteracting electrons with a hybridization b ; hence, the condensation of b signals Kondo screening (see Sec. V for details). Antiferromagnetism is obtained from a mean-field decoupling^{9,17} of the intermoment exchange interaction I_{ij} , which results in a staggered mean field for the f electrons.

We consider the following effective Hamiltonian:

$$\begin{aligned} \mathcal{H}_{\text{mf}} = \sum_{k\sigma} [& (\epsilon_{\vec{k}} - \mu) c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} + (\epsilon_{\vec{k}f} - \lambda) f_{\vec{k}\sigma}^\dagger f_{\vec{k}\sigma} + V(c_{\vec{k}\sigma}^\dagger f_{\vec{k}\sigma} + \text{H.c.}) \\ & + m_s \sigma c_{\vec{k}+\vec{Q}\sigma}^\dagger c_{\vec{k}\sigma} + M_s \sigma f_{\vec{k}+\vec{Q}\sigma}^\dagger f_{\vec{k}\sigma}]. \end{aligned} \quad (3)$$

It consists of two bands hybridized by V , with dispersions $\epsilon_{\vec{k}}$

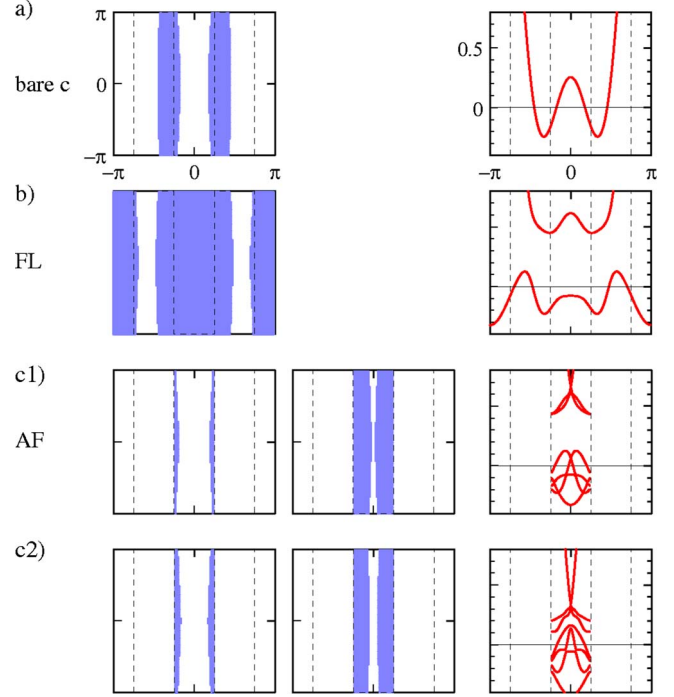


FIG. 1. (Color online) Fermi surfaces (left) and band structures (right) for a mean-field Kondo-lattice model, Eq. (3), on a two-dimensional (2D) rectangular lattice, with $n_c=0.5$ and bare band dispersions as given in the text. The dashed lines show the boundary of the reduced Brillouin zone of the antiferromagnet with $\vec{Q}=(\pi/2,0)$. (a) Bare c band. (b) Paramagnetic heavy Fermi liquid (FL), $V=0.3$. (c) Antiferromagnetic Fermi liquid (AF) with (c1) $V=0.29$, $M_s=10^{-4}$, and $m_s=10^{-5}$ (no changes occur for $M_s, m_s \rightarrow 0$) and (c2) $V=0.01$, $M_s=0.1$, and $m_s=10^{-2}$. From (b) to (c1), the system undergoes a standard SDW transition, whereas (c2) is close to a “local-moment” antiferromagnet [i.e., obtained by backfolding of the band structure from (a), together with a fully gapped f band]. Note that (c) has two completely filled bands after backfolding.

and $\epsilon_{\vec{k}f}$, respectively. Note that within a mean-field theory for the Kondo lattice, $\epsilon_{\vec{k}f}$ and λ are renormalized *effective* parameters of the f band, the latter playing the role of a Lagrange multiplier fixing $n_f=1$. Collinear antiferromagnetism is accounted for via the mean fields m_s and M_s (for c and f electrons) encoding the magnetic order parameter with wave vector \vec{Q} (see Appendix A for the general case). Typically, order will primarily arise in the f electron sector; hence, we expect $|M_s| > |m_s|$. \vec{Q} corresponds to an N -site unit cell in the AF ordered state, for even N the AF bands will be spin degenerate (Appendix A).

As an example we focus on a quasi-one-dimensional situation of a $2d$ array of coupled chains where the AF phase has a 4×1 unit cell, i.e., a collinear period-4 AF order in each chain. In Fig. 1 we show the Fermi-surface evolution and the band structures for parameters $\epsilon_{\vec{k}} = -2 \cos k_x + \cos(2k_x) - (\cos k_y)/30$, $\epsilon_{\vec{k}f} = 0.2[\cos k_x - \cos(2k_x)] - (\cos k_y)/50$, $n_c = 0.5$, $n_f = 1$, and different values of V , M_s , and m_s . The bare c Fermi surface is shown in Fig. 1(a). Backfolding into the AF zone results in two partially filled bands—this is the FS structure of the local-moment antiferromagnet where the f subsystem is gapped [Fig. 1c2]. On the other hand, the para-

magnetic large-FS state for sizeable V is shown in Fig. 1(b). Entering the AF phase via an SDW transition leaves us with two full and two partially filled bands [Fig. 1c1]. Importantly, this topology is identical to the one in Fig. 1c2. Together with the continuity arguments in Sec. II B, this constitutes a proof that a continuous evolution from itinerant [Fig. 1c1] to local-moment [Fig. 1c2] antiferromagnetism is possible.

A few remarks are in order: (i) Due to the $1d$ geometry, there are no closed orbits, and the large Fermi surface of FL does not intersect the AF zone boundary [Fig. 1(b)]. As a result, there is no Landau damping of the AF order parameter at the SDW transition. However, both features can be easily changed by including a second c band with a closed FS intersecting the AF zone boundary. (Heavy-fermion metals often feature a complicated band structure with numerous bands.) If this band is only weakly hybridized with the f band, then its Fermi surface will not differ in topology between the itinerant and local-moment limits. We shall give an additional example in Appendix C, which displays both closed orbits and Landau damping. (ii) For an AF unit cell with N a half-integer multiple of 4 ($N=2, 6, \dots$), topological reasons require that the Fermi surface crosses at least one van Hove singularity between the itinerant and local-moment limits (see Appendix B).

IV. RENORMALIZATION GROUP AND FIXED POINTS

In this section, we discuss the fate of Kondo screening in the framework of the renormalization-group (RG) treatment of the Kondo coupling between local moments and conduction electrons. In this language, Kondo screening (in the paramagnetic phase) is signaled by a runaway flow to strong coupling of the Kondo interaction.

What happens in the antiferromagnetic phase? Reference 14 presented an RG calculation starting from a local-moment antiferromagnet, with the result that the Kondo coupling is an exactly marginal perturbation to the fixed point of decoupled c and f electrons (dubbed AF_S). This qualitative difference to the paramagnetic case was used to conclude that AF_S and the Kondo-screened AF_L situations represent distinct *phases*, and a phase transition has to separate the two.

For comparison, let us review the well-studied problem of a single Kondo impurity in a magnetic field.¹⁹ Here, no zero-temperature phase transition occurs as a function of the field, i.e., all observables evolve smoothly from $B=0$ to $B \rightarrow \infty$. For $B > 0$, the low-energy theory takes the form of a spin-dependent potential scatterer with phase shifts varying continuously as a function of the field. In the RG language, this situation corresponds to a *line* of fixed points parametrized by the phase shifts. This line connects the fixed points of the screened zero-field impurity and the fully polarized impurity. The topology of the RG flow implies the existence of an exactly marginal operator—for a finite fixed field, this is the Kondo coupling J itself. Importantly, the distinct RG flow of J for zero and finite fields does *not* imply the existence of a quantum phase transition.

Adapting this knowledge to the Kondo lattice, we believe that the RG calculation of Ref. 14 is correct but does not

imply the necessity for a phase transition inside the antiferromagnetic phase (if the latter is reached via a SDW transition). We can offer two lines of arguments: (i) Within DMFT, the antiferromagnetic phase of the Kondo lattice is mapped onto a single Kondo impurity in a field; hence, the knowledge sketched above can be carried over.²⁴ (ii) Beyond DMFT, we know that both AF_L and AF_S are Fermi-liquid phases, which generically display a set of marginal operators (corresponding, e.g., to band-structure parameters). As the RG expansion in Ref. 14 is performed around a Fermi liquid, finding marginal operators is no surprise. (This is different from an expansion starting from decoupled moments in the paramagnetic Kondo lattice—this is a non-Fermi liquid due to the degenerate local-moment states.) In fact, it is straightforward to check that all Fermi-liquid renormalizations are generated in the expansion of Ref. 14. Hence, no qualitative differences exist between the local-moment and itinerant AF regimes.

In summary, the RG result of Ref. 14 is not in contradiction with itinerant and local-moment AF regimes being continuously connected. Instead, the AF phase should be interpreted as a family of RG fixed points of Fermi-liquid type. Depending on band-structure details, topological transitions may occur along a path from itinerant to local-moment AF, but this is not required, see Sec. III.

V. SLAVE PARTICLES, GAUGE FIELDS, AND PHASE DIAGRAM

A popular description of the low-temperature Kondo-lattice physics is based on a representation of the local moments by auxiliary fermions and a decoupling of the Kondo interaction by slave-boson fields b_i . Fluctuation effects are captured via a compact $U(1)$ gauge field. An additional intermoment exchange interaction J_H is decoupled using a non-local field χ , such that the low-energy action takes the form,⁹

$$\begin{aligned} S = \int d\tau \left\{ \sum_k \bar{c}_k (\partial_\tau - \epsilon_k) c_k + \sum_i \bar{f}_i (\partial_\tau - ia_0) f_i \right. \\ \left. - \sum_i \left(b_i \bar{c}_i f_i + \text{c.c.} - \frac{4|b_i|^2}{J} \right) \right. \\ \left. - \sum_{\langle ij \rangle} \left[\chi_{ij} (e^{ia_{ij}} \bar{f}_i f_j + \text{c.c.}) - \frac{4|\chi_{ij}|^2}{J_H} \right] \right\}. \quad (4) \end{aligned}$$

Here, the time component a_0 of the gauge field implements the occupation constraint for the f fermions, whereas the space component a_{ij} represents phase fluctuations of the decoupling parameters.

In the saddle-point approximation, gauge-field fluctuations are ignored. This mean-field approach has well-known deficiencies, such as an artificial breaking of the internal gauge symmetry in the FL regime where $\langle b \rangle \neq 0$, leading to an artificial finite-temperature phase transition. These deficiencies are cured once the gauge-field physics is taken into account. After integrating out the fermions, the effective theory is given by a compact $U(1)$ gauge field coupled to the charged scalar b . The Fermi-liquid phase corresponds to the

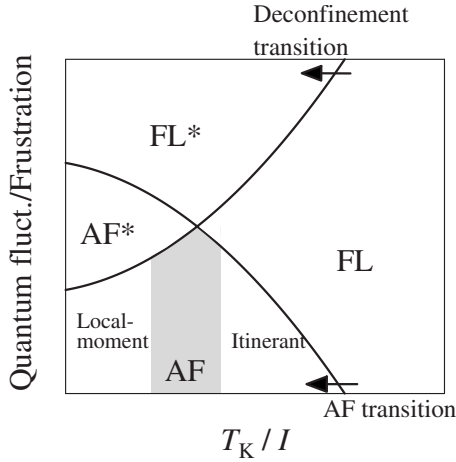


FIG. 2. Schematic zero-temperature phase diagram of the Kondo-Heisenberg model $\mathcal{H}_{\text{KLM}} + \mathcal{H}_I$ as a function of the dimensionless ratio T_K/I (formed from Kondo and intermoment exchange energy scales) and the amount of quantum fluctuations (e.g., due to frustration). The solid lines show continuous phase transitions associated with the onset of antiferromagnetism and deconfinement/topological order. In the absence of antiferromagnetism, the deconfinement transition is equivalent to a Kondo breakdown or f Mott transition. The shaded area denotes the crossover from itinerant to local-moment AF; in this region FS-topology-changing transitions *may* occur depending on the type of magnetic order and the FS topology, see Appendix B. (The structure of the phase boundaries follows from Refs. 8 and 9.) A scenario of deconfined criticality modifies the phase diagram (Ref. 10), see text.

Higgs phase of the gauge theory; due to the compactness of the $U(1)$ gauge field, no finite-temperature transition occurs. Most importantly, for this gauge theory, the confined and the Higgs phases are smoothly connected, i.e., identical²⁵ (and hence FL-like). The gauge theory also has a deconfined (or Coulomb) phase characterized by topological order. Without magnetism, the result is the fractionalized Fermi liquid FL^* . No Kondo screening occurs here, i.e., $b=0$ at the mean-field level. The transition from FL to FL^* is the Kondo-breakdown transition advocated in Refs. 8 and 9, which can also be interpreted as a Mott transition of the f electron subsystem.²⁶ Adding antiferromagnetic order to the FL^* phase results in an AF^* phase—this is a fractionalized antiferromagnet.⁹

The zero-temperature phase diagram from this discussion is in Fig. 2. The smooth connection between Higgs and confined phases of the gauge theory allows us to conclude that in the presence of antiferromagnetism, there is only a single *conventional* phase (AF). Inside the AF phase, a transition toward the fractionalized AF^* phase is possible, accompanied by the onset of topological order. Such a transition may be driven by increasing quantum fluctuations or magnetic frustration.¹² However, it is usually assumed that local-moment antiferromagnetism in heavy-fermion metals is conventional, such that the AF^* phase is unlikely to be realized.²⁷ (Mean-field theories display a zero-temperature transition where b vanishes upon increasing the magnetic order parameter. This transition—which may be interpreted as the AF– AF^* transition—does not coincide with a possible Lifshitz transition.)

Finally, we note that a Kondo-breakdown transition from FL to AF in Fig. 2 is only possible with fine tuning via the multicritical point. In contrast, in the scenario of deconfined criticality²⁸ proposed for the Kondo lattice,¹⁰ the FL^* phase is assumed to display a secondary instability toward antiferromagnetism (accompanied by confinement). Then FL^* (together with AF^*) disappears from the $T=0$ phase diagram rendering a Kondo-breakdown transition from FL to AF possible without fine tuning. The RG flow near this transition displays multicritical behavior.²⁸

VI. CONCLUSIONS

We have argued that local moment and itinerant antiferromagnetism in heavy-fermion compounds are not necessarily distinct phases. To this end, we have demonstrated adiabatic continuity along the path (i) itinerant Kondo-lattice AF, (ii) noninteracting two-band system with small exchange field and strong hybridization, (iii) noninteracting two-band system with large exchange field and vanishing hybridization, and (iv) local-moment Kondo-lattice AF. Here, the connection (i)–(ii) follows from the Fermi-liquid properties of the heavy FL, the connection (ii)–(iii) was established using an explicit example for a continuous Fermi-surface evolution in Sec. III, and the connection (iii)–(iv) builds on the continuity between antiferromagnetic band and Mott insulators in one-band models together with the Fermi-liquid properties of the local-moment antiferromagnet. This provides a proof of principle that a continuous evolution from itinerant to local-moment antiferromagnetism is possible without intervening topological or other quantum phase transitions.

These arguments do not exclude the existence of (continuous or first-order) Lifshitz or van Hove transitions within the antiferromagnetic phase. However, those transitions depend on band structure and topology and cannot be associated with the breakdown of Kondo screening in the magnetic phase: The concepts of quasiparticles and Fermi surfaces remain well defined across such transitions.¹⁶ Our reasoning, which rests on the broken translational symmetry in the AF phase, applies similarly to other variants of translational symmetry breaking in the local-moment regime of Kondo lattices, e.g., the formation of valence-bond solids.

Let us briefly consider the implications for the much discussed Kondo-breakdown scenario for the antiferromagnetic quantum critical point. Our arguments imply that the two distinct quantum phase transitions, namely conventional SDW and Kondo breakdown, connect the *same* phases, namely a paramagnetic and an antiferromagnetic Fermi-liquid metal. Then, it is clear that measurements only taken *inside* the antiferromagnetic phase (even close to the critical point) do not allow to draw sharp conclusions about the nature of the quantum phase transition. Only (i) the finite-temperature quantum critical behavior and (ii) the evolution of observables at low temperatures *across* the quantum phase transition can distinguish between the transition being of conventional SDW type or of Kondo-breakdown type. In the latter case, e.g., a jump in the zero-temperature limit of the Hall coefficient⁶ across the quantum phase transition can be expected. (Such a jump also occurs at a first-order transition

between FL and AF as in the theory work of Ref. 15; however, there will be no finite-temperature quantum critical region, but instead the first-order behavior will continue to finite T .)

On the experimental side, CeNi₂Ge₂ appears to fit into the standard SDW transition scenario, whereas CeCu_{6-x}Au_x and YbRh₂Si₂ have been discussed as candidates for AF transitions accompanied by the breakdown of the Kondo effect.² In particular, Hall-effect measurements on YbRh₂Si₂ support a jump in the Hall coefficient across the QPT.²⁹ Recent substitution experiments³⁰ in YbRh₂Si₂ gave indications for a separation of the magnetic and Kondo-breakdown transition signatures (e.g., upon replacing Rh with Ir or Co), opening an exciting opportunity to study the global phase diagram in more detail. In line with our arguments, we predict the signatures of the Kondo breakdown to be weakened or smeared inside the antiferromagnetic phase even in the low-temperature limit. For CeCu_{6-x}Au_x, we note that several transport experiments inside the AF phase^{31,32} could be nicely explained by a competition between AF order and Kondo screening—this may be taken as evidence *against* a Kondo-breakdown scenario for the magnetic QPT in this material. More detailed studies (e.g., Hall effect under pressure) are desirable.

An interesting case is that of CeRhIn₅.^{33,34} Under pressure, de-Haas-van-Alphen measurements detected a change in the Fermi-surface properties at a critical pressure of $p_c \approx 2.3$ GPa.³⁴ In zero field, this system displays an intricate pressure-driven interplay of antiferromagnetism and superconductivity. However, the experiment was performed in fields up to 17 T where superconductivity is suppressed, but antiferromagnetism is believed to persist for $p < p_c$. Thus, the experimental data may be consistent with a Kondo-breakdown transition upon lowering p , which occurs concomitantly with the onset of AF order. Evidence for a transition inside an AF phase with a Fermi-surface reconstruction has been recently found³⁵ in CeRh_{1-x}Co_xIn₅. This transition, however, is strongly first order and is also accompanied by a change in the magnetic structure.

Last but not least, we note that metallic spin-liquid behavior has been observed in the geometrically frustrated Kondo-lattice compound Pr₂Ir₂O₇ (Ref. 36) rendering it a candidate for the FL* phase. Here, experimental efforts to drive a transition toward FL [by doping or (chemical) pressure] seem worthwhile.

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APPENDIX A: BAND STRUCTURE OF ITINERANT ANTIFERROMAGNETS

In this Appendix, we highlight the distinctions between collinear and noncollinear AF regarding band degeneracy.

Those are relevant for the possible existence of FS topological transitions inside the AF phase of Kondo lattices, to be discussed in Appendix B.

Consider the local-moment electrons only, with one-electron per paramagnetic unit cell and a dispersion $\epsilon_{\vec{k}}$, in the presence of commensurate antiferromagnetic order described by a single ordering wave vector \vec{Q} . The electrons move in a mean field given by $\vec{h}(\vec{r}_i) = \text{Re}[\vec{M} \exp(i\vec{Q} \cdot \vec{r}_i)]$, where \vec{M} is a complex vector encoding the order parameter, such that, e.g., spiral order has $\vec{M} = \vec{M}_1 + i\vec{M}_2$ with real \vec{M}_1 and \vec{M}_2 obeying $\vec{M}_1 \cdot \vec{M}_2 = 0$. For a unit cell with N sites, $N\vec{Q}$ is a reciprocal-lattice vector, and the band structure is given by the eigenvalues of the $2N \times 2N$ matrix

$$\begin{pmatrix} \epsilon_{\vec{k}} & 0 & M_{\uparrow\uparrow} & M_{\uparrow\downarrow} & 0 & 0 & \dots \\ 0 & \epsilon_{\vec{k}} & M_{\downarrow\uparrow} & M_{\downarrow\downarrow} & 0 & 0 & \dots \\ M_{\uparrow\uparrow}^* & M_{\uparrow\downarrow}^* & \epsilon_{\vec{k}+\vec{Q}} & 0 & M_{\uparrow\uparrow} & M_{\uparrow\downarrow} & \dots \\ M_{\downarrow\uparrow}^* & M_{\downarrow\downarrow}^* & 0 & \epsilon_{\vec{k}+\vec{Q}} & M_{\downarrow\uparrow} & M_{\downarrow\downarrow} & \dots \\ 0 & 0 & M_{\uparrow\uparrow}^* & M_{\uparrow\downarrow}^* & \epsilon_{\vec{k}+2\vec{Q}} & 0 & \dots \\ 0 & 0 & M_{\downarrow\uparrow}^* & M_{\downarrow\downarrow}^* & 0 & \epsilon_{\vec{k}+2\vec{Q}} & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}, \quad (\text{A1})$$

where odd (even) rows and columns correspond to spin-up (down) electrons, and $M_{\sigma\sigma'} = \vec{M} \cdot \vec{\tau}_{\sigma\sigma'}$ with $\vec{\tau}$ as the vector of Pauli matrices. For collinear AF, $M_{\sigma\sigma'}$ can be chosen diagonal $\propto \tau_z$.

We are interested in the degeneracy of the $2N$ bands. The simplest situation is collinear AF with even N : Here, the up and down sectors decouple and are degenerate, as the eigenvalues of Eq. (A1) depend only on $|\vec{M}|^2$. For noncollinear order with even N the spin sectors mix, but the double degeneracy is preserved, because there exists a translation operation which reverses all spins (i.e., the combined action of time reversal plus translation is a symmetry of the state).

For odd N , the spin degeneracy is in general lifted. The only exception is the case of a purely imaginary $M_{\sigma\sigma'}$: Here, one site within the unit cell (more generally, an odd number of sites) has exactly zero magnetization. This situation requires an exotic spin liquid, further symmetry breaking, or coupling to other degrees of freedom like Kondo screening of these moments.

We conclude that for both the cases of (i) even N and (ii) odd N with spin degeneracy lifted, the itinerant antiferromagnet with one electron per site has an *integer* band filling (after taking into account backfolding and spin). Then, in the presence of sufficiently large exchange fields (i.e., band splitting) the magnet will be insulating. This AF band insulator is adiabatically connected to an AF Mott insulator.

APPENDIX B: CRITERIA FOR THE NONEXISTENCE OF FS TOPOLOGICAL TRANSITIONS

As transitions with changes in the FS topology may always occur within Fermi-liquid phases, we discuss under which circumstances topological transitions in the AF phase

of Kondo lattices are *not* required to occur: An example without transitions was given in Sec. III. The discussion will concentrate on the momentum-space volume and topology of the occupied fermionic states of the c plus f electron system where we allow for K different c electron bands. The strategy is to find conditions for the backfolded band structures of the FL phase and the c bands alone to be identical in topology—then a smooth evolution from itinerant to local-moment AF is possible.

We denote the total occupied volumes of the partially filled bands in the FL phase and the c bands alone with $K_d n_L$ and $K_d n_S$, respectively. Hence, $n_L \equiv (n_c + 1) \bmod 2$ and $n_S \equiv n_c \bmod 2$; in other words, n_L and n_S differ by an odd integer. After backfolding, both total occupied volumes (again of the partially filled bands) need to be identical to avoid topological transitions in the AF phase. The volumes can change by $2/N$ if bands after backfolding (i.e., in the reduced Brillouin zone) are fully occupied [as in Fig. 1(b)]. Hence, the number F of completely filled *reduced* BZ must differ by an odd multiple of $N/2$ between the FL phase and the c bands alone, $(F_L - F_S)2/N = 1 \bmod 2$.

This condition can obviously not be met for odd N ; here “large” and “small” Fermi volumes are only equivalent in the AF phase after taking into account the broken spin degeneracy of the bands. Thus, for odd N , at least one topological transition occurs inside the AF phase.

For even N , we now focus on the number P of partially filled bands in the AF phase (after backfolding) where those $(d-1)$ dimensional surface areas of the reduced BZ boundary, which were not part of the original BZ boundary, are fully occupied. For the discussion we furthermore assume inversion symmetry. P receives *even* contributions from all bands of the paramagnetic phase, except for situations where a reduced BZ is fully occupied: Each of these cases give an *odd* contribution to P , hence, $P \equiv F \bmod 2$. To avoid topological transitions, P must be equal for the itinerant AF (derived from FL) and the localized AF (derived from the c bands alone), $P_L = P_S$. Hence, $F_L \equiv F_S \bmod 2$. The above condition $F_L - F_S = (N/2) \bmod N$ translates into the necessary condition of N to be a multiple of 4 for not having a topological transition (in the presence of inversion symmetry). An example with $N=4$, $K=1$, and $P=2$ is in Fig. 1.

Further considerations now have to include the $(d-2)$ dimensional “edges” of the BZ. Here, we have found that at least in low-symmetry situations topological transitions can be avoided. One truly $2d$ example, which also includes closed electron orbits, with $N=4$, $K=1$, and $P=0$ is in Fig. 3.

APPENDIX C: FERMI-SURFACE EVOLUTION: ANOTHER EXAMPLE

We provide an additional example for a continuous Fermi-surface evolution within a model of effectively noninteracting electrons similar to Sec. III.

The model is defined on a $2d$ square with inequivalent diagonals (equivalent to a rhomboid lattice). The AF phase has $N=4$ with a 2×2 unit cell originating from 4-sublattice coplanar AF order characterized by two ordering wave vectors $\vec{Q}_1 = (\pi, 0)$ and $\vec{Q}_2 = (0, \pi)$, where \vec{Q}_1 (\vec{Q}_2) correspond to

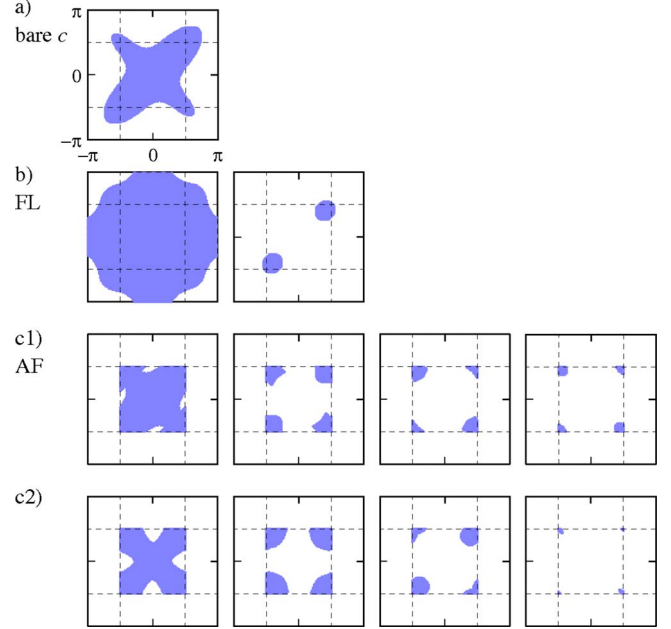


FIG. 3. (Color online) Fermi surfaces as in Fig. 1, but now for a situation with a 2×2 AF unit cell as described in the text. (a) Bare c band. (b) Paramagnetic heavy FL, $V=0.45$. (c) AF Fermi liquid with (c1) $V=0.44$, $M_s=10^{-4}$, and $m_s=10^{-5}$ and (c2) $V=0.01$, $M_s=0.1$, and $m_s=10^{-2}$.

a spin-density wave with spin polarization in z (x) direction with an equal amplitude. The model parameters are $\epsilon_{\vec{k}} = (\cos k_x - \cos k_y)^2 + (\cos 2k_x + \cos 2k_y)/2 - \cos(k_x - k_y) + [(1 - \cos k_x)^8 + (1 - \cos k_y)^8]/50$, $\epsilon_{\vec{k}f} = -(\cos k_x + \cos k_y)/10 + [\cos(k_x - k_y) + \cos(k_x + k_y)]/20 + (\cos 2k_x + \cos 2k_y)/20$, $n_c = 0.65$, and $n_f = 1$.

The Fermi-surface evolution is shown in Fig. 3. Backfolding of the FL bands [Fig. 3(b)] results in two completely filled plus four partially filled bands in the itinerant antiferromagnet [Fig. 3c1]. Again, these Fermi surfaces are topologically identical to those of the local-moment antiferromagnet [Fig. 3c2], obtained from backfolding the bare c band structure of Fig. 3(a). Note that this example displays both closed electron orbits and Landau damping of the order parameter.

APPENDIX D: INCOMMENSURATE MAGNETISM

So far, the discussion applied to antiferromagnetism with a spatial period being commensurate with the crystal lattice. Incommensurate order is qualitatively different, at least at $T=0$ in an ideal crystal. Here, the volume of the reduced Brillouin zone (after backfolding) is zero, and the resulting band structure has quasicrystalline properties with a hierarchy on infinitely many gaps.^{29,37} Hence, the Fermi volume is no longer a well-defined concept. Another way to think about incommensurate ordering is to approach the incommensurate \vec{Q} via a sequence of commensurate \vec{Q} with increasing size of the unit cell and decreasing size of the Brillouin zone. A small Brillouin zone implies that changes of the band structure cause frequent topological transitions. Then, the passage

from itinerant to local-moment antiferromagnetism in the incommensurate case will be accompanied by a dense sequence of topological transitions—which may be interpreted as adiabatic continuity.

In the presence of finite temperature or disorder, the small band gaps will be smeared, and the structure effectively behaves as commensurate (for fixed T). Then, our above consideration in the body of the paper applies.

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