Quantum phase transitions out of the heavy Fermi liquid

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Abstract

We review recent work on the instability of the heavy Fermi liquid state (FL) of the Kondo lattice towards a magnetic metal in which the local moments are not part of the Fermi sea. Using insights drawn from the theory of deconfined quantum criticality of insulating antiferromagnets, we discuss the possibility of a direct second order transition between the heavy Fermi liquid and such a magnetic metal. We suggest the presence of at least two distinct diverging time scales - the shorter one describes fluctuations associated with the reconstruction of the Fermi surface, while a longer one describes fluctuations of the magnetic order parameter. The intermediate time scale physics on the magnetic side is suggested to be that of a novel fractionalized Fermi liquid (FL*) state with deconfined neutral $S = 1/2$ excitations. This could ultimately devolve into the magnetic phase with conventional order at one of the larger time scales. Experimental implications for this scenario are noted.

Key words: quantum criticality, Kondo lattice, deconfinement

1. Introduction

A remarkable realization of Landau’s Fermi liquid theory of metals occurs in the ‘heavy fermions’ class of materials. Indeed, it has long been known that at low temperatures these can typically be described within the Fermi liquid paradigm, albeit with strongly renormalized parameters (for instance, effective masses of order $10^2 - 10^3$ the band mass). Microscopically, this class of material may be modelled as possessing localized magnetic moments coupled to a separate set of conduction electrons. The heavy Fermi liquid (see Section 2 below) is understood by a lattice analog of the Kondo screening of the localized moments. Crudely speaking, the localized moments “dissolve” into the Fermi sea. Luttinger’s theorem for the volume of the resulting Fermi surface includes both the conduction electrons and those forming the local moments.

In contrast, recent experimental work has focused on situations where the Fermi liquid description of such metals appears to break down in a rather strong manner. Such non-Fermi liquid behavior occurs most strikingly in the vicinity of zero temperature phase transitions out of the heavy Fermi liquid - typically to a magnetically ordered metal. However there is little theoretical understanding of this breakdown of the Fermi liquid paradigm.

Quite generally, two distinct kinds of magnetically ordered metals are possible in heavy fermion materials. In one the magnetism is to be viewed as a spin density wave instability arising out of the parent heavy Fermi liquid state. Crudely speaking, this magnetism may be viewed as arising from imperfectly Kondo-screened local moments. We will refer to such a state as the SDW metal. A different kind of magnetic metallic state is also possible where the localized moments order due to RKKY exchange interactions, and do not participate in the Fermi surface of the metal. The “Kondo order” present in the heavy Fermi liquid is absent in
2. The heavy Fermi Liquid, FL

Much of our understanding of the heavy fermion compounds is based on the Kondo lattice model:

\[ H_K = \sum_k \varepsilon_k c_{k \alpha}^\dagger c_{k \alpha} + \frac{J_K}{2} \sum_r \bar{S}_r \cdot \bar{\sigma}_{\alpha \alpha'} \bar{c}^\dagger_{ra} \bar{c}_{ra'}. \]  

This model consists of a density \( n \) of conduction electrons \( c_{k \alpha} \) with dispersion \( \varepsilon_k \) (\( k \) is momentum and \( \alpha = \uparrow, \downarrow \) is a spin index) interacting with \( f \) electron spins \( \bar{S}_r \) (\( r \) is a lattice position, and \( \bar{\sigma} \) are the Pauli matrices) via an antiferromagnetic Kondo exchange coupling \( J_K \).

There is a well accepted theory of the formation of a heavy fermion liquid state (hereafter referred to as the FL state) in this model [2,3,4]. The charge of the \( f_{ra} \) electrons is fully localized on the rare-earth sites, and so one initially imagines that these electrons occupy a flat dispersionless band, as shown in Fig 1a. This band has to be half-filled, and so we must place it at the Fermi level. The \( c_{ra} \) electrons are imagined to occupy their own conduction band. Next, it is argued [2], that such a material. We will denote this second magnetically ordered metal as a ‘local moment magnetic metal’ or LMM metal. Often the distinction between these two kinds of magnetic states can be made sharply: the Fermi surfaces in the two states may have different topologies (albeit the same volume modulo that of the Brillouin zone of the ordered state) so that they cannot be smoothly connected to one another.

There is a well developed theory for the quantum transition between the heavy Fermi liquid and the SDW metal [1] which, however, often fails to produce the non-Fermi liquid physics observed in experiments. It is therefore tempting to assume that when non-Fermi liquid physics is seen at a magnetic ordering transition out of the heavy Fermi liquid, the resulting magnetic state is the LMM metal rather than the SDW metal. However, there is no theoretical understanding of such a transition. Indeed, a number of basic conceptual questions arise. Can there be a second order transition where the ‘Kondo order’ of the heavy Fermi liquid disappears concomitantly with the appearance of magnetic long range order? What is the theoretical description of such a transition? Will it reproduce the observed non-Fermi liquid physics in the heavy fermion metals near their magnetic ordering transition?

The answers to these questions are not known with confidence at present. In this paper we will review our recent work on related questions in a number of simpler contexts. Based on the lessons from these studies we will present some ideas on the transition from the heavy Fermi liquid to the LMM metal, and their implications for experiments.

Fig. 1. Conventional theory of the FL state. A completely flat \( f \) electron “band” (dashed line in (a)) mixes with the conduction electrons to obtain the renormalized bands in (b). There is a single Fermi surface at \( k_F \) in the FL state containing states whose number equals that of the \( f \) and \( c \) electrons combined. The Kondo exchange is equivalent to turning on a small hybridization between these two bands. We represent this hybridization by a non-zero expectation value of the bosonic operator

\[ b_r \sim \sum_\alpha c_{ra}^\dagger f_{ra}. \]

With \( (b_r) \) non-zero, the two bands will mix and lead to the renormalized bands shown in Fig 1b. A crucial point is that because the \( f \) band was initially dispersionless, there is absolutely no overlap between the renormalized bands. Hence the occupied states are entirely within the lower band, and one obtains a single Fermi surface within wavevector \( k_F \): the volume within \( k_F \) is determined by the total density of \( c \) and \( f \) electrons. This is precisely the Fermi volume predicted in the limit of weak interactions between the electrons by the Luttinger theorem. Moreover, as in Fig 1b, the Fermi surface is in a region where the electrons are primarily have a \( f \) character, and consequently the band is still quite flat—this accounts for the large effective mass of the fermionic quasiparticles.

A key technical feature of the theory of the FL state is presence of an emergent compact U(1) gauge field. This is a consequence of the quenching of the charge fluctuations on the \( f \) electron sites \( i.e. \) the constraint

\[ \sum_\alpha f_{ra}^\dagger f_{ra} = 1 \]

is obeyed at every rare earth site. This constraint implies that that theory is invariant under the spacetime dependent U(1) gauge transformation

\[ f_{ra} \rightarrow f_{ra} e^{i \phi_r(r)} \]

where \( r \) is imaginary time. After integrating out high energy degrees of freedom, this invariance leads to the emergence of a dynamical compact U(1) gauge field \( A_\mu \) (\( \mu \) is a spacetime index, and ‘compact’ refers to the
invariance of the theory under $A_\mu \rightarrow A_\mu + 2\pi$. Notice also that the bosonic field $b$ in Eq. (2) also carries a U(1) gauge charge. The $b$ field is condensed in the FL state, and so in this state the U(1) gauge theory can be considered to be in a ‘Higgs’ phase. The appearance of the $b$ Higgs condensate also means that $A_\mu$ fluctuations are quenched, and so are relatively innocuous in the FL state.

We are interested here in the manner in which this heavy FL state may be destroyed by perturbations at zero temperature ($T$). An important early proposal made by Doniach [5] was that the state could be unstable to magnetic ordering of the $f$ moments, induced by a RKKY exchange coupling between them:

$$\mathcal{H}_H = \sum_{rr'} J_H(r,r') S_r \cdot S_{r'}.$$  \hspace{1cm} (5)

Assuming this metallic state is the SDW metal noted in Section 1, such a quantum phase transition can be analyzed [1] in a manner similar to the SDW instability in an ordinary Fermi liquid. In such an approach one assumes that once the heavy FL state has formed between the $f$ and $c$ electrons, the resulting quasiparticles lose memory of their origin, and behave like ordinary ‘light’ quasiparticles.

As discussed in Section 1, here we will review our recent work [6,7] exploring another route to the breakdown of the FL state of $\mathcal{H}_K + \mathcal{H}_H$. Here, the Kondo lattice origins of the FL state play a central role, and the focus is on the breakdown of the ‘hybridization’ or ‘Kondo screening’ between the $f$ and $c$ bands. Magnetic order may well appear at very low energies (in a LMM metal) once the FL state has been disrupted; however, this will be viewed as a secondary or ‘epiphenomenon’, and the primary physics is that of the destruction of the Higgs phase of the U(1) gauge theory.

Other distinct points of view are in Refs. [8,9,10].

3. The fractionalized Fermi liquid, FL*

As noted above, the only active degrees of freedom on the $f$ sites are the spins, and this is captured by the $f_{\alpha \sigma}$ operators. The exchange coupling in $\mathcal{H}_H$ can move this spin between sites, and so the initial assumption above of a dispersionless $f$ band may be questioned. So let us reconsider the above argument starting from a $f$ band which has a dispersion of order $J_H$, as shown in Fig 2a. When the hybridization energy, in Eq. (2), is on a scale larger than $J_H$, the physics is as is in Section 2. However, as the hybridization decreases, it is clear that eventually there will be band overlap, and the FL state will have 2 occupied bands, as shown in Fig 2b, with two Fermi wavevectors, $k_{F1}$ and $k_{F2}$. Nevertheless, this is still a conventional FL state, in that the total number of states contained between both Fermi surfaces still equals the total number of $c$ and $f$ electrons, and the conventional weak-coupling Luttinger theorem is still obeyed. However, it has been argued [1,6] that the transition from a state with $(b) \neq 0$ to a state with $(b) = 0$ is indeed a sharp phase transition at $T = 0$. However, there is no conventional Landau order parameter for this transition, and there is no analog of such a transition at $T > 0$ (although a $T > 0$ transition between a state with $(b) \neq 0$ and a state with $(b) = 0$ does appear in mean field theory [12]). Rather, it is a transition characterized by a change in the ‘topological’ character of the ground state wavefunction, in that the fate of the $A_{\mu}$ field dynamics undergoes a qualitative change.

So what is the nature of the state, which we denoted FL*, with $(b) = 0$ obtained by increasing $J_H$? First, it is a Fermi liquid in the sense that the $c$ electrons form a conventional Fermi surface, with sharp electron-like quasiparticles at $k_F^c$ (see Fig 2a). However, the volume enclosed by this Fermi surface contains states whose number equals only the number of $c$ electrons; this violates the conventional Luttinger theorem. Closely linked with this non-Luttinger Fermi volume is the fate of the spin moments on the $f$ electrons. These form a ‘spin liquid’ state, which does not break any lattice translational symmetries and fully preserves spin rotation invariance (i.e. there is no magnetic moment). The spin liquid state contains $S = 0$ excitations of the gauge field, $A_\mu$, which remain gapless if the U(1) gauge group remains unbroken (spin liquid states with a $Z_2$ gauge group are also possible), along with the now charge neutral $S = 1/2 f_{\alpha}$ fermions. A fairly rigorous
argument can be made [6,13] showing that the unusual Fermi volume of the FL* phase requires the emergent collective gauge excitations represented by $A_\mu$.

Our work also presented [6] a description of the quantum critical point between the FL and FL* phases. Within the FL phase, as one moves towards the FL* phase, the two Fermi surfaces at $k_{F1}$ and $k_{F2}$ behave differently. The Fermi surface at $k_{F1}$ evolves into the Fermi surface at $k_{F*}$ in the FL* state, and this remains ‘cold’ near the quantum critical point: there is no strong scattering of these quasiparticles, and the electron quasiparticle residue remains finite across the transition. In contrast, the Fermi surface at $k_{F2}$ becomes ‘hot’: the lifetime of the quasiparticles becomes short, and the quasiparticle residue decreases and ultimately vanishes at the quantum critical point. The dynamics of the quasiparticles exhibits non-Fermi liquid behavior at the quantum critical point. Note that this anomalous behavior extends across the entire hot Fermi surface, in contrast to the isolated ‘hot spots’ that appear in the SDW theory [1]. The self energies also have a full momentum dependence, in contrast to theories of ‘local’ criticality [9].

4. Deconfined quantum criticality in insulating antiferromagnets

It is useful to interpret the approach of the FL state to the FL* state described above as a approach to a deconfinement transition of the $f_\sigma$ fermions. In the FL state these are ‘bound’ to the $c_\sigma$ by the Higgs condensate of (2), the ultimate low energy quasiparticles carry charge $-e$ and $S = 1/2$, and there are no strong $A_\mu$ fluctuations. At the quantum critical point, neutral $f_\sigma$ quanta are liberated, and the $A_\mu$ fluctuations become much stronger. The present theory [6] of this critical point treats these gauge fluctuations perturbatively - for reasons explained in Ref. [6] this may be legitimate in spatial dimension $d = 3$, but not necessarily so in $d = 2$. In the latter case it is entirely possible that there are additional non-perturbative effects which have not been fully accounted for.

To explore the possible consequences of such deconfinement-driven quantum criticality, we consider here a simpler insulating system for which much progress has recently been made [7] in understanding the non-perturbative consequences of gauge fluctuations. We describe the square lattice $S = 1/2$ Heisenberg antiferromagnet, important in its applications to the physics of the cuprates. This is a model in the class $\mathcal{H}_H$ of the $f$ moments alone, with no metallic charge carriers. When the exchange interactions are predominantly nearest neighbor, the ground state long-range Néel order, in which the moments are polarized along opposite collinear directions on the two sublattices. As is conventional, we characterize the local orientation of this order by a unit vector field $\vec{n}_x \propto (-1)^{x+y} \hat{S}_x$. It turns out to be useful to further express the vector $\vec{n}_x$ in spinor variables by

$$\vec{n}_\mu = z_\alpha \sigma_{\alpha\beta} z_{\beta}$$

where $z_{\uparrow}, z_{\downarrow}$ are complex spinors obeying

$$|z_{\uparrow}|^2 + |z_{\downarrow}|^2 = 1.$$  

As in Eqs. (3), (4), Eq. (7) implies that the theory for the $z_\alpha$ has a compact U(1) gauge invariance

$$z_{\alpha} \to z_{\alpha} e^{i \phi_\alpha(r)},$$

and an associated compact U(1) gauge field $A_\mu$. In the present situation, it is possible to use spin and lattice symmetries, and the absence of gapless Fermi surfaces, to write down an explicit effective action for the gauge theory in the continuum limit:

$$S_z = \int d^2r d\tau \left[ \left| \left( \partial_\mu - i A_\mu \right) z_\alpha \right|^2 + s |z_\alpha|^2 + u (|z_\alpha|^2)^2 \right].$$

Here $s$ is a tuning parameter which we use to destroy Néel order, and will we then describe the consequences of gauge fluctuations at the resulting quantum critical point. The Néel phase is obtained when $s < 0$, and the $z_\alpha$ are condensed with $\langle z_\alpha \rangle \neq 0$. In other words, the Néel phase is the Higgs phase of the present gauge theory, in close analogy to our discussion in Sections 2, 3 for the FL phase. Here too the Higgs condensate quenches the gauge fluctuations, and morphs them into a $S = 0$ collective mode of pairs of spin waves.

Now let us approach the quantum critical point, which is at $s = s_c$ (say). Here, the $z_\alpha$ are gapless $S = 1/2$ quanta which interact via exchange of the gapless U(1) gauge quanta of $A_\mu$. In a sense, the $z_\alpha$ quanta have been deconfined, but some care has to used with this terminology because the $z_\alpha$ also acquire an anomalous dimension [14].

We can continue the same analysis into the paramagnetic phase with $s > s_c$ and $\langle z_\alpha \rangle = 0$, where the properties of the theory $S_z$ are really quite simple, and describe a U(1) spin liquid ground state. The $z_\alpha$ quanta are sharply defined $S = 1/2$ quasiparticles (spinons) and they interact via exchange of $A_\mu$ quanta, which now have a true Maxwell-photonic form.

While simple and direct, the above story turns out to be fundamentally incomplete, and this breakdown likely has implications for the FL to FL* transition we described earlier. In taking the continuum limit to Eq. (9), we have lost information on the compactness of $A_\mu$ (i.e., invariance under $A_\mu \to A_\mu + 2\pi$). A compact U(1) gauge theory in 2+1 dimensions allows monopole point defects, which are tunnelling events
between sectors whose total flux differs by $2\pi$. In the language of the $\vec{n}$ field, these are ‘hedgehog’ defects. Furthermore, a lattice scale analysis of the action of these monopoles shows that they carry Berry phases. We refer the reader to Ref. [14] for a review of the physics of these monopoles at and near the quantum critical point, and merely summarize the results of such an analysis here. As shown in Fig 3, it is useful to consider a two-dimensional renormalization group (RG) flow in the tuning parameter, $s$, and a certain quadrupole monopole fugacity, $\lambda_4$.

The properties of the theory $S_2$ are described by the line $\lambda_4 = 0$. There is an unstable fixed point at $s = s_c$, separating a flow towards the magnetically ordered Néel state for $s < s_c$, from a $s > s_c$ flow towards the paramagnetic spin liquid with a gapless U(1) photon and gapped spinon excitations. The relevant RG eigenvalue at $s = s_c$ determines a spin correlation length $\xi_{\text{spin}} \sim |s - s_c|^{-\nu}$ which diverges as the critical point is approached. For $s > s_c$, there is an energy gap towards spinful excitations $\sim \xi_{\text{spin}}$ which vanishes as $s \rightarrow s_c$.

Now consider a nonzero $\lambda_4$. Notice that $\lambda_4$ is irrelevant at the $s = s_c$, $\lambda_4 = 0$ fixed point. This means that the above description of the critical properties of $S_2$ applies also to the underlying antiferromagnet. There is, however, a crucial caveat. While $\lambda_4$ is irrelevant at the quantum critical point, for $s > s_c$ the flow of $\lambda_4$ eventually turns around and is attracted towards large values of $\lambda_4$. This happens because $\lambda_4$ is a relevant perturbation to the large $s$ fixed point describing the U(1) spin liquid phase. This phenomenon characterizes $\lambda_4$ as a dangerously irrelevant coupling at the critical point. For $s$ just above $s_c$, the value of $\lambda_4$ becomes very small at length scales of order $\xi_{\text{spin}}$ (or energy scales of order $\sim \xi_{\text{spin}}^{-1}$), but eventually becomes of order unity or larger at a second length scale which we denote $\xi_{\text{VBS}}$. This behaves like $\xi_{\text{VBS}} \sim \xi_{\text{spin}}^\lambda$, where $\lambda > 1$ is a critical exponent; so we have $\xi_{\text{VBS}} \gg \xi_{\text{spin}}$. There is also a corresponding energy scale $\sim \xi_{\text{VBS}}^{-1}$ which is much smaller than the energy gap to spin excitations.

### 5. Implications for heavy electron criticality

We now turn to our discussion to the instability of the heavy Fermi liquid. The analogy with our discussion in Section 4 should now be evident. In the insulating magnets there is a direct second order transition between the Néel state and a state with a very different kind of order (the valence bond solid, VBS). This may be viewed as being analogous to a direct second order transition between the heavy Fermi liquid and the LMM metal where the loss of ‘Kondo order’ happens concomitantly with the appearance of magnetic order. Indeed, both the Néel state (of the insulating magnet) and the FL state (of the Kondo lattice) are stable Higgs phases of a compact U(1) gauge theory. They are un-
stable to a 'deconfinement' transition to the U(1) spin liquid and the FL* phases respectively. However, such deconfined phases are rather fragile states of matter, and can ultimately be unstable to confined phases with conventional order. We reviewed above the instability of the U(1) spin liquid into a VBS state. It is then natural to explore the instability of the FL* state to the LMM, but in a manner that the quantum criticality remains 'deconfined'. In the insulating magnets, the separation between the two competing orders (Neel and VBS) occurs not as a function of a tuning parameter, but dynamically as a function of length/time scale. Indeed, in the paramagnet, the loss of Neel correlations occurs on one length scale $\xi$ while the pinning of the VBS order appears on a much longer length scale $\xi_{\text{VBS}}$ that diverges as a power of $\xi$. By analogy, for the heavy electron systems this strongly suggests that a direct second order transition between the two appropriate competing orders (Kondo order in FL and magnetic order in the LMM metal) is possible but requires at least two diverging length/time scales at the quantum critical point, with deconfinement evident only at the shorter scale(s).

These ideas suggest interesting and important directions for experimental work on heavy electron systems. Are there indeed two or more distinct diverging time/length scales near heavy fermion critical points? In particular, we might expect that the reconstruction of the Fermi surface happens (if it does so at all) at a time scale which diverges slower than the time scale associated with magnetic fluctuations. An immediate consequence is that the Neel temperature, $T_N$, at which magnetism appears in the LMM state, will vanish faster (i.e. with a larger power of the tuning parameter across the quantum phase transition) than the temperature scale, $T_{\text{coh}}$, at which well-defined quasiparticles appear at the large Fermi surface on the FL side (see Fig 5). Further, on the LMM side, there should be an intermediate temperature regime $T_N \ll T \ll T_{\text{coh}}$ in which the properties are those of the small Fermi surface state FL* described in Section 3. The two temperature scales $T_{\text{coh}}$ and $T_{\text{coh}}^*$ must vanish identically on approaching the quantum critical point from opposite sides.

More generally, the presence of two or more diverging length scales will affect the scaling properties of a number of physical quantities near the quantum critical point - probes of the magnetic fluctuations will scale with a different length/time scale from probes of fluctuations associated with the Fermi surface structure. Experiments that elucidate the character of these two possibly different kinds of fluctuations are important, and would be extremely helpful in clarifying the physics behind the non-Fermi liquid behavior near heavy fermion quantum critical points.

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