How do Fermi liquids get heavy and die?

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Abstract

We discuss non-Fermi liquid and quantum critical behavior in heavy fermion materials, focussing on the mechanism by which the electron mass appears to diverge at the quantum critical point. We ask whether the basic mechanism for the transformation involves electron diffraction off a quantum critical spin density wave, or whether a break-down in the composite nature of the heavy electron takes place at the quantum critical point. We show that the Hall constant changes continously in the first scenario, but may "jump" discontinuously at a quantum critical point where the composite character of the electron quasiparticles changes.

1. *Introduction: Mass divergence and the break-down of the quasiparticle concept.*

A key element in the Landau Fermi liquid theory[1, 2, 3] is the idea of quasiparticles: excitations of the Fermi sea that carry the original charge and spin quantum numbers of the non-interacting particles from which they are derived, but whose mass m^* is renormalized by interactions. What is the fate of quasiparticles when interactions become so large that the ground state is no longer adiabatically connected to a non-interacting system? It is known that the quasi-particle mass diverges in the approach to a zero temperature ferromagnetic instability[4, 5, 6, 7]. Recent measurements on three dimensional heavy fermion compounds suggest[8, 9, 11, 12, 13] that the quasiparticle mass also diverges in the approach to an antiferromagnetic quantum critical point. A central property of the Landau quasiparticle, is the existence of a finite overlap "Z", or "wavefunction renormalization" between a single quasiparticle state, denoted by $|\mathrm{qp}^-\rangle$ and the state formed by adding a single electron to the ground-state, denoted by $|e^-\rangle = c^\dagger_{\mathbf{k}\sigma}|0\rangle$,

$$Z = |\langle e^-|\mathrm{qp}^-\rangle|^2. \tag{1}$$

This quantity is closely related to the ratio m/m^* of the electron to quasiparticle mass, $Z \sim m/m^*$ and if the quasiparticle mass diverges, the overlap between the quasiparticle and the electron state from which it is derived is driven to zero, signalling a break-down in the quasiparticle concept. Thus the divergence of the electron mass at an antiferromagnetic quantum critical point (QCP) has important consequences, for it indicates that antiferromagnetism causes a break-down in the Fermi liquid concept[15].

In the late seventies, unprecedented mass renormalization was discovered in heavy fermion compounds. In these materials, quasiparticle masses of order 100, but sometimes in excess of 1000 bare electron masses have been recorded, a significant fraction of which is thought to derive from their close vicinity to an antiferromagnetic quantum critical point. The discovery of the cuprate superconductors in the late eighties further sharpened interest in the effects of strong antiferromagnetic interactions. In these materials, unconventional normal state properties have led many to believe that a combination of strong antiferromagnetic correlations and low dimensionality may lead to a complete break-down of the electron quasiparticle. Against this backdrop, heavy fermion materials acquire a new significance. The appearance of non-Fermi liquid behavior, often in conjunction with anisotropic superconductivity near a heavy fermion quantum critical point tempts us to believe that there may

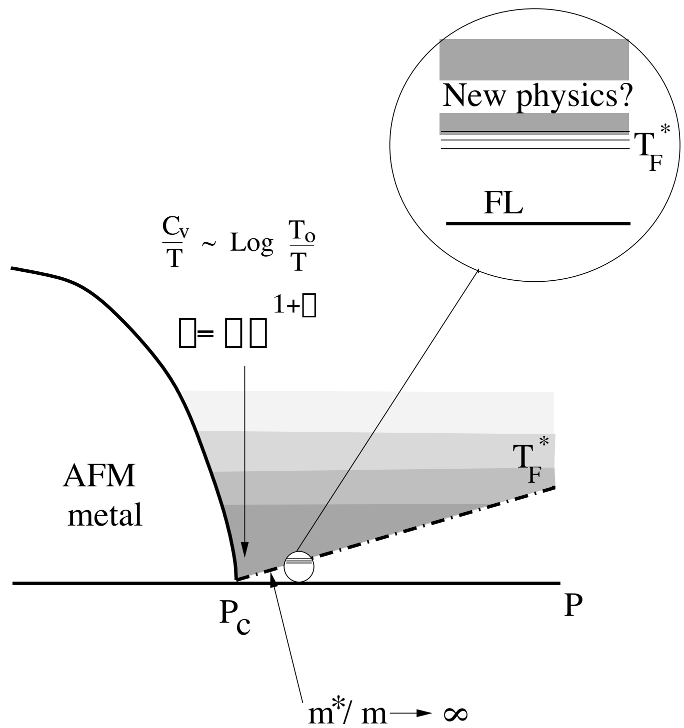


FIG. 1: Schematic illustration of quantum critical point physics in heavy fermion metals. In cerium and uranium heavy fermion systems, pressure drives the system from the antiferromagnet, into the paramagnetic phase. In ytterbium systems, the situation is reversed, and pressure induces antiferromagnetism. The inset emphasizes the point that if the Fermi temperature goes to zero at the quantum critical point, then a new class of universal excitations is expected above T_F^*.

be certain aspects of the quantum critical physics that are shared between heavy fermion and cuprate materials.[10] The clear advantage of heavy fermions lies in the ability to use pressure [14] or chemical pressure [11, 12, 13], to tune them continuously from an unambiguous three dimensional fermi liquid into an antiferromagnetic quantum critical point where non-Fermi liquid behavior is consistently manifested, permitting a first systematic study of the break-down of the Fermi liquid in the presence of critical antiferromagnetism (see figure 1).

Table. 1. Selected Heavy Fermion compounds with quantum critical points.

Compound	P_c/x_c	$\frac{C_v}{T} \to \infty$?	$\rho \sim T^a$	Reference
$CeNi_2Ge_2$	$P_c = 0$	$Log\left(\frac{T_o}{T}\right)^{(a)}$	$T^{1.2}$	[16, 17, 18, 19]
$YbRh_2(Si_{1-x}Ge_x)_2$	$x_c = 0.05$	$Log\left(\frac{T_o}{T}\right)^{(b)}$	T	[20]
$Ce(Cu_{1-x}Au_x)_6$	$x_c = 0.016$	$Log\left(\frac{T_o}{T}\right)$	$T + c$	[11, 12, 13]
$CeCu_{6-x}Ag_x$	$x_c = 0.09$	$Log\left(\frac{T_o}{T}\right)$	$T^{1.1}$	[21]
U_2Pt_2In	$P_c = 0$	$Log\left(\frac{T_o}{T}\right)$	T	[22]
U_2Pd_2In	$P_c < 0$	?	$T + c$	[22]
$CePd_2Si_2$	$P_c > 0$	?	$T^{1.2}$	[16]
$CeIn_3$	$P_c > 0$	?	$T^{1.5}$	[14, 16]
$U_3Ni_3Sn_4$	$P_c > 0$	no	?	[23]
$CeCu_2Si_2$	$Pc = 0$	no	$T^{1.5}$	[24]

$^{(a)}$ New data[25] show a stronger divergence at lower temperatures, and $\gamma \sim A - B\sqrt{T}$ at intermediate temperatures.

$^{(b)}$ At low temperatures, γ diverges more rapidly than $Log\left(\frac{T}{T_o}\right)$[20].

There are several heavy fermion systems that have been tuned to an antiferromagnetic quantum critical point.(See table 1.) Two stoichiometric heavy fermion systems, $CeNi_2Ge_2$[16], U_2Pt_2In[22] lie almost at a quantum critical point at ambient pressure, whilst the compounds $CeCu_6$[13, 21] and $YbRh_2Si_2$[20] can be tuned to a quantum critical point with a tiny amount of chemical pressure, applied by doping. There is a growing list of antiferromagnetic cerium and uranium systems that can be driven paramagnetic by the application of pressure, including $CePd_2Si_2$[14], U_2Pd_2In[22], $CeIn_3$[14] and $CeRh_2Si_2$[26]. Diamond anvil methods are expected to substantially add to this list in the near future.

By its very nature, quantum criticality is hyper-sensitive to disorder, which can never be totally eliminated [27]. Nevertheless, the quantum critical point in the idealized limit of a perfectly clean system poses an intellectual challenge in its own right that must be understood before moving on to the more complex effects of disorder. With this guiding philosophy in mind, we will *not* discuss those materials far from stoichiometry, in which large inhomogeneities are suspected. The discussion here will focus on materials that are explicitly stoichiometric and tuned to the critical point by pressure, or those where critical behavior is insensitive to whether small doping or pressure was used to tune them to criticality. These materials show many common properties:

The key properties of these compounds are:

- Fermi liquid behavior in the paramagnetic phase.[23, 28] One of the classic features of Fermi liquid behavior, a quadratic temperature dependence of the resistivity $\rho = \rho_o + AT^2$ develops at ever lower temperatures, in the approach to the the quantum phase transition, indicating that Fermi liquid behavior survives right up to the quantum critical point.

- Divergent specific heat coefficients at the critical point. In many cases, the divergence displays a logarithmic temperature dependence,

$$\gamma(T) = \frac{C_v(T)}{T} = \gamma_0 \log \left[\frac{T_o}{T} \right]. \tag{2}$$

  This suggests that the Fermi temperature renormalizes to zero and the quasiparticle effective masses diverge

$$T_F^* \to 0, \qquad \frac{m^*}{m} \to \infty \tag{3}$$

  at the quantum critical point of these three dimensional materials. Further support for this conclusion is provided by the observation that the quadratic coefficient A of the resistivity grows in the approach to the quantum critical point[22]. As yet however, surprisingly little is known about the variation of the zero-temperature linear specific heat coefficient in the approach to the quantum critical point.

- Quasi-linear temperature dependence in the resistivity

$$\rho \propto T^{1+\epsilon}, \tag{4}$$

  with ϵ in the range $0 - 0.6$. The most impressive results to date have been observed in $YbRh_2Si_2$, where a linear resistivity over three decades develops at the quantum critical point[20].

- Non-Curie spin susceptibilities

$$\chi^{-1}(T) = \chi_0^{-1} + cT^a \tag{5}$$

with $a < 1$ observed in critical $CeCu_{6-x}Au_x$ (x=0.1), $YbRh_2(Si_{1-x}Ge_x)_2$ (x=0.05) and $CeNi_2Ge_2$. In critical $CeCu_{6-x}Au_x$, the differential magnetic susceptibility dM/dB also exhibits B/T scaling in the form

$$(dM/dB)^{-1} = \chi_0^{-1} + cT^a g[B/T], \tag{6}$$

and extensive inelastic neutron measurements show that the dynamical spin susceptiblity exhibits E/T scaling[29, 30] throughout the Brillouin zone, parameterized in the form

$$\chi^{-1}(\mathbf{q}, \omega) = T^a f(E/T) + \chi_0^{-1}(\mathbf{q}) \tag{7}$$

where $a \approx 0.75$ and $F[x] \propto (1 - ix)^a$. Scaling behavior with a single exponent in the momentum-independent component of the dynamical spin susceptibility suggests an emergence of *local* magnetic moments which are *critically correlated in time* at the quantum critical point. E/T and B/T scaling, with unusual exponents, represent important signatures of universal critical fluctuations, as we now discuss.

3. *Is there Universality at a Heavy Fermion QCP?*

Usually, the physics of a metal above its Fermi temperature depends on the detailed chemistry and band-structure of the material: it is non-universal. A divergence in the linear specific heat of heavy fermion systems at the quantum critical point offers the possibility of a very different state of affairs, for if the renormalized Fermi temperature $T_F^*(P)$ can be tuned to become arbitrarily small compared with the characteristic scales of the material, we expect that the "high energy" physics *above* the Fermi temperature T_F^* is itself, universal. This is an unusual situation, more akin to that in particle physics. This potential for universal fixed point physics above the Fermi temperature is of particular interest, for we expect that like a Fermi liquid, it should involve a robust set of universal excitations, or quasiparticles, describing the emergence of magnetism, whose interactions and energies only depend on the symmetry of the crystal plus a small set of relevant parameters.

In classical statistical mechanics, universality manifests itself through the appearance of scaling laws and critical exponents that are so robust to details of the underlying physics, that they re-occur in such diverse contexts as the critical point of water and the Curie point of a ferromagnet. Dimensionality plays a central role in this universality. Provided that the dimensionality of the classical critical point lies below its "upper critical dimension", then the thermodynamics and correlation functions near the critical point are dominated by a single length scale. The emergence of a single length in the correlation functions and thermodynamics is called "hyperscaling". At the critical point, the Fourier transformed correlation function takes the form

$$S(\mathbf{q}) \propto \frac{1}{|\mathbf{q}-\mathbf{Q}|^{2-\eta}} \ , \tag{8}$$

where $\mathbf{Q}$ is the ordering wavevector. Suppose the system has finite spatial extent L in one or more directions. Below the upper-critical dimension, L is the only spatial scale in the problem, and the correlation function now develops a finite correlation length $\xi \propto L$, so that

$$S(q) = \frac{1}{q^{2-\eta}} F(qL). \tag{9}$$

where $F(x)$ is a universal function of dimensionless parameters. The short-distance physics does not affect the finite correlation length induced by the finite size.

By contrast, if the system is above the upper critical dimension, the quantum critical point is no longer dominated by a single length scale and "naive" scaling laws involve corrections associated with the short-range interaction between the critical modes. [31]. For example, the critical theory governing the liquid gas critical point, the so called ϕ^4 theory has an upper critical dimension $d_u = 4$. Above four dimensions, the short-range interactions, denoted by a parameter U affect the correlation length when the system is near the critical point, so that now the correlation function above the upper critical dimension takes the form

$$S(q) = \frac{1}{q^2} F(q\xi). \tag{10}$$

where the correlation length is now *more* than L, determined by a function of the form

$$\xi^{-1} = L^{-1} G(U, L) \tag{11}$$

where $G(x)$ is a dimensionless function determined by the Gaussian fluctuations about the mean-field theory. Indeed, above $d = 4$, the scaling dimensions of U are $[U] = L^{d-4}$, so that

U and L must enter in the combination U/L^{d-4}. Detailed calculations show that $G \propto U^{\frac{1}{2}}$, so that

$$\xi^{-1} \propto L^{-1} \left(\frac{U}{L^{d-4}} \right)^{\frac{1}{2}} \tag{12}$$

above the upper critical dimension $d = 4$.

Universality in the context of quantum criticality implies the extension of these same principles to the quantum fluctuations that develop at a second-order instability in the ground-state. Quantum critical behavior implies a divergence in both the long distance and long-time correlations in the material. In quantum statistical mechanics, temperature provides a natural cutoff timescale

$$\tau_T = \frac{\hbar}{k_B T} \tag{13}$$

beyond which coherent quantum processes are dephased by thermal fluctuations. We are thus dealing with a problem of finite size scaling in the time direction[31]. If a quantum critical system exhibits hyperscaling, then τ_T must set the temporal correlation length τ, i.e $\tau \propto \tau_T$, so that at the quantum critical point the correlation functions in the frequency domain take the form

$$F(\omega, T) = \frac{1}{\omega^\alpha} f(\omega\tau) = \frac{1}{\omega^\alpha} f(\hbar\omega/k_B T). \tag{14}$$

Since dynamic response functions at energy $E = \hbar\omega$ are directly proportional to correlation functions at frequency ω via the fluctuation dissipation theorem, it follows that dynamic response functions at a quantum critical point below its upper critical dimension are expected to obey E/T scaling[32]

$$F(E, T) = \frac{1}{E^\alpha} f(E/k_B T) \tag{15}$$

Above the upper critical dimension, naive scaling no longer applies. In this case the strength of the short-range interactions between the critical modes play the role of "dangerous irrelevant variables" which affect the correlation time[33]. In a quantum ϕ^4 or "Hertz Millis" field theory,[35, 36], the temporal correlation time above the upper critical dimension takes the form

$$\tau^{-1} = \tau_T^{-1} R(T, U) \tag{16}$$

where $R(T, U)$ is a dimensionless universal function. Near a quantum critical point, the dynamical correlation time τ scales with the spatial correlation length ξ through a dynamical exponent z such that

$$\tau^{-1} \propto \xi^{-z} \ . \tag{17}$$

For a "Hertz Millis" theory of a critical spin density wave[35, 36], $z = 2$ and T and U enter into R as the dimensionless combination $UT^{(d+z-4)/z} = UT^{\frac{1}{2}}$. Furthermore, $R(X) \propto X$, thus $\tau^{-1} \sim UT^{3/2}$ in three spatial dimensions, corresponding to $E/T^{3/2}$ scaling[33].

$$F(E, T) = \frac{1}{E^{\alpha}} f(E\tau) = \frac{1}{E^{\alpha}} f(E/T^{3/2}). \tag{18}$$

For a generic effective Lagrangian ω/T scaling will not occur above the upper critical dimension[34]. Thus the observation of E/T scaling in the dynamical spin susceptibility indicates that the underlying physical theory lies beneath its upper critical dimension. What is this universal "non-Fermi liquid" physics, and what is the mechanism by which the mass of the heavy electrons diverges in the approach to the anti-ferromagnetic instability?

The existence of a Fermi liquid either side of the antiferromagnetic quantum critical point in heavy fermion materials affords a unique perspective on the above question, for it tells us that the universal Lagrangian governing the quantum criticality must find expression in terms of fields that describe the quasiparticles in the Fermi liquid. If we write the low-energy physics of the Fermi liquid in terms of a Lagrangian, we expect to be able to divide it into three terms

$$L = L_F + L_{F-M} + L_M. \tag{19}$$

where L_F describes the free energy of the paramagnetic Fermi liquid, far from the magnetic instability: this term would involve the short-range interactions between the quasiparticles and the band-structure. The last term, L_M describes the magnetic excitations that emerge above the energy scale $T_F^*(P)$ and L_{F-M} describes the way that the quasiparticles couple to and decay into these magnetic modes. We may then ask:

1. what is the nature of the quantum fields that carry the magnetism, whose activation at energy scales above $T_F^*(P)$ is described by the Lagrangian L_M, and

2. what are the interaction terms L_{F-M} that couple the low-energy quasiparticles to these universal, high energy excitations?

4. Spin Density Waves versus Composite Quasiparticles

We shall now contrast two competing answers to this question, one in which non-Fermi liquid behavior derives from Bragg diffraction of the electrons off a critical spin density wave, the other in which the bound-state structure of the composite heavy fermions breaks down at the QCP.

If we suppose first that the QCP is a spin-density wave instability[37] of the Fermi surface, then non-Fermi liquid behavior results from the Bragg scattering of electrons off a critical spin density wave. In this "weak-coupling" approach L_{F-M} is a classical coupling between the modes of a spin density wave and the Fermi liquid

$$L^{(1)}_{F-M} \;=\; g \sum_{\mathbf{k},\mathbf{q}} \vec{\sigma}_{-\mathbf{q}} \cdot \vec{M}_{\mathbf{q}} \tag{20}$$

where $\vec{\sigma}_{-\mathbf{q}} = \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k}-\mathbf{q}} \vec{\sigma} c_{\mathbf{k}}$ is the electronic spin density and $\vec{M}_{\mathbf{q}}$ represents the amplitude of the spin-density wave at wavevector $\mathbf{q}$. In the paramagnetic Fermi liquid, the spin fluctuations have a finite correlation length and correlation time: it is the virtual emission of these soft fluctuations via the process

$$e^{-} \rightleftharpoons e^{-} + \text{spin fluctuation} \tag{21}$$

that then gives rise to mass renormalization. Ultimately, once the magnetic order develops, electron Bragg scattering off the spin density wave causes the Fermi surface to "fold" along lines in momentum space. In this picture, the electrons which form the Fermi surface on the paramagnetic and the antiferromagnetic side of the quantum critical point are closely related to one-another.

The alternative "strong coupling" response to these questions treats the heavy fermion metals as a Kondo lattice of local moments[38]. From this perspective, heavy electrons are *composite* bound-states formed between local moments and high energy conduction electrons. Here, the underlying spinorial character of the magnetic fluctuations plays a central role in the formation of heavy quasiparticles. For instance, the Fermi surface volume, or Luttinger sum rule[39] in the paramagnetic phase "counts" both the number of conduction electrons *and* the number of heavy-electron bound-states, given by the number of spins:

$$2\frac{\mathcal{V}_{FS}}{(2\pi)^3} = n_e + n_{spins} \tag{22}$$

where $\mathcal{V}_{FS}$ is the volume of the Fermi surface, n_e is the number of conduction electrons per unit cell and n_{spins} is the number of spins per unit cell.[40, 41] This scenario departs fundamentally from the spin-density wave scenario if we suppose that at the critical point, the bound-states which characterize the Kondo lattice disintegrate. In this case, the Fermi

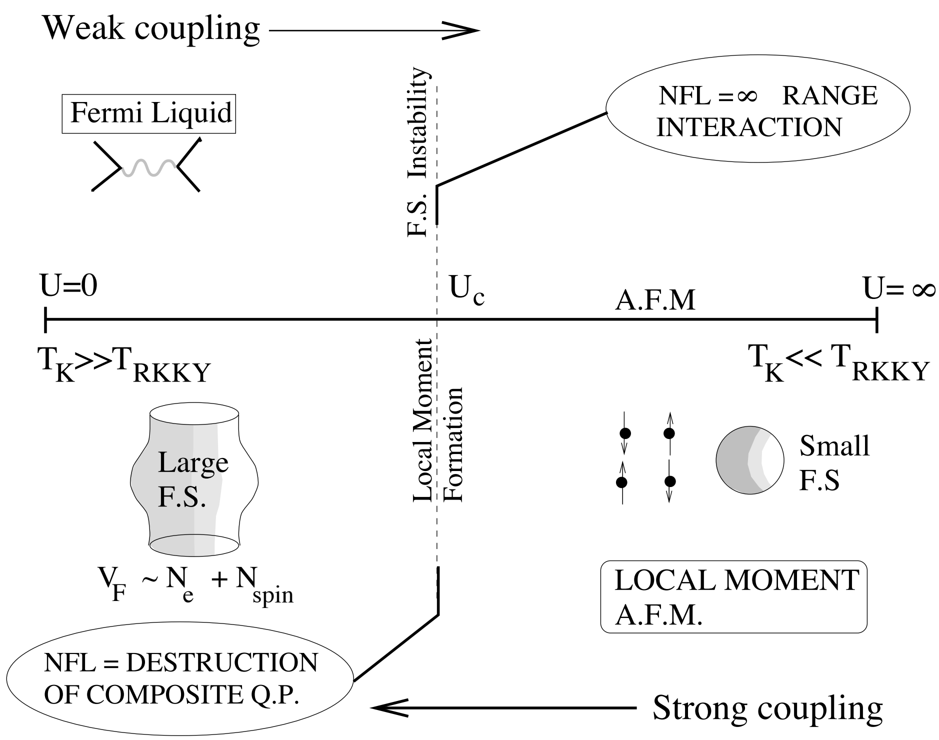


FIG. 2: Contrasting the weak, and strong-coupling picture of an antiferromagnetic QCP.

liquid in the paramagnetic and magnetic phases involve different electron quasiparticles. The antiferromagnet involves a fluid of conduction electrons immersed in a lattice of ordered moments. By contrast, the heavy fermion paramagnet involves quasiparticles built from a bound state between conduction electrons and the local moments: the magnetic degrees of freedom are confined and manifest themselves as new spinorial degrees of freedom. The Fermi surface reconfigures at the QCP to accomodate the changing character and density of the quasiparticles. From this point of view, it is natural to suppose that the spinorial character of the magnetic degrees of freedom seen in the heavy fermion phase will *also* manifest itself in the decay modes of the heavy quasiparticles. For example, the heavy quasiparticles could decay into a neutral "spinon" and a spinless, charge e fermion, schematically $e^-_\sigma \rightleftharpoons s_\sigma + \chi^-$, corresponding to

$$L_{F-M}^{(2)} = g \sum_{\mathbf{k},\mathbf{q}} [s^{\dagger}_{\mathbf{k}-\mathbf{q}\sigma} \chi^{\dagger}_{\mathbf{q}} c_{\mathbf{k}\sigma} + \text{H.c}],$$

where $s^{\dagger}_{\mathbf{q}}$ is a neutral spin-1/2 boson and χ a spinless charge e fermion, reminiscent of a hole in a Nagaoka ferromagnet.[42, 43] Indeed, if the magnetism enters as a spinorial field, its coupling to the electron field can only occur via an inner product over the spin indices as shown in $L_{F-M}^{(2)}$. The collective magnetic correlations of the spinor field oblige us to cast it as a boson, and likewise, statistics forces us to introduce the additional spinless fermion into the coupling. In other words, the idea that magnetism enters into the decay modes as a spinorial field constrains the coupling Lagrangian to the above form.

In this second picture, the scale $T_F^*(P)$ is the threshold energy above which the composite particles decay into their constituent particles and magnetism develops via the condensation of the spinon field. This in turn, transforms the Fermi surface by opening up a resonant channel between the heavy electrons and the spinless fermions.

Let us now examine these alternatives in greater detail (see figure 2).

In the spin-density wave picture, the internal structure of the quasiparticles is unimportant: the physics is entirely described by the interaction between the Fermi surface and critical antiferromagnetic spin fluctuations (Fig 3(a)) Bragg reflections off these critical fluctuations strongly couple the lines of excitations on the Fermi surface that are separated by the critical wavevector $\mathbf{Q}$. Along the hot lines, the electron energies are given by

$$\epsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}-\mathbf{Q}} = 0. \tag{23}$$

Beyond the critical point, the Fermi surface folds along these "hot lines", pinching into two separate and smaller Fermi surfaces, as shown in (Fig 3 (a)). At the quantum critical point, quasiparticles along the "hot lines" are critically scattered with divergent scattering rate and effective mass.

The quantum critical behavior predicted by this model has been extensively studied,[35, 36] and the effective "Hertz-Millis" action describing the critical fluctuations takes the form

$$L_M = \sum_{i\omega_n} \int \frac{d^3q}{(2\pi)^3} |M(q,\omega_n)|^2 \chi_o^{-1}(\mathbf{q},\omega_n) + U \int d^3r d\tau M(\mathbf{r},\tau)^4 \tag{24}$$

where

$$\chi_o^{-1}(\mathbf{q},\omega_n) = \left[(\mathbf{q}-\mathbf{Q})^2 + \xi^{-2} + |\omega_n|/\Gamma_{\mathbf{Q}}\right] \chi_0^{-1} \tag{25}$$

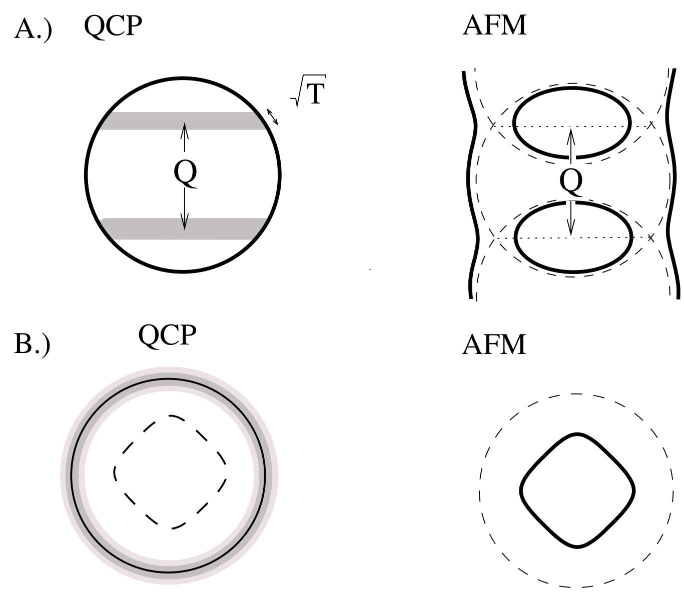


FIG. 3: Competing scenarios for the antiferromagnetic QCP in heavy fermion materials (a) spin density wave scenario, where the Fermi surface "folds" along lines separated by the magnetic Q vector, pinching off into two separate Fermi surface sheets; (b) sudden reconfiguration of the fermi-surface accompanies break-down of composite heavy fermions. The fermi surface in the antiferromagnetic phase only incorporates the conduction electrons.

is the inverse dynamical spin susceptibility of the magnetic fluctuations. The linear damping rate of the magnetic fluctuations is derived from the density of particle-hole excitations in the Fermi sea. $\xi^{-1} \sim (P - P_c)^{\frac{1}{2}}$ is the inverse spin correlation length, whilst $\tau^{-1} = \Gamma_{\mathbf{Q}}\xi^{-2}$ is the inverse spin correlation time. An important feature of this "ϕ^4" Lagrangian is that the momentum dependence enters with twice the power of the frequency dependence and $\tau \sim \xi^z$, where $z = 2$ (the dynamical critical exponent of this theory), so that the time dimension counts as *two* space dimensions, and the effective dimensionality of the theory is

$$D = d + z = d + 2 \tag{26}$$

Assuming $d = 3$ in heavy fermion systems then $D = 5$ exceeds the upper critical dimension $D_c = 4$ for a ϕ^4 theory. This has three immediate consequences

- the interactions amongst the critical modes are "irrelevant", scaling to zero at large scales, so that the long-wavelength antiferromagnetic modes are non-interacting Gaussian modes, or over-damped "phonons". The absence of non-linearities in the interactions means that singularities in the magnetic response will remain confined to the region around the Bragg point, and will not manifest themselves in the uniform susceptibility.

- the temporal correlation time entering into the magnetic response functions will involve $E/T^{3/2}$, rather than E/T scaling [32] (see earlier discussion).
- the correlation functions and thermodynamics will not exhibit anomalous scaling exponents.

The first point is difficult to reconcile with the observation of a singular temperature dependence in the uniform magnetic susceptibility. The second and third points are incompatible with the divergence of the specific heat and the observation of E/T scaling with anomalous exponents[13]. To gain more insight into the physics that lies behind these difficulties, let us examine the nature of the spin fluctuations predicted in this picture. The Gaussian critical spin fluctuations predicted by the quantum spin density wave picture mediate an effective interaction given by

$$V_{eff}(\mathbf{q},\omega) = g^2 \frac{\chi_0}{(\mathbf{q}-\mathbf{Q})^2 - \frac{i\omega}{\Gamma_{\mathbf{Q}}}} \tag{27}$$

In real-space, this corresponds to a "modulated ", but unscreened Coulomb potential

$$V_{eff}(r,\omega=0) \propto \frac{1}{r} e^{i\mathbf{Q}\cdot\mathbf{r}} \tag{28}$$

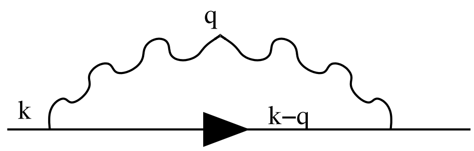
The rapid modulation in the above potential produces Bragg scattering. Unlike a critical ferromagnet, where the singular scattering potential affects all points of the Fermi surface, here the modulated potential only couples electron quasiparticles along "hot lines" lines on the Fermi surface that are separated by the wave-vector $\mathbf{Q}$.

In practice, thermal spin-fluctuations of frequency $\omega \sim k_B T$ are excited, so that electrons within a strip of momentum width

$$\Delta k \sim \sqrt{\frac{k_B T}{\Gamma_{\mathbf{Q}}}} \tag{29}$$

around the hot lines are strongly scattered by the critical fluctuations. The spin-fluctuation self-energy produced by these critical fluctuations is denoted by the Feynman diagram given by

$$\Sigma(\mathbf{k},\omega) = -T\sum_{\mathbf{q},\nu} g^2\chi_o(\mathbf{q},\nu)G(\mathbf{k}-\mathbf{q},\omega-\nu) \tag{30}$$



where g is the strength of the coupling between spin fluctuations and conduction electrons and $G(\mathbf{k},\omega) = [\omega - \epsilon_{\mathbf{k}}]^{-1}$ is the Green function of the conduction electrons. Along the hot lines, this produces a Marginal self-energy of the form $\Sigma(\mathbf{k}_{hot},\omega) \sim \omega\ln[\max(\omega,T)/\Gamma]$, giving rise to a mass renormalization with a weak logarithmic divergence

$$\frac{m^*}{m} \sim 1 - \frac{\partial\Sigma}{\partial\omega} \sim \ln(\Gamma/T) \tag{31}$$

This weak logarithmic divergence only extends along the narrow "hot band" of width $\Delta k \sim \sqrt{T}$: elsewhere on the Fermi surface the electrons are essentially unaffected by the critical fluctuations. For this reason the critical spin fluctuations should only produce a weak singularity in the specific heat, if the quantum critical behavior is described by a spin density wave instability. The residual contribution to the specific heat produced by this narrow band of non-Fermi liquid behavior is expected to depend on $\sqrt{T}$. This can been seen by noting that the singular contribution to the Free energy at the quantum critical point is due to the gaussian fluctuations of the critical antiferromagnetic modes, given by

$$\begin{aligned} F_{sing} &= T\sum_{i\omega_n}\int \frac{d^3q}{(2\pi)^3}\log[\chi_o^{-1}(\mathbf{q},\omega_n)] \\ &= \int \frac{d^3q}{(2\pi)^3}\int\frac{d\nu}{\pi}\left[n(\nu)+\frac{1}{2}\right]\tan^{-1}\left[\frac{\nu/\Gamma_{\mathbf{Q}}}{[(\mathbf{q}-\mathbf{Q})^2]}\right] \end{aligned} \tag{32}$$

By rescaling $\nu = uT$ and $(\mathbf{q}-\mathbf{Q}) = \mathbf{x}\left(\frac{T}{\Gamma_{\mathbf{Q}}}\right)^{\frac{1}{2}}$, we see that

$$F_{sing} = \frac{T^{\frac{5}{2}}}{\Gamma_{\mathbf{Q}}^{\frac{3}{2}}}\int\frac{d^3x}{(2\pi)^3}\int\frac{du}{2\pi}[\coth(u/2)]\tan^{-1}\left[\frac{u}{\mathbf{x}^2}\right] \tag{33}$$

scales as $T^{5/2}$, giving rise to a contribution to the linear specific heat coefficient $\partial^2F/\partial T^2 \sim \sqrt{T}$. Thus the specific heat at the QCP of a critical three dimensional spin density contains a singular $\sqrt{T}$ component, but it is <u>not divergent</u>.

Some aspects of the above picture are modified by disorder. Rosch[44] has argued that a disorder can significantly modify the transport properties of the spin density wave picture. Thus in a strictly clean system, the resistivity should be short-circuited by the electrons far from the hot lines, giving rise to a T^2, rather than a quasi-linear resistivity. High temperatures plus disorder give rise to a resistivity dominated by the average scattering rate, given approximately by a product of the width of the hot line and the linear scattering rate on the hot line ($\sqrt{T} \times T = T^{1.5}$). Rosch has pointed out that the cross-over between these two limits is extremely broad, and gives a quasi-linear resistivity. However, this still does not account for the divergence of the specific heat and the E/T scaling.

One proposed resolution to this paradox is to suppose that the spin fluctuations in the heavy fermion quantum critical systems form a two, rather than three dimensional spin fluid. If, for example, due to the effects of frustration, over the observed temperature range, the spin fluctuations were confined to decoupled planes in real space, then the critical spin physics would be two-dimensional and the effective dimensionality of the quantum critical point would be $2 + z = 4$, putting the fluctuations at their critical dimensionality. This explanation was first advanced by Rosch et al to account for the logarithmic dependence of the specific heat coefficient in $CeCu_{6-x}Au_x$, (x=0.1)[48]. Inelastic neutron scattering experiments on this material do provide circumstantial support for reduced dimensionality, showing that the critical scattering appears to be concentrated along linear, rather than at point-like regions in reciprocal space[13, 48]. In an independent discussion, Mathur et al [14] have suggested that the spin fluctuations in quantum critical $CePd_2Si_2$ and $CeGe_2Ni_2$ might be driven to be two dimensional by frustration.

This two-dimensional SDW picture, however, cannot explain the anomalous exponents – both at and far away from the ordering wavevector $\mathbf{Q}$ – in the neutron and magnetization data. Together with the E/T scaling, the experiments instead suggest a fundamentally new *interacting* fixed point. There are two approaches in the search for such a new universality class. Si et al [45] have recently proposed that quasi-two dimensional spin fluctuations interact with the Kondo effect to produce a "local quantum critical point " which gives rise to localized spin fluctuations with critical correlations in time that exhibit E/T scaling. This picture raises many questions. Do the quasi-2D fluctuations, seen in $CeCu_{6-x}Au_x$, also occur in the other heavy fermion systems with a divergent specific heat coefficient ? More microscopically, why should quantum critical heavy fermion systems have a tendency towards quasi-two dimensional spin fluids, when the transport is highly three dimensional?

On the other hand, Coleman, Pepin and Tsvelik[46], advance the view that the anomalous quantum critical behavior seen in these systems is a feature of a truly three dimensional spin system, but one governed by a new class of quantum critical behavior with upper critical dimension larger than three. But this too raises many questions- in particular- can a field theory of the form (19) be found in which the upper critical spatial dimension is greater than three, and what experimental signatures would this lead to?

The two issues - whether the quantum criticality in heavy fermions is quasi-two dimensional or purely three dimensional, and whether or not it represents a fundamentally new class of quantum critical behavior, lie at the heart of the current debate about these systems. Experimentally, it remains a task of high priority to examine the momentum distribution of the critical scattering, and the extent to which E/T scaling prevails, in stoichiometric quantum critical heavy fermion systems. More detailed information on manifestly three-dimensional systems, such as cubic quantum-critical $CeIn_3$ would also be useful in this respect.

5. *Does the Hall Constant Jump at a QCP?*

We should like to end this discussion by asking what other independent experimental signatures, over and beyond the divergence of the linear specific heat and neutron scattering, can be used to test the mechanism by which the Fermi surface transforms between the paramagnet and the antiferromagnet? Here, one of the most promising, but surprisingly, untested probes is the Hall constant. If the same quasiparticles are involved in the conduction process on both the paramagnetic and the antiferromagnetic side of the quantum critical point, then we expect the Hall constant to vary continuously through the quantum phase transition. If by contrast, the entire character of the Fermi surface changes, for instance, via the creation or destruction of fermionic resonances at the Fermi energy, then we expect that the Hall constant will encounter a discontinuity at the quantum critical point. In the most extreme example, it may even change sign.

To see the logic in this discussion more clearly, consider first the case of a spin density wave. In a Boltzmann transport approach, the Hall conductivity of the Fermi surface is [47]

$$\sigma_{xy} \propto \int dk_z \int \left(\frac{\mathbf{v} \times d\mathbf{v}}{\Gamma^2_{tr}(\mathbf{k})} \right) \tag{34}$$

where $\mathbf{v} = \nabla_{\mathbf{k}} E_{\mathbf{k}}$ is the group velocity on the Fermi surface. The above integral corresponds to the average area swept out by the group-velocity vector around the Fermi surface. When the spin density wave develops, Bragg reflections cause the Fermi surface to fold and pinch into two separate sheets, as illustrated in Fig. 3. The group-velocity on the two separate Fermi surfaces that develop is determined by the renormalized energy

$$E^{\pm}_{\mathbf{k}} = \frac{1}{2}(\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k+Q}}) \pm \sqrt{\left(\frac{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+Q}}}{2}\right)^2 + g^2 M^2_{\mathbf{Q}}} \tag{35}$$

where $\pm$ refers to the dispersion on the two separate sheets, $M_{\mathbf{Q}}$ is the staggered magnetization at wavevector $\mathbf{Q}$ and $\epsilon_{\mathbf{k}}$ is the quasiparticle dispersion in the heavy fermi liquid. Notice that away from the hot lines, the change in the group velocity induced by the magnetic order is second order in the staggered magnetization and that furthermore, the Fermi surface volume is conserved through the transition

$$\begin{aligned} \Delta v_{\mathrm{FS}} &= 0 \\ \nabla_{\mathbf{k}} E^{\pm}_{\mathbf{k}} &= \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}} + O(M^2_{\mathbf{Q}}) \end{aligned} \tag{36}$$

Away from the hot lines we also expect the scattering rate to change no faster than the square of the magnetization. Near the quantum critical point, the Fermi surface becomes increasingly sharp in the vicinity of the hot lines which develop into "corners" of the Fermi surface. (Fig. 4.) Approaching the quantum critical point from the magnetic side, the Hall conductivity can be divided into two parts

$$\sigma_{xy} \sim \left\{ \int_{sheets} dk_z + \int_{corners} dk_z \right\} \int \left(\frac{\mathbf{v} \times d\mathbf{v}}{\Gamma^2_{tr}(\mathbf{k})} \right) \tag{37}$$

The contribution to this integral from the "sheets" of the Fermi surface converge to that of the paramagnetic Fermi liquid. The corners of the Fermi surface correspond to saddle points in the electron dispersion, and close to the quantum critical point the corner regions on the two daughter Fermi surfaces are exact mirror images of one-another with identical scattering rates but equal and opposite group velocities and mass tensors: for this reason the contributions to the Hall conductivity from the saddle point region of one Fermi surface identically cancel the corresponding contribution from the corners of the second. (Fig 4 (c))

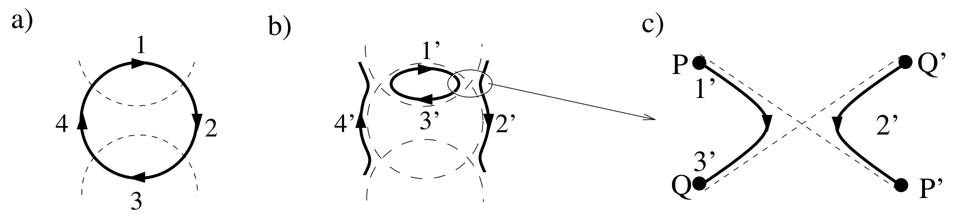


FIG. 4: Fermi surface in (a) paramagnetic phase and (b) spin density wave phase, showing how regions 1-4 have folded and pinched to form two new Fermi surfaces. (c) Expanded detail of the "corners" of the Fermi surface in the vicinity of the saddle point along the hot line. Points P and P', Q and Q' correspond to quasiparticles with the same group velocity and scattering rate, but equal and opposite effective masses. Thus the integrals $\int_P^Q d\mathbf{l} \times \mathbf{l} = -\int_{Q'}^{P'} d\mathbf{l} \times \mathbf{l}$ and the total contribution to the Hall conductivity from the corners of the Fermi surfaces identically cancel.

In the remaining portions of the Fermi surface, the change in the quasiparticle energy and group velocity is proportional to $M_{\mathbf{Q}}$. Since the change in dispersion of the electrons away from the hot lines is dependent on the square of the magnetization, we expect the change in the Hall constant to grow quadratically with the staggered magnetization a quantum critical point is driven by diffraction off a spin density wave.

$$\Delta R_H \propto M_{\mathbf{Q}}^2, \qquad (S.D.W.) \tag{38}$$

which in the simplest models, with $M_{\mathbf{Q}} \propto |P - P_c|^{\frac{1}{2}}$ would imply a jump in dR_H/dP, but no jump in R_H. The continuity of the Hall constant in this scenario is a direct consequence of the continuity in the quasiparticle character, through the transition.

By contrast, if a break-down of composite heavy fermions develops at the quantum critical point, then we expect the more abrupt changes in the Fermi surface to manifest themselves in the Hall constant. In the simplest possible models of heavy electron behavior, the quasiparticles in the Kondo lattice paramagnet are holes with a Hall constant that is opposite in sign to the conduction electrons from which they are formed. If the change in character from conduction electron to heavy electron were to take place at the quantum critical point, the Hall constant might not just jump- it could even change sign at the quantum critical point. To emphasize this more fully, consider the following toy model in which the spinorial character of the magnetism appears in L_{FM},

$$H=\sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+g\sum_{\mathbf{k},\mathbf{q}}[s^{\dagger}_{\mathbf{k}-\mathbf{q}\sigma}\chi^{\dagger}_{\mathbf{q}}c_{\mathbf{k}\sigma}+\mathrm{H.c}]+\lambda\sum_{\mathbf{k}}\chi^{\dagger}_{\mathbf{k}}\chi_{\mathbf{k}}+L_M[s]\ ,$$

where λ is the chemical potential of the spinless fermions. Antiferromagnetism results from a condensation of the spinorial field, $\langle s_{\mathbf{q}\sigma}\rangle=\sqrt{2M_{\mathbf{Q}}}z_{\sigma}\delta_{\mathbf{q}-\sigma\mathbf{Q}/2}$, so that the effective effective Hamiltonian takes the form

$$H=\sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+g\sqrt{M_{\mathbf{Q}}}\sum_{\mathbf{k}\sigma}[\chi^{\dagger}_{\mathbf{k}-\sigma\mathbf{Q}/\mathbf{2}}c_{\mathbf{k}\sigma}+\mathrm{H.c}]+\lambda\sum_{\mathbf{k}}\chi^{\dagger}_{\mathbf{k}}\chi_{\mathbf{k}}+L_M[s]\ . \tag{39}$$

Once the magnetization develops, the the hybridization with the χ fermions has two effects. First, it changes the dispersion of the up and down spin quasiparticles according to

$$\omega^{(\pm)}_{\mathbf{k}}=\frac{\epsilon_{\mathbf{k}}+\lambda}{2}\pm\sqrt{[(\epsilon_{\mathbf{k}}-\lambda)/2]^2+g^2M_{\mathbf{Q}}}. \tag{40}$$

Notice that the change in the dispersion is now first order in the magnetization. Second, the staggered magnetization induced by the condensation of the spin-bosons causes Bragg diffraction which mixes up and down bands to producing fermions with dispersion $E_{\mathbf{k}}$ determined from the roots of the equation

$$\prod_{\pm}(E-\omega^{(\pm)}_{\mathbf{k}})(E-\omega^{(\pm)}_{\mathbf{k}+\mathbf{Q}})=(g^2M_{\mathbf{Q}})^2 \tag{41}$$

There are two main consequences of the disintegration of the heavy fermions- first, the Fermi surface volume now has to change to accomodate the resonances formed by the disintegration of the heavy electrons and second, the change in the dispersion is *first order* in the staggered magnetization:

$$\begin{aligned}\delta v_{\mathrm{FS}}&=n_{\chi}/2\\ \nabla_{\mathbf{k}}E_{\mathbf{k}}&=\nabla\epsilon_{\mathbf{k}}+O(M_{\mathbf{Q}})\end{aligned} \tag{42}$$

Suppose the spinless fermions are in equilibrium with the heavy quasiparticles at the Fermi surface, so that the chemical potential $\lambda=0$ at the quantum critical point, in this case n_{χ} starts out with a finite value, and the Fermi surface volume jumps at the transition. If by contrast, $\lambda\neq 0$ at the transition, then n_{χ} would start out from zero, but the change in the dispersion would still be first order in the staggered magnetization. In the former scenario, the Hall constant jumps at the transition, whereas in the latter it evolves in direct proportion to the change in the staggered magnetization. Summarizing:

$$\Delta R_H \propto \begin{cases} O(1) & (\lambda = 0) \\ M_{\mathbf{Q}} & (\lambda \neq 0) \end{cases} \qquad \text{(composite heavy fermions)} \tag{43}$$

The main point (Table 2.) is that, a large discontinuity in the gradient or jump in the Hall constant is expected in a picture where the quantum critical point involves a break-down of composite heavy fermions, whereas a spin density wave picture predicts a continuous change in the Hall constant with a finite jump in dR_H/dP at the quantum critical point.

6. Conclusion

To conclude, we have discussed the challenge posed by the apparent divergence in quasi-particle masses that appears to develop at a heavy fermion quantum critical point. We have emphasized in some length how this poses severe difficulties for a model based on the development of a spin density wave instability.

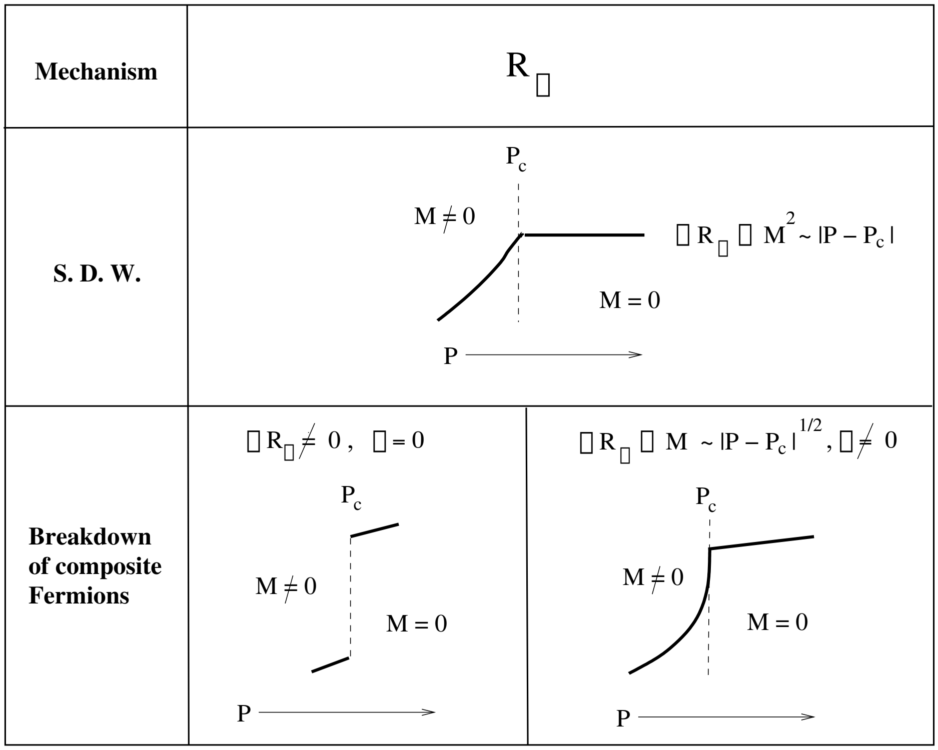


Table 2. Variation of the Hall constant expected in a spin density wave scenario, and a scenario where the composite heavy fermions disintegrate at the quantum critical point. For the purposes of illustration, it is assumed that the magnetization grows as the square-root of the control parameter, $M \propto \sqrt{|P - P_c|}$.

This has set the ground for a lively debate on two different fronts. First and foremost, do the experiments require a more complete break-down in quasiparticle physics than that expected from a quantum spin density wave instability? Second, are the quantum critical fluctuations quasi-two dimensional in character, or is the quantum critical behavior signal a new class of three dimensional quantum criticality? It is hoped that these discussions will stimulate further experimental work . In particular, further experimental clarification would be immensely useful in two separate respects:

- Further evidence for the divergence of the linear specific heat and the collapse of the Fermi temperature near a heavy fermion quantum critical point is needed. More direct specific heat capacity measurements and further measurements of the quadratic coefficient of the resistivity in the approach to the quantum critical point would help to elucidate this issue.

- Careful examination of the evolution of the Hall constant at a heavy fermion quantum critical point will provide the means to check directly whether the Fermi surface "folds and pinches" under the influence of Bragg diffraction off a spin density wave, with no discontinuity in the Hall constant, or whether it undergoes a fundamental transformation due the introduction of new fermionic resonances into the Fermi sea, producing a jump in the Hall constant.

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