Comments on heavy-fermion criticality

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A variety of heavy fermion compounds show quantum critical behavior of some sort

But not much universality

So each is entitled to study their own favorite

Hilbert's is $CeCu_{6-x}Au_x$, mine is $YbRh_2Si_2$ (YRS)

Why YRS?

A bit of history:

Superconductivity in $CeCu_2Si_2$ discovered in 1979.

$T_c = 0.6$ K, $E_F = 10$ K, $m^* \approx 200$

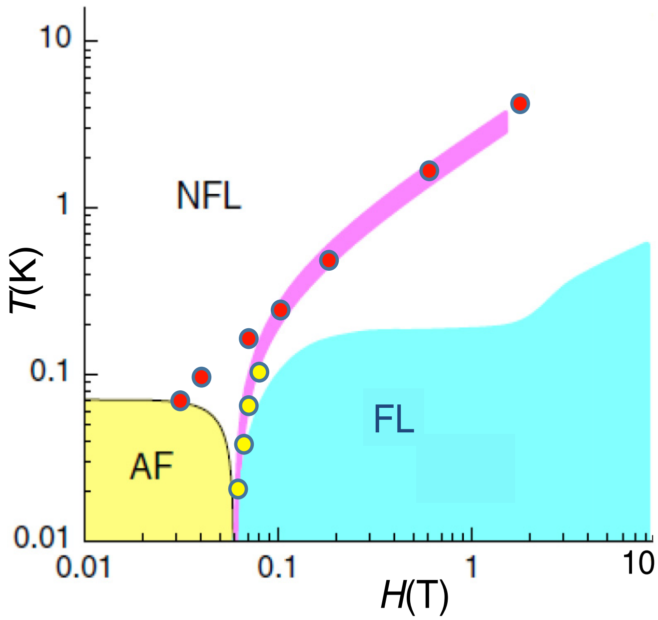
The first high-T_c superconductor!

in $CeCu_2Si_2$, the Ce ion has one f-electron. YRS has the same crystal structure

But the Yb ion has one f-hole. This particle-hole transformation reduces T_c to nearly zero, if not zero

The phase diagram of YRS has interesting features all of which are very small:

- An antiferromagnetic phase, $T_N = 70$ mK with tiny ordered moment $< 0.02\mu_B$ that is shut down at a QCP tuned by H = .070 T
- Perhaps superconductivity at $H = 0$ with $T_c < 3$ mK
- A "T^*-line" (purple), across which various transport quantities appear to jump. Sometimes interpreted as a change from a small Fermi surface to a large one, left to right



Yellow and red dots represent a theoretical alternative to "Kondo breakdown"

"Conventional ('Hertz-Millis') picture of antiferromagnetic metals near QCP

Quantum fluctuations of the of the order parameter (spin fluctuations) described by a bosonic field theory weakly coupled to conduction electrons

The corresponding action is of G-L-W type with $d_{eff} = d + z > 4$, hence in the Gaussian regime

This theory gives predictions for thermodynamic and transport properties, often confirmed.

But sometimes not! *e.g.* $CeCu_{6-x}Au_x$ and $YbRh_2Si_2$.

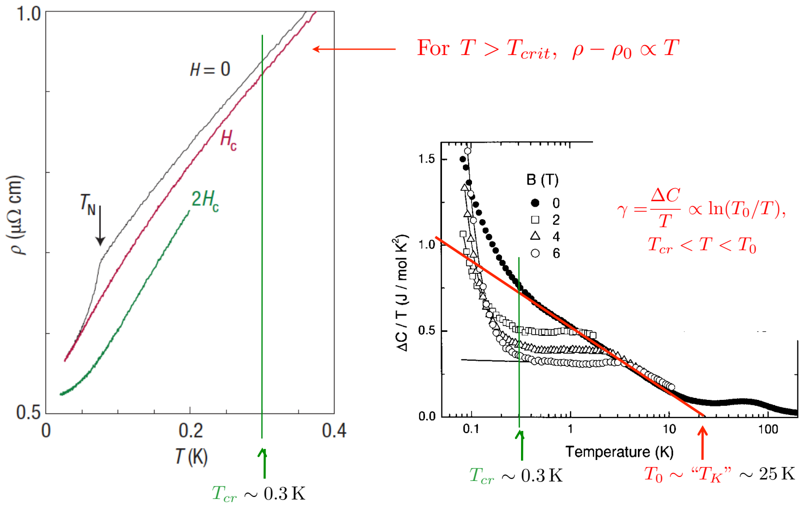
In YRS, at 300 mK there appears to be a crossover from "conventional" non-Fermi liquid behavior

$$\rho(T) = \rho_0 + c/T$$
$$C(T)/T = \log(T/T_0)$$

$T = 300$ mK corresponds to the crossover to $3d$ spin fluctuations and anomalous critical behavior that needs explaining

Theory of critical qps

When the Fermions themselves develop critical behavior (*e.g.* $Z \to 0$, they act back on the boson spectrum.



Anomalous properties of YRS

The latter in turn modifies the qp spectrum- A self-consistent problem.

Formulation with Peter Wölfle and Jörg Schmalian:

Quasiparticle self energy determined by interaction with magnetic fluctuations:

$$\chi''(q,\omega) \sim \frac{(\lambda^2\omega/v_F Q)}{(r+q^2)^2 + (\lambda^2\omega/v_F Q)^2}$$

$r \propto H - H_c$ is the distance to the critical point , q is measured from the ordering vector Q,

λ contains all the feedback effects of the quasiparticles on the spin fluctuation spectrum: Renormalization of v_F, DOS and Landau damping as well as corrections at the spin fluctuation-electron vertex.

Problem presented: The fluctuations couple only the "hot spots" on the FS, connected by $\vec{Q}$.

For critical behavior over the whole FS, invoke impurity averaging.

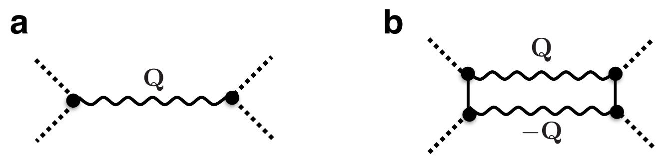
OR -Problem solved courtesy Subir and co workers (PRB 2011):

Couple to composite operator consisting of *two* spin fluctuations peaked at Q and -Q

We view this as an energy fluctuation:

$$K_E \sim \langle \vec{S}_i \cdot \vec{S}_j, \vec{S}_k \cdot \vec{S}_l \rangle \sim \langle S_i^+ S_l^- \rangle \langle S_k^+ S_j^- \rangle + K_{connected}$$

Our energy fluctuation propagator is then built as $\chi_E(q+q') \sim \lambda^4 \sum GG\chi(q)\cdot\chi(q')$ with q, q' near $Q, -Q$ so $\chi_E(q)$ is peaked near $q = 0$ and scattering from energy fluctuations involves the whole FS



Critical fluctuations: **a**. Single spin fluctuation $\mathbf{Q}$. **b**. Structure of the energy fluctuation χ_E. A second contribution has the two spin fluctuation lines crossed.The dashed lines represent the particle-hole excitations at the Fermi surface to which the fluctuations couple. The full lines are excitations far from the Fermi surface, and the black dots represent vertex function λ.

Critical quasiparticles:

The quasiparticle propagator $G(k, \omega)$ has the form $Z(k, \omega)/(\omega - E_k + i\Gamma)$

$Z = 1/(1 - \partial \text{Re}\Sigma/\partial\omega)$ is the quasiparticle weight.

If $Z = 0$, usual case of "non-Fermi liquid" - no qp peak in the spectral function

But - a well-defined peak at $\omega = E_k$ when $\Gamma < E_k$. Then $E_k \to Z\epsilon_k$.

Then $1/Z$ is interpreted as a correlation-induced mass enhancement m^*/m

Suppose $\Sigma \propto \omega^{1-\eta}$. Compare $\Gamma(= Z\text{Im}\Sigma)$ to E_k, get $\Gamma/|E_k| = \tan(\pi\eta/2)$

Then if $0 < \eta < 1/2$, qp peak is well-defined and $Z \propto \omega^\eta$.

Although $Z \to 0$ at the FS, as long as $Z \neq 0$ at non-zero ω (or T) there are defined "critical qps". And Z is contained in the vertex functions λ by various Ward identities

Self-consistent scheme:

1. Compute energy fluctuation propagator and use it to (re)compute qp self energy
2. The result contains powers of Z and ω.
3. Use the new self energy to (re)compute $Z(\omega)$
4. Solve the equation with Ansatz $Z \propto \omega^\eta$
5. Result: $\eta = 1/4\,(d = 3),\ \ 1/8\,(d = 2)$.

The qp condition is satisfied!

Exponents

Because of the dependence of the spin fluctuation propagators on $\lambda(Z)$ and Z, the critical exponents may be read off immediately:

$$z = 4d/3$$
$$\nu = 3/(3+2d)$$

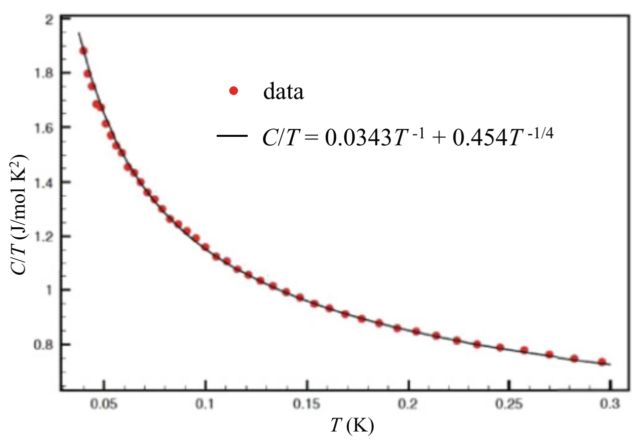
Comparison to experiment: Thermodynamics and Transport

The free energy of the qps involves an integral over the qp self energy.

The actual expression for Σ involves quantities from the self-consistently determined fluctuation propagator, hence z and ν as well as η. One obtains scaling form for free energy density. Example:

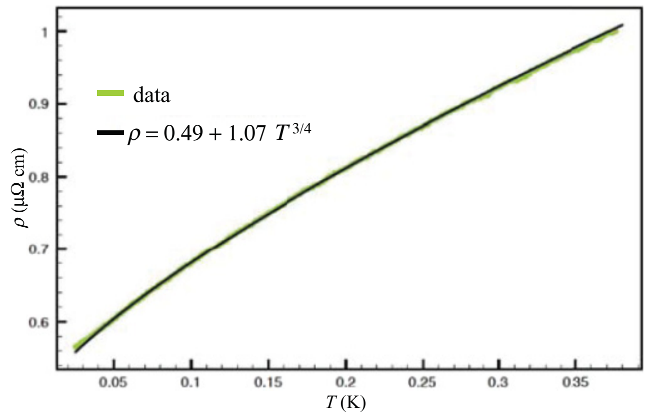
$$f(T,r) \propto T^{2-\eta}[1 + c(r^{z\nu}/T)^{\eta}]^{-1}$$

Specifc heat: $C/T \propto T^{\beta}$ $\beta = -1/4, -1/8$ for $d = 3, 2$



Also power laws for magnetization, susceptibility, magnetic Grüneisen ratio

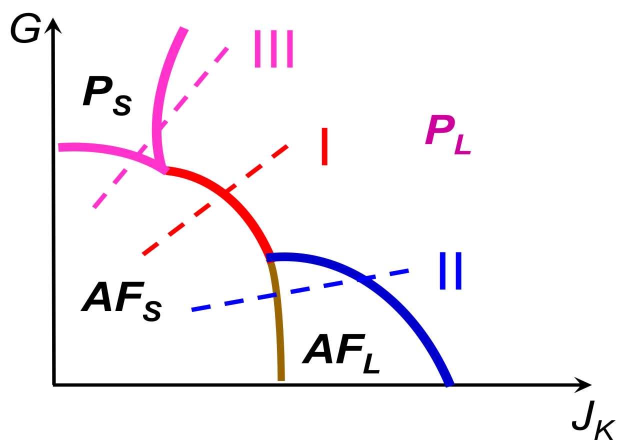
Resistivity: Obtained from the qp $\Gamma = Z\text{Im}\Sigma$. Find $\rho \propto T^{\alpha}$ $\alpha = 3/4, 7/8$ for $d = 3, 2$



Good agreement for $CeCu_{6-x}Au_x$ and $YbRh_2Si_2$: New critical exponents for measured quantities

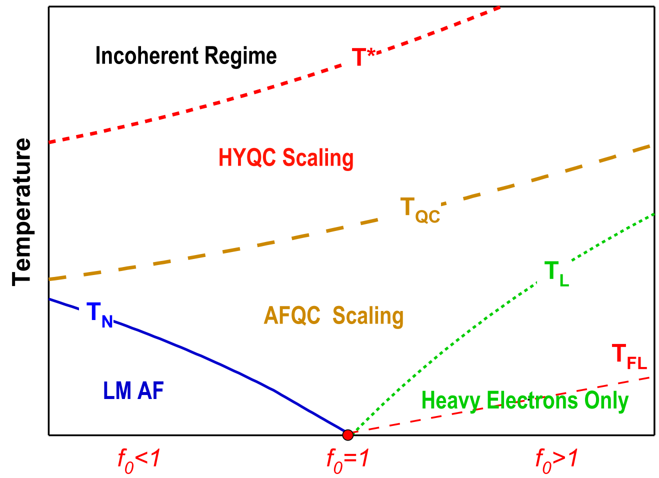
Conclusion: This was an advertisement for our semi-phenomenological theory of critical quasiparticles.

To be fair, there do exist efforts to make more universal statements. For example, a "Global Phase Diagram" (QM Si 2011):



$T = 0$ phase diagram of Kondo lattice. $G \sim$ magnetic frustration (of the RKKY). $J \sim$ Kondo coupling. 4 phases with L(arge) and S(mall) FS

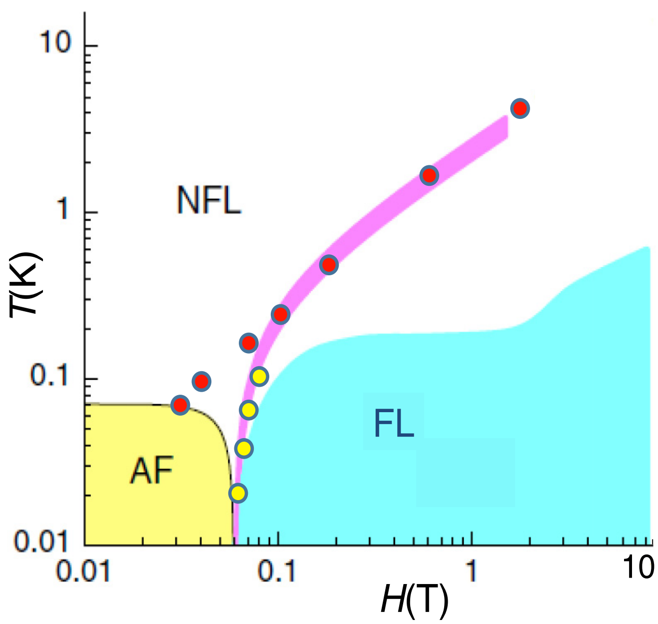
And another: A suggested phase diagram for one of three types of heavy fermion quantum criticality (Yang, Pines, Lonzarich PNAS 2017)



HY="hybridization", LM ="local moment", f_0 ="hybridization strength"

Maybe someone is interested in the colored dots on the T^* line in the first figure?

- Red dots: As T is lowered, onset of scattering of critical qp from electron spin resonance, as observed in ESR.
- Yellow dots: Onset of spin-flip scattering from critical spin fluctuations - depends on renormalized Zeeman splitting



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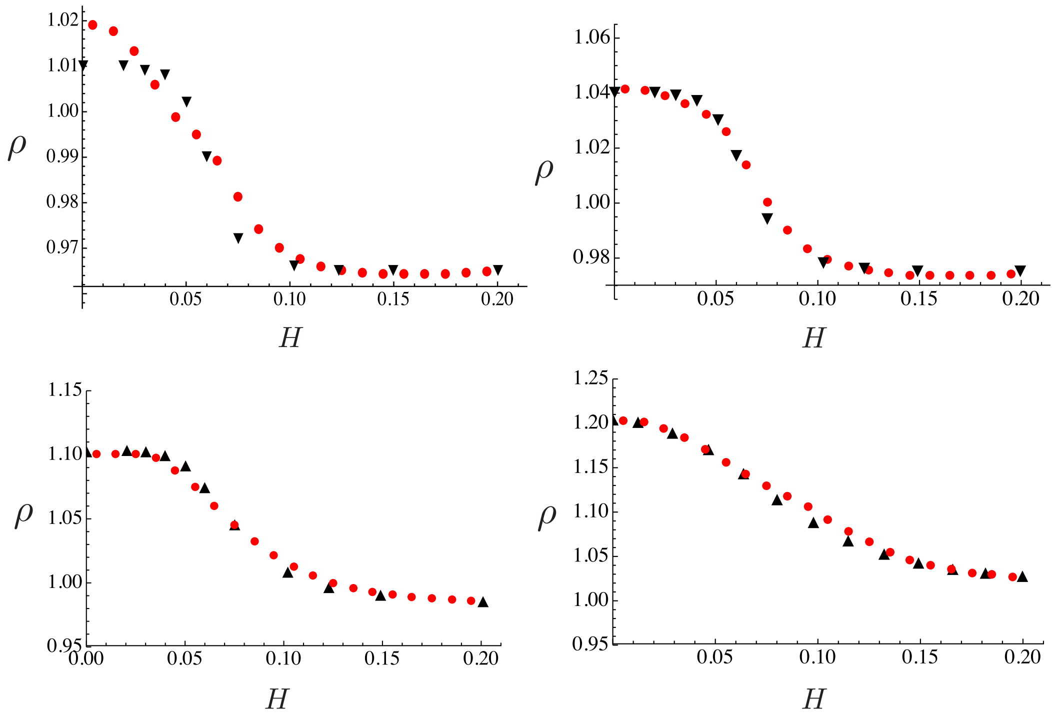
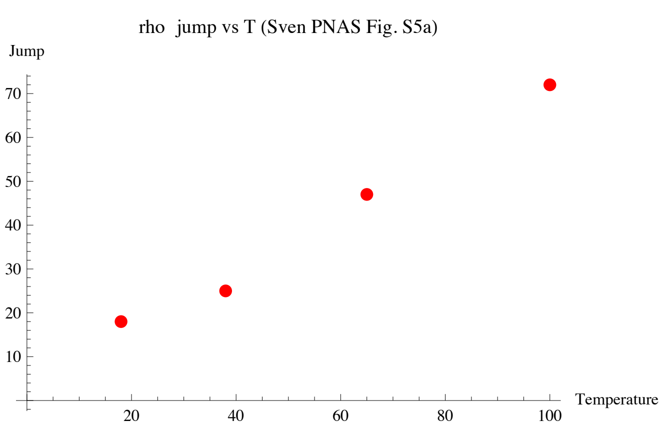
These scattering processes depend on T, H and effect transport. Example: Magnetoresistivity



Magnetoresistivity: Dots are theory, triangles are data. Clockwise from upper left, $T = 18, 38, 65, 100$ mK

One may eyeball the jump at the four temperatures and plot the result

The issue is: Is the jump non-zero as $T \to 0$? In the "Kondo breakdown" scenario, it is. In our scattering scenario, the jump $\to 0$. In my rough estimation, shown here, it is inconclusive.



Jump in the magnetoresistance as function of temperature