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Breakdown of Kondo Effect at a Quantum Critical Point Quantum Critical Point

PAUL Indranil

Centre d'Etudes de Saclay - CEA, Service de Physique Theorique
Orme des Merisiers
Batiment 774
F-91191 Gif sur Yvette
FRANCE

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Breakdown of Kondo Effect At a Quantum Critical Point

Indranil Paul

Institut Laue-Langevin, Grenoble

Collaborators

Catherine Pépin (CEA, Saclay)

Mike Norman (Argonne)

PRL **98**, 026402 (2007)

PRB **78**, 035109 (2008)

Outline

1. Introduction to quantum criticality in the heavy fermions:
   (a) Spin fluctuation theory
   (b) Breakdown of Kondo effect

2. Kondo-Heisenberg model: calculation of thermodynamics & transport

3. Open questions & summary

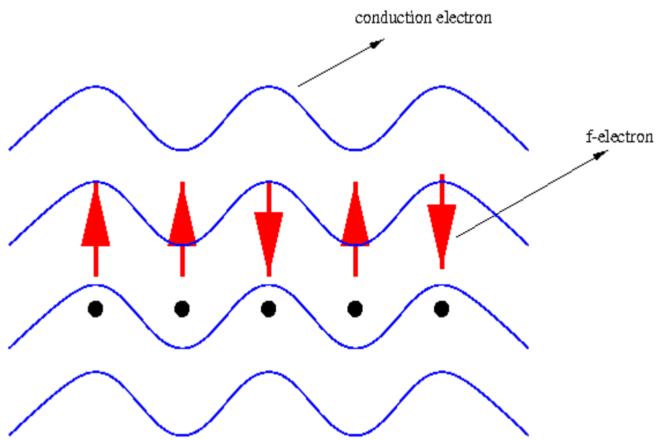
Heavy Fermion Quantum Criticality

Heavy Fermions

Lattice of quantum spins + conduction electrons

Spin exchange interaction (Kondo, Heisenberg)

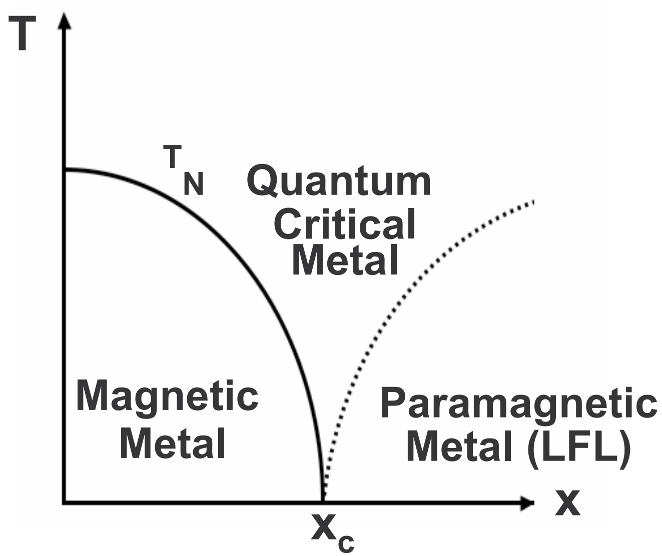
$CeCu_{6-x}Au_x$, $YbRh_2Si_2$, $CeNi_2Ge_2$, $CeCoIn_5$, etc.



Competing mechanisms for entropy reduction

(i) Long range magnetic order

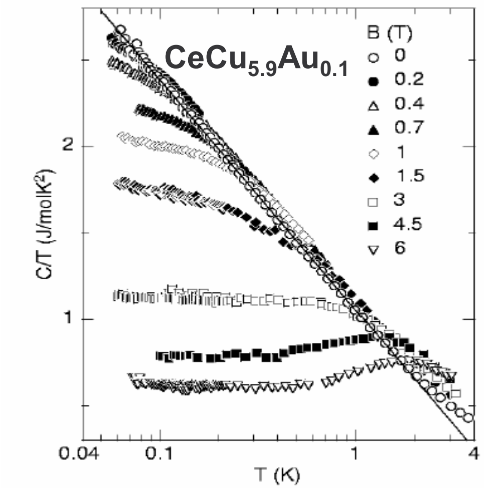
(ii) Kondo screening of quantum spins



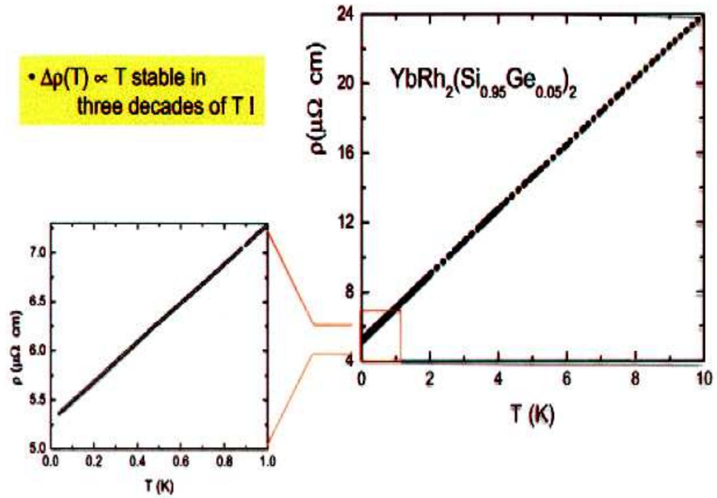
G. R. Stewart, Rev. Mod. Phys., 2001

H. v. Löhneysen *et al*, Rev. Mod. Phys., 2007

Thermodynamics and transport near quantum criticality



H. v. Löhneysen, *et al*, Physica B, **223-224**, 471 (1996)



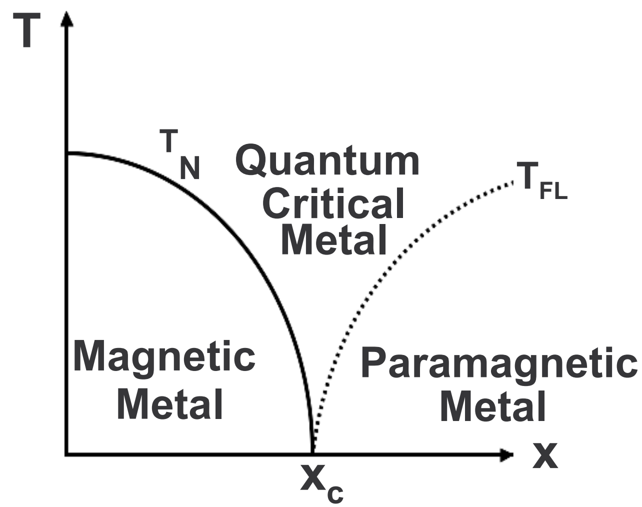
J. Custers, *et al*, Nature **424**, 524 (2003)

Specific heat $C(T) \propto T \log(1/T)$

Resistivity $\rho(T) \propto T$

Normal metals (Landau Fermi liquids)

$C \propto T, \quad \rho \propto T^2$



Challenge

What are the elementary excitations of a quantum critical metal?

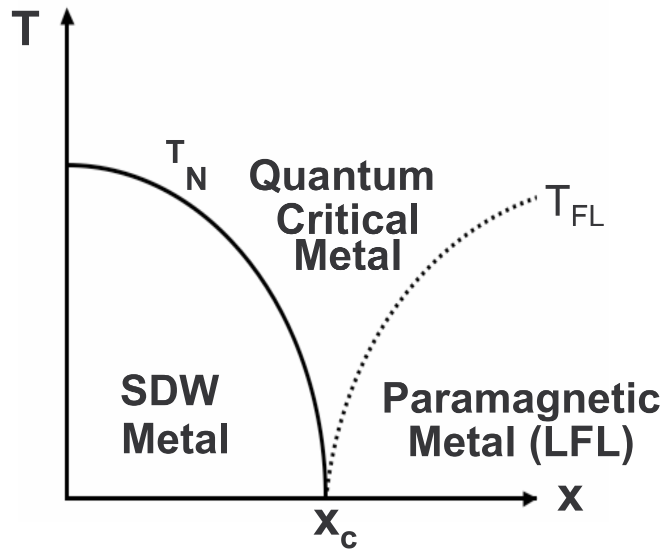
Spin Fluctuation Theory

Assumption
Finite Kondo energy scale below which local moments are screened, and system is a Fermi liquid.

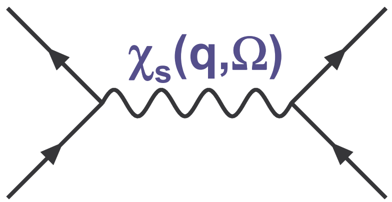
QCP $\rightarrow$ spin density wave instability.
Divergence of spin susceptibility $\chi_s(Q_0)$.

$$\chi_s(q) = \frac{1}{T_{FL} + (q - Q_0)^2}$$

$x \rightarrow x_c$, $T_{FL} \rightarrow 0$



Spin density wave transition of a metal



short range interaction $\rightarrow$ Landau Fermi liquid ($T < T_{FL}$)
long range interaction $\rightarrow$ non-Fermi liquid ($T > T_{FL}$)

- Does not work for most materials
- Requires fine tuning
- Anything qualitatively new possible?

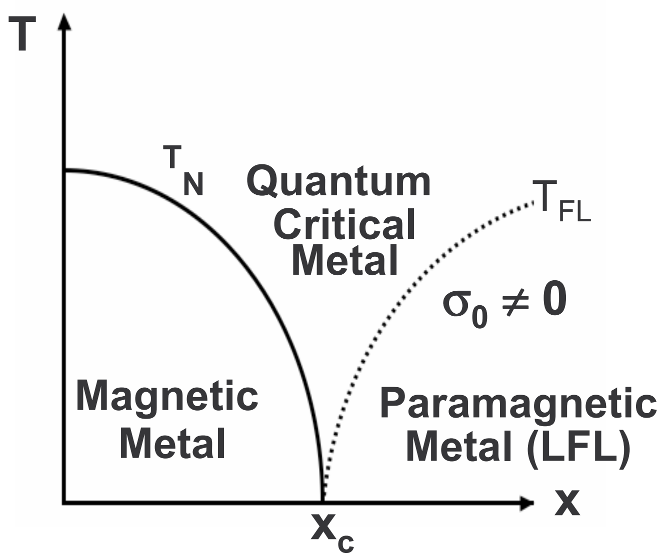
Hertz, PRB 1976; Millis, PRB 1993; Rosch, PRL 1999

Concept of Kondo breakdown

$T_{FL} \rightarrow$ **Kondo energy scale below which FL forms**

Local moments participate in quantum criticality

Coleman *et al*, J Phys Condens Matter 2002
Si *et al*, Nature 2001; Pépin, PRL 2005



"Kondo breakdown" QCP

Kondo hybridization = σ_0

$T_{FL} \approx (\pi\, \sigma_0^2)/E_F$

$\sigma_0 \rightarrow 0$**, vanishing Kondo hybridization gives QCP**

Gapless spin excitation + no long range order = spin liquid (Anderson)

What kind of spin liquid?

Uniform spin liquid

T. Senthil, S. Sachdev, M. Vojta
PRL **90** (2003), PRB **69** (2004)

P. Coleman, J. B. Marston, A. J. Schofield, PRB **72** (2005)
C. Pépin, PRL **98** (2007), arXiv:0802.1498
L. De Leo, M. Civelli, G. Kotliar, PRB **77** (2008)
N. Lanata, P. Barone, M. Fabrizio, arXiv:0807.3849

Effect of critical fluctuations of hybridization on system properties.

Kondo-Heisenberg model (3d)

$$\mathcal{H} = \underbrace{\sum \epsilon_k c^\dagger_{k,\alpha} c_{k,\alpha}}_{\text{cond band}} + \underbrace{J_K \sum \left(c^\dagger_{r,\alpha} \sigma_{\alpha\beta} c_{r,\beta} \right) S^i_r}_{\text{Kondo}} + \underbrace{J_H \sum S^i_r S^i_{r'}}_{\text{Heisenberg}}$$

J_H is *independent* of J_K

J_H can be generated by RKKY and by *super-exchange*

Fermionic representation of spin: $S_{\alpha\beta}(r) = f^\dagger_\alpha(r) f_\beta(r)$

Constraint: $\sum f^\dagger_\alpha(r) f_\alpha(r) = N/2, \quad \forall r$

Hubbard-Stratanovich: $\underbrace{(\sigma^*_K(r), \sigma_K(r))}_{\text{Kondo boson}}$ $\underbrace{\left(\phi^*_H(r,r'), \phi_H(r,r')\right)}_{\text{Heisenberg boson}}$

Uniform spin liquid phase: $\phi_H(r,r') = \phi_0 e^{i \int_r^{r'} \vec{A}\cdot\vec{dl}}$

$$\sigma^\dagger_i \rightarrow \sum_\alpha f^\dagger_{i\alpha} c_{i\alpha}$$

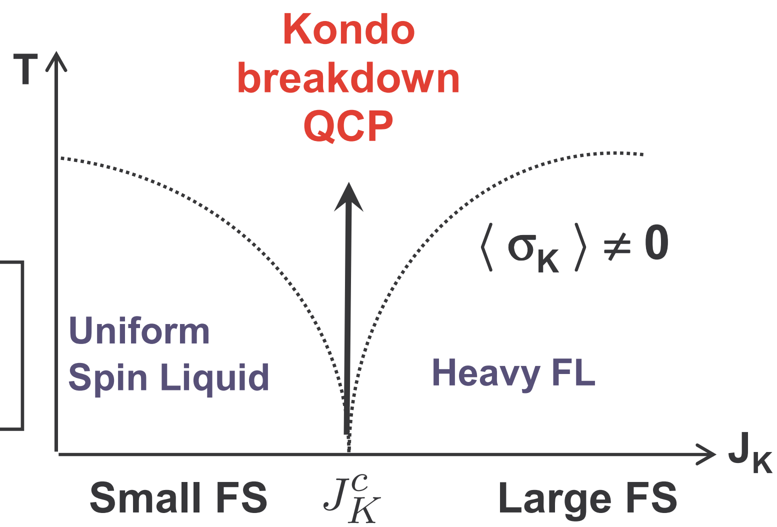
$$\phi_{ij} \rightarrow \sum_\alpha f^\dagger_{i\alpha} f_{j\alpha}$$

ϕ_0 gives dispersion to spinons. Bandwidth = J_H

Mean Field Phase Diagram

Un-hybridized

c- and f- bands



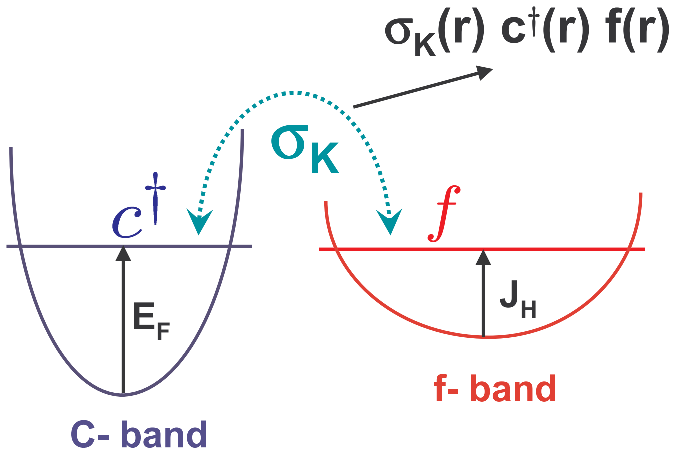
Hybridized

c- and f- bands

Senthil, Sachdev, M. Vojta, PRL **90**

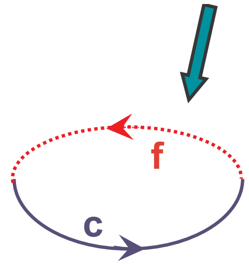
Heavy Fermi liquid phase sets in only for $J_K > J_K^c$
Very different from Coleman ('87); Millis, Lee ('87)
Crucial ingredient: dispersion of the spinons (J_H)
No phase with magnetic LRO !

Mean Field Theory



Kondo boson condensation:

$$\frac{\partial^2 F_{\mathrm{MF}}}{\partial |\sigma_K(q)|^2} = \frac{1}{J_K} + \Pi_{fc}(q,0) = 0$$



$$\frac{1}{J_K} - \frac{1}{E_F} \ln\left(\frac{1}{\alpha}\right) = 0$$

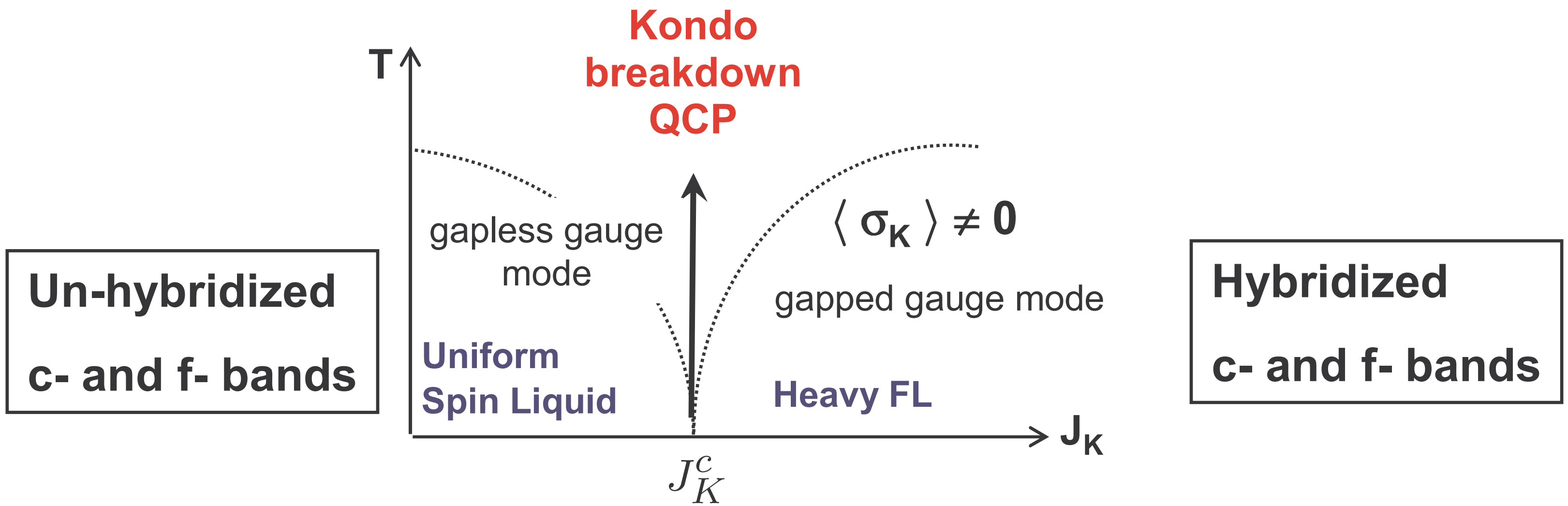
$\alpha = J_H/E_F$

$T_K^0 (J_K) = E_F \exp[- E_F/J_K]$ (1-impurity Kondo-T)

At QCP $T_K^0 (J_{Kc}) \approx J_H$ (Doniach's competition of scales)
$T_K^0 \sim 10$ K, $E_F \sim 10^4$ K $\Rightarrow \alpha \sim 10^{-3}$
FL phase is indeed heavy!

IP, C. Pépin, M. Norman PRL **98**

S. Burdin et. al., PRB **66**



U(1) Higgs phenomena: For $J_K > J_{Kc}$
σ_K condenses, and gauge field is gapped

Senthil, Sachdev, Vojta PRL **90**

Competition between Kondo effect and spin liquid. At QCP $T_K^0 (J_{Kc}) \approx J_H$.
Demanding consistency with experiments give $\alpha = J_H/E_F \ll 1$.
FL phase is indeed heavy!

IP, C. Pépin, M. Norman PRL **98**

Fluctuations: Gauge theory

Gapless excitations:

1. **Gauge fluctuations:** $\phi_H(r,r') \to \phi_0 e^{i\vec{A}\cdot(\vec{r}-\vec{r}')}$
2. **Hybridization fluctuations:** $\sigma_K(r) \to \langle \sigma_K \rangle + \delta\sigma_K(r)$

Gauge fluctuations **($\nabla \cdot$ A = 0)** **Senthil *et al*, PRB, 69 (2004)**

$$D_{\mu\nu}(q,i\Omega) \equiv \langle A_\mu A_\nu \rangle \propto \left[\delta_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}\right] \frac{1}{q^2 + |\Omega|/q}$$

(over-damped dynamics)

z=3

$$\boxed{\gamma \equiv -\partial^2 F/\partial T^2 \propto \log\left(\frac{\alpha E_F}{T}\right)}$$

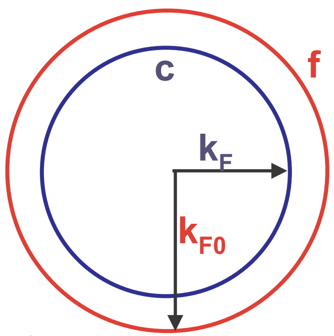
Band Structure Dependence

1. Spinon bandwidth = $J_H = \alpha E_F$

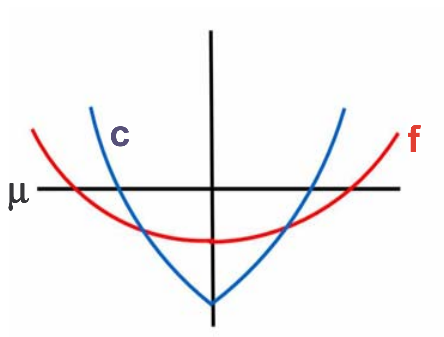
$E_F \sim 10^4$ K, $T_K^0 \sim J_{\mathcal{H}} \sim 10$ K $\Rightarrow$ $\alpha \approx 10^{-3}$

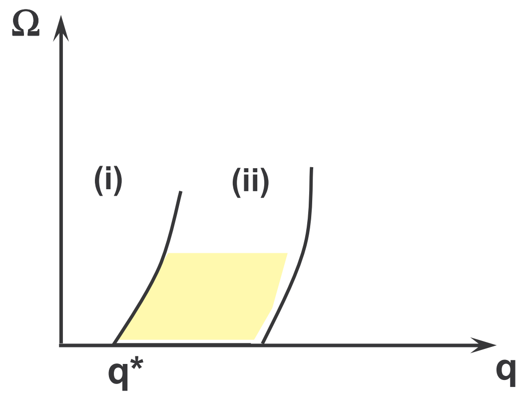
2. Spinon band is 1/2- filled, conduction band is not.

$(q^*/k_F) \approx 0.1$ (non-universal parameter)



$$\underbrace{q^* \equiv k_{F0} - k_F}_{\text{Fermi surface mismatch}}$$

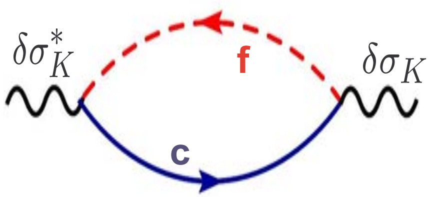




2-band particle-hole continuum starts at finite wave-vector q*

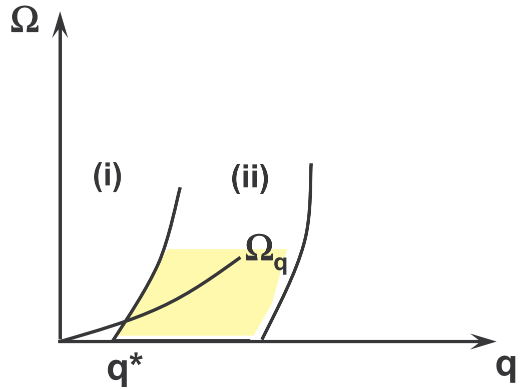
Hybridization Fluctuations

Kondo boson propagator: $D_\sigma(q, i\Omega) \equiv \langle \delta\sigma_K^* \delta\sigma_K \rangle$



(i) q < q*: $D_\sigma(q, i\Omega_n)^{-1} \approx \frac{q^2}{k_F^2} - \frac{i\Omega_n}{\alpha v_F q^*}$ **(z=2)**

(ii) q > q* : $D_\sigma(q, i\Omega_n)^{-1} \approx \frac{q^2}{k_F^2} + \frac{|\Omega_n|}{\alpha v_F q}$ **(z=3)**



regime (ii) gives leading contribution

$E^* \equiv \alpha\, E_F\, (q^*/k_F)^3 \sim 10$ mK

UV cut-off = $\alpha\, E_F \sim 10$ K

$(q^*/k_F) \approx 0.1$

$\alpha = (T_K^0/E_F) \approx 10^{-3}$

Thermodynamics

Free energy:

$$F = T \, \mathrm{Tr} \log \left[D_\sigma^{-1}(q, i\Omega_n) \right]$$

Specific heat coeff:

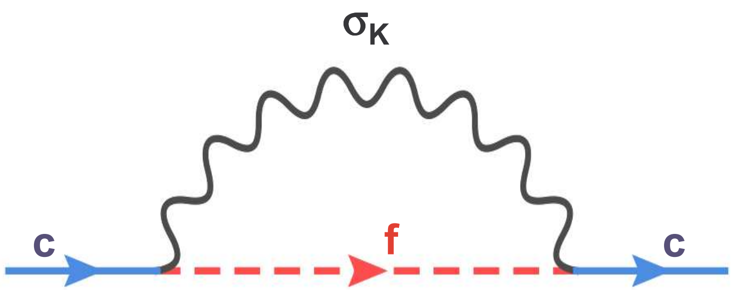
$$C/T \equiv \gamma \propto \begin{cases} \log(\alpha E_F / T) & E^* < T < \alpha E_F \\ \mathrm{const} & T < E^* \end{cases}$$

(d=3, z = 3, IR cutoff)

$E^* \equiv \alpha\, E_F\, (q^*/k_F)^3 \sim 10$ mK

UV cut-off = $\alpha\, E_F \sim 10$ K

Conduction Electron Self Energy



$$\text{Im}\Sigma_c(k_F,\omega) \propto \begin{cases} \omega & E^* < \omega < \alpha E_F \\ \omega^2 & \omega < E^* \end{cases}$$

(d=z, IR cutoff)

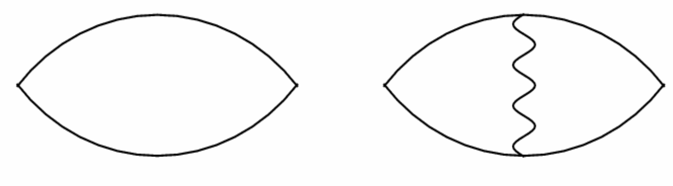
$$\text{Im}\Sigma_c(k_F,\omega=0,T) \propto \begin{cases} T\log(T/E^*) & E^* < T < \alpha E_F \\ T^2 & T < E^* \end{cases}$$

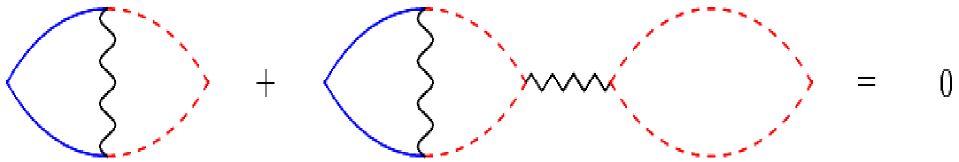
A microscopic mechanism to obtain *marginal Fermi liquid* in three dimensions

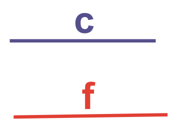
Resistivity

Transport time (τ_{tr}) & particle lifetime (τ_{QP})

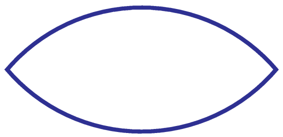
In single band model $\tau_{tr} \neq \tau_{QP}$
(vertex correction gives partial cancellation)







Spinon current vertex is zero. (gauge invariance)

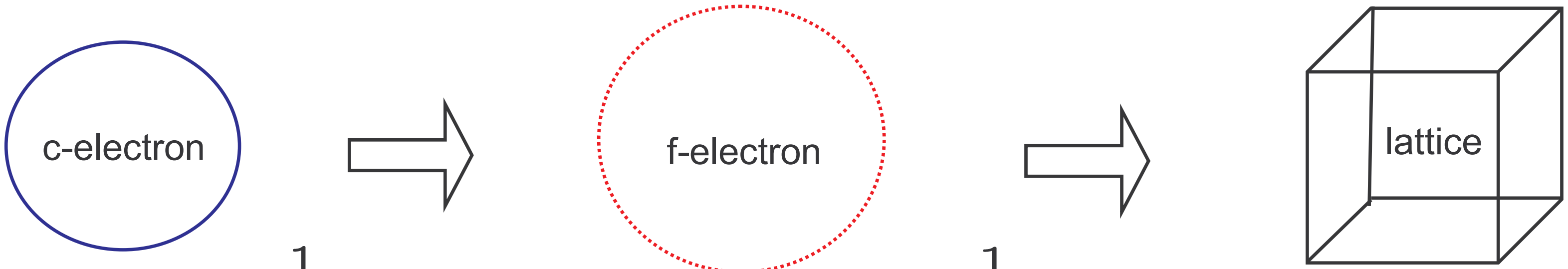


Survives in Kondo-Heisenberg model
$\tau_{tr} \approx \tau_{QP}$

Spinons provide a bath for conduction electrons to relax momentum

$$\rho(T) - \rho(0) \equiv \delta\rho(T) \propto \begin{cases} T \log(T/E^*) & E^* < T < \alpha E_F \\ T^2 & T < E^* \end{cases}$$

Transport Rate



$\frac{1}{\tau_{cf}} \propto \mathrm{Im}\Sigma_c$

$\frac{1}{\tau_f}$ **(Umklapp)**

For $E^* < T < \alpha E_F$:

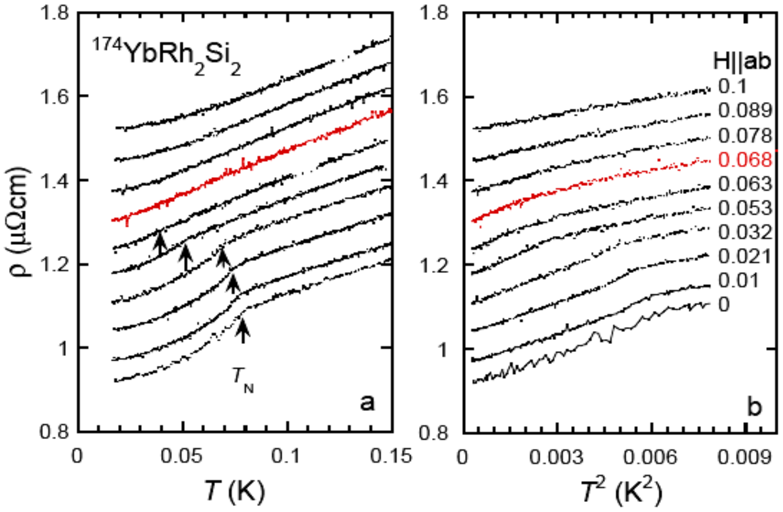
$1/\tau_{cf} \propto T/E_F$

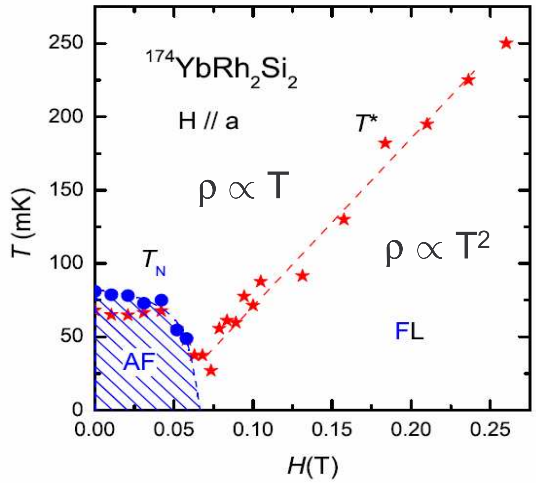
$1/\tau_f \propto T^2/(\alpha E_F)^2$

$\Bigg\}$ $1/\tau_f >> 1/\tau_{cf}$

$$\rho(T) - \rho(0) \equiv \delta\rho(T) \propto \begin{cases} T \log(T/E^*) & E^* < T < \alpha E_F \\ T^2 & T < E^* \end{cases}$$

Finite Energy Scale in Quantum Critical Regime





Finite T* at QCP from resistivity

J. Phys. Soc. Japan **75**, 114709
(group at Grenoble)

Finite low-energy scale near Kondo breakdown QCP ?

Conclusion

Breakdown of Kondo effect

Transition from uniform spin liquid to heavy Fermi liquid.

Microscopic realization of Doniach's competition of energy scales.

$T_K^0 (J_{Kc}) \approx J_H$

Critical fluctuations of hybridization

Infrared cutoff $T^* \sim 10$ mK

dynamical exponent $z=3$

Marginal Fermi liquid in three dimensions

$\mathrm{Im}\, \Sigma_c (\omega) \propto \omega$, above T*

Resistivity has quasi-linear T-dependence

$\rho (T) \propto T \log (T/E^*)$, above T*