Transport and optical properties of heavy fermions

Theo Costi
Institute for Solid State Research,
Research Centre Jülich, Germany

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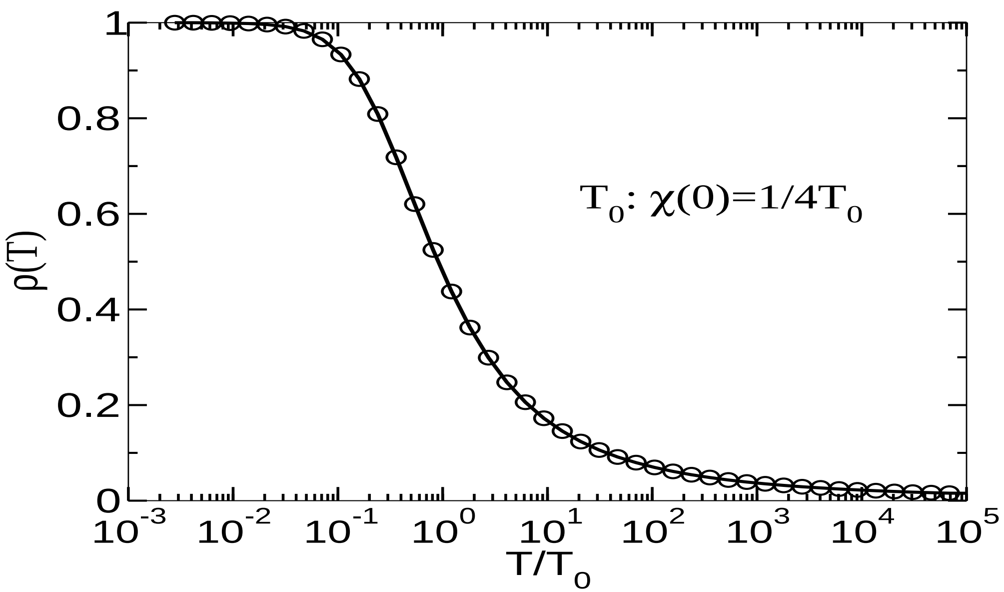
- What are the low energy scales in (paramagnetic) heavy fermions ?
- How are these manifested in physical properties such as
  - spectra,
  - dynamical susceptibilities,
  - resistivities,
  - optical conductivities ?
- In what sense is there universality and scaling in heavy fermions ?

T. A. C., N. Manini, JLTP 2002 & unpublished

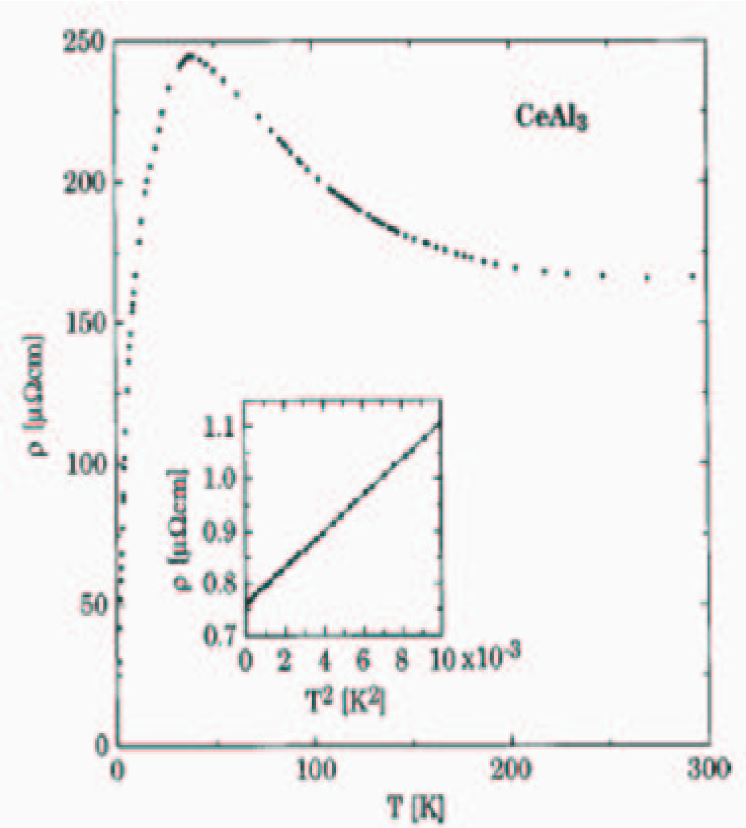
Motivation:single Kondo impurity

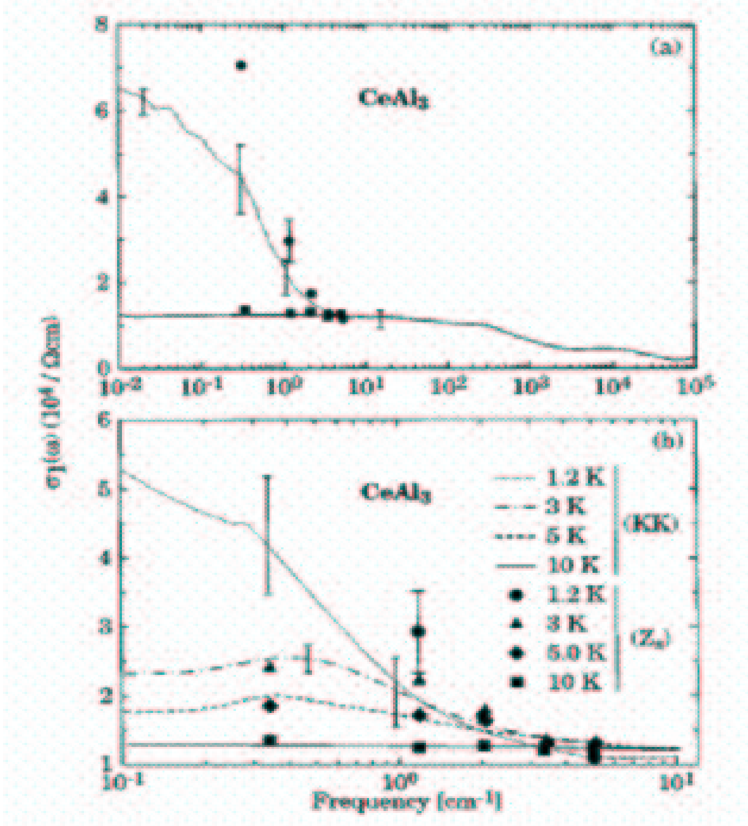
$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + J\, \mathbf{S}_0 \cdot \mathbf{s}_0$$

- One low energy scale:
  - $T_K = f(J/D)$
  - Fermi liquid scale $T_0 = T_K$
- universal scaling functions:
  - $\rho(T, J/D) \Rightarrow f_\rho(T/T_K)$
  - $A(\omega, T, J/D) \Rightarrow f_A(\omega/T_K, T/T_K)$



Motivation:experiments, e.g. Andres et al 1975





- Fermi liquid coherence scale $T_0 \approx 3K$.
- $T_{max} = 35K \approx 10T_0$. However, $T_{max} \neq T_K$!
- In fact T_K generally absent in $\rho(T), \sigma(\omega, T)$.

Kondo Lattice Model

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \; c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{j} J \; \mathbf{S}_j \cdot \mathbf{s}_j$$

Solve for paramagnetic solutions by DMFT(NRG) on a Bethe-Lattice :

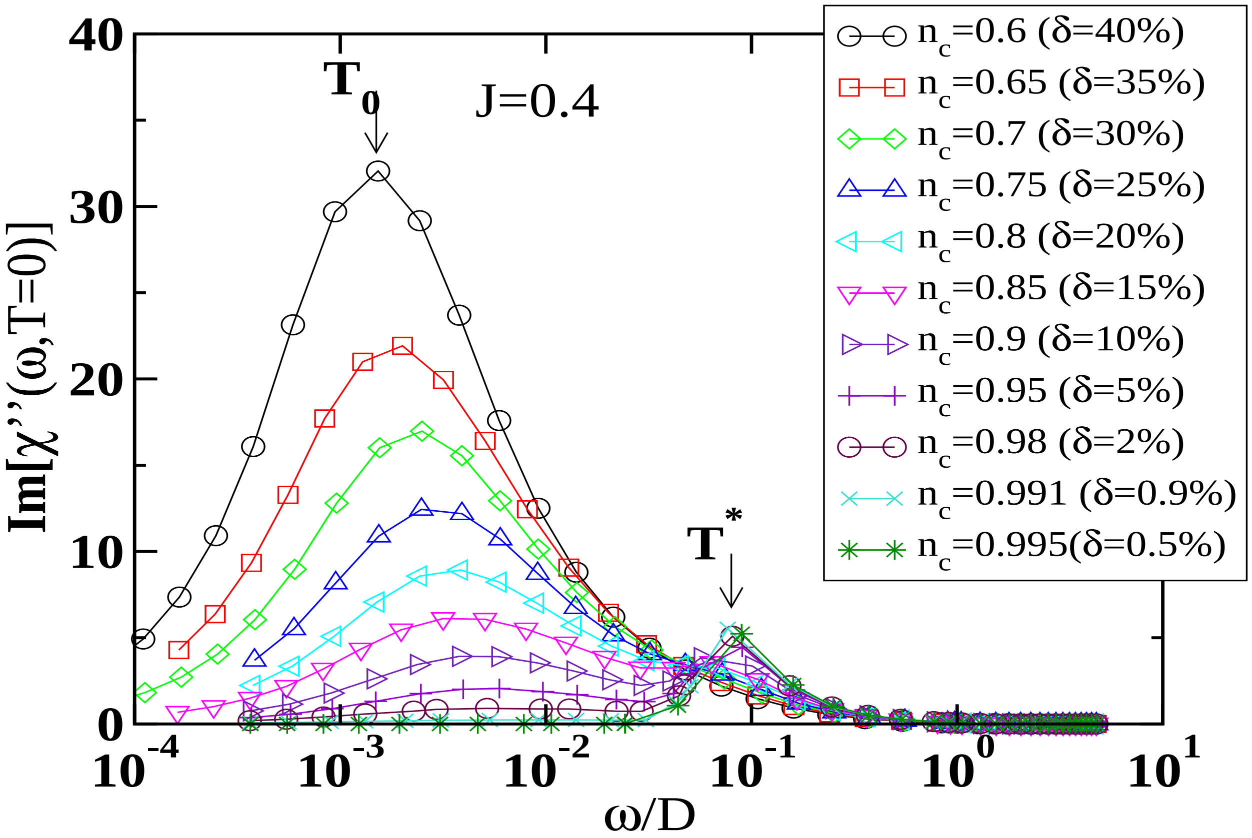
$$N_0(\varepsilon_k) = \frac{2}{\pi D^2} \sqrt{D^2 - {\varepsilon_k}^2}$$

Consider c-electron fillings $0 < n_c < 1$ (hole dopings $0 \leq \delta \leq 1$).

Calculate :

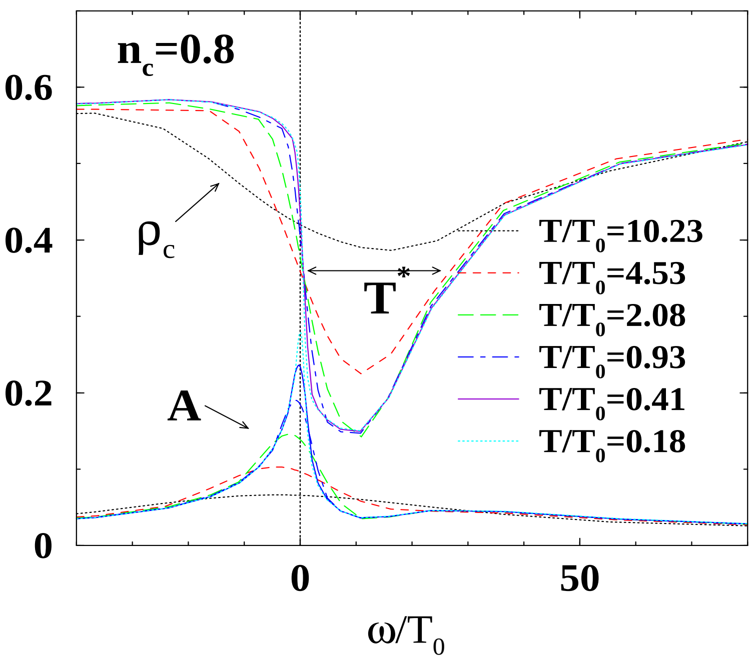
- $\Sigma_\sigma(\omega, T)$, c-electron self-energy
- $\rho_c(\omega, T)$, c-electron DOS
- $A(\omega, T)$, f-electron DOS
- $\chi(\omega, T)$, dynamical susceptibility
- $\sigma(\omega, T)$, optical conductivity
- $\rho(T)$, resistivity

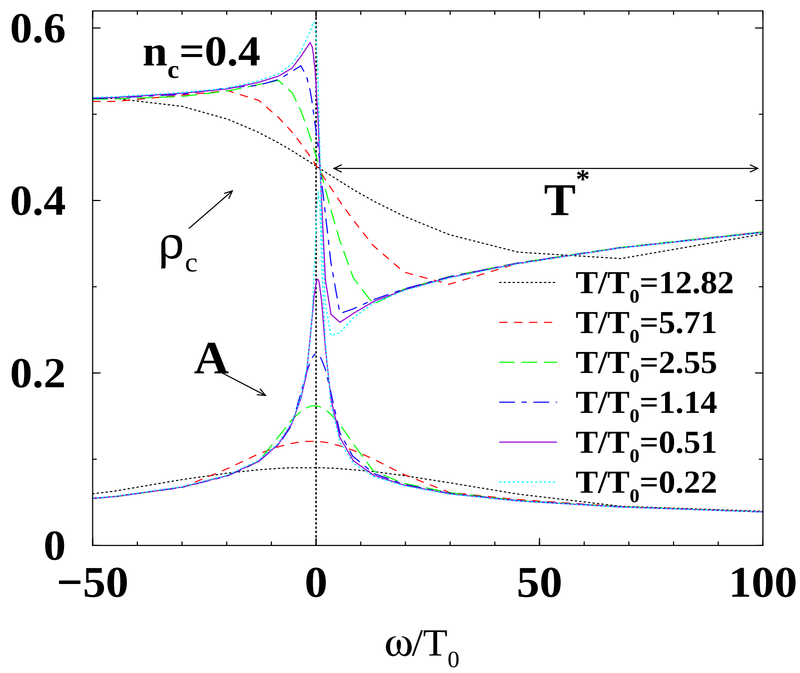
Low energy scales in $\chi(\omega, T)$



- Fermi lquid scale T_0, discernible in χ for all $\delta > 0$.
- Single-ion Kondo scale $T^* = T_K$, descernible in χ for $\delta < 20\%$

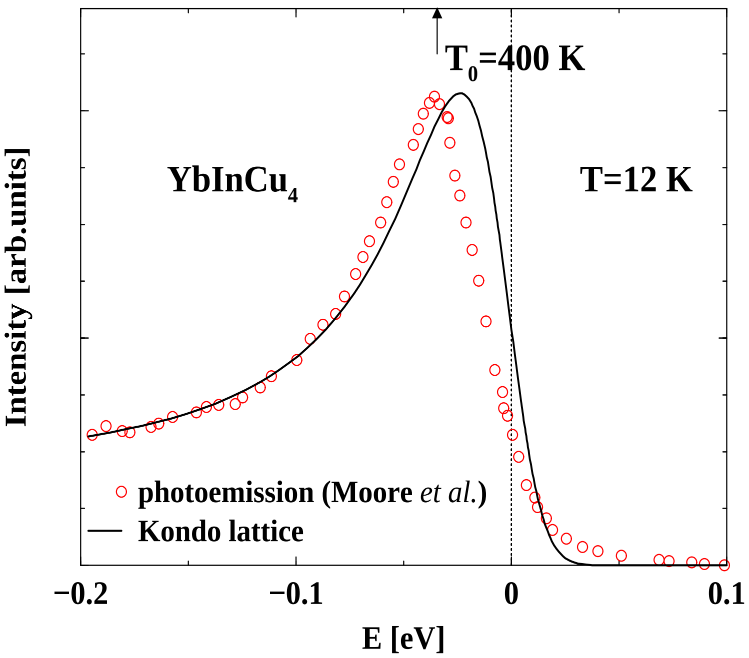
Low energy scales in spectra

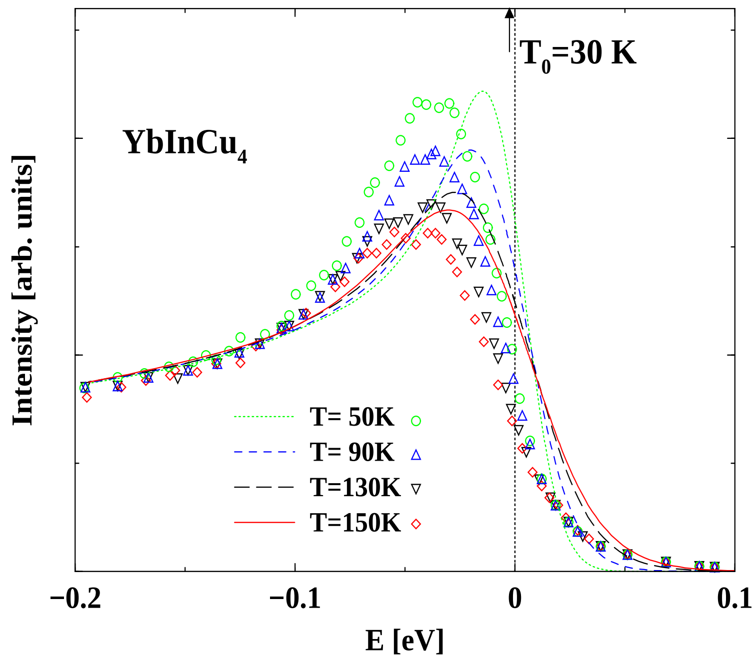




- $T^* = T_K$ discernible in f-electron spectrum $A(\omega)$ only for $\delta < 20\%$
- $T^* = T_K$ allways discernible in c-electron spectrum $\rho_c(\omega)$.
  Suggests tunneling measurement to obtain $T^* = T_K$ from local c-electron DOS.
- T_0 sets T-dependence of $A(\omega = 0, T)$, $\rho_c(\omega = 0, T)$.
- $T_0/T_K \longrightarrow 0, n_c \longrightarrow 0$ (Pruschke et al. Anderson Lattice, PRB 1999)

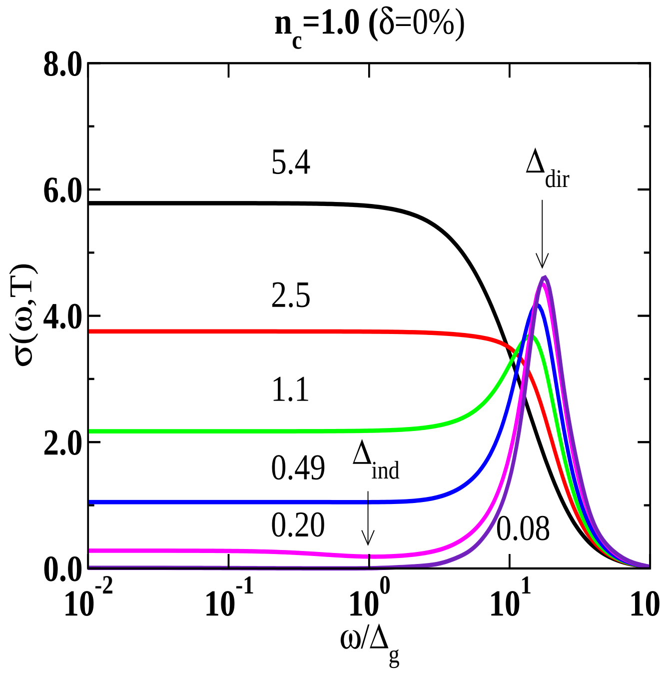
Comparison of Spectra with Photoemission

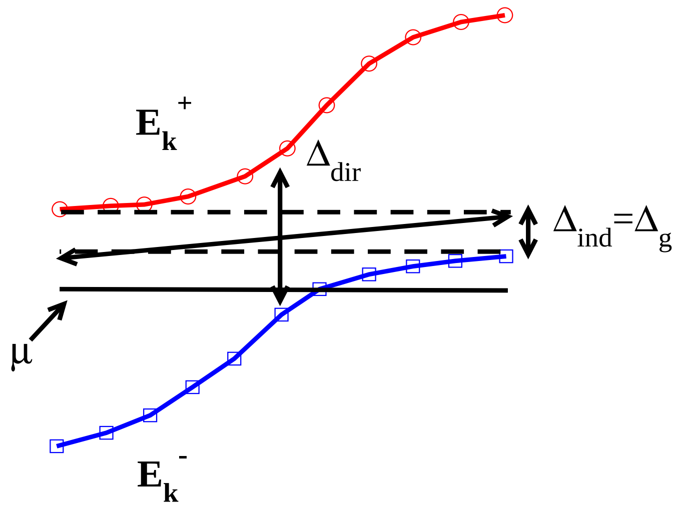




- YbInCu$_4$: volume collapse at $T_v = 42$K. High $T_0 = 400$K phase for $T < T_v$. Low $T_0 = 30$K phase for $T > T_v$. Kondo system with $14 - n_f = 0.85 - 0.96$.
- Single crystals, $\Delta E = 25$meV FWHM resolution
- Lineshape and T-dependent intensity consistent with KL scenario.

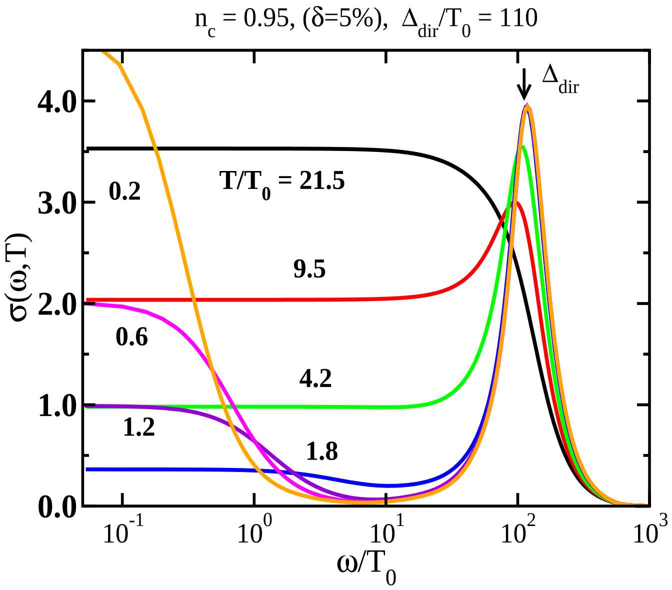
Optical conductivity: Kondo insulator

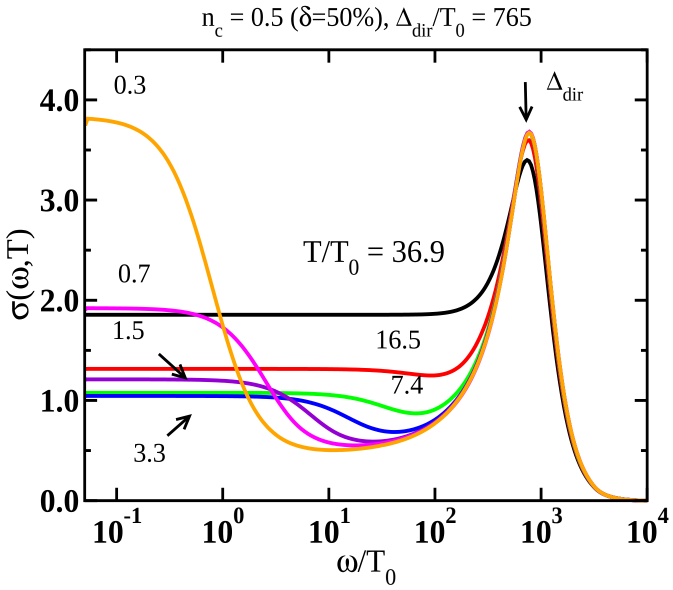




- No Drude peak as $T \to 0$.
- $T = 0$ threshold set by *indirect gap* $\Delta_{ind} = \Delta_g = T_K$ (see Logan's talk).
- T-dependence set by $T^* = T_K = \Delta_{ind}$
- mid-infrared peak; transitions across quasiparticle bands

Optical conductivity: $\delta > 0$



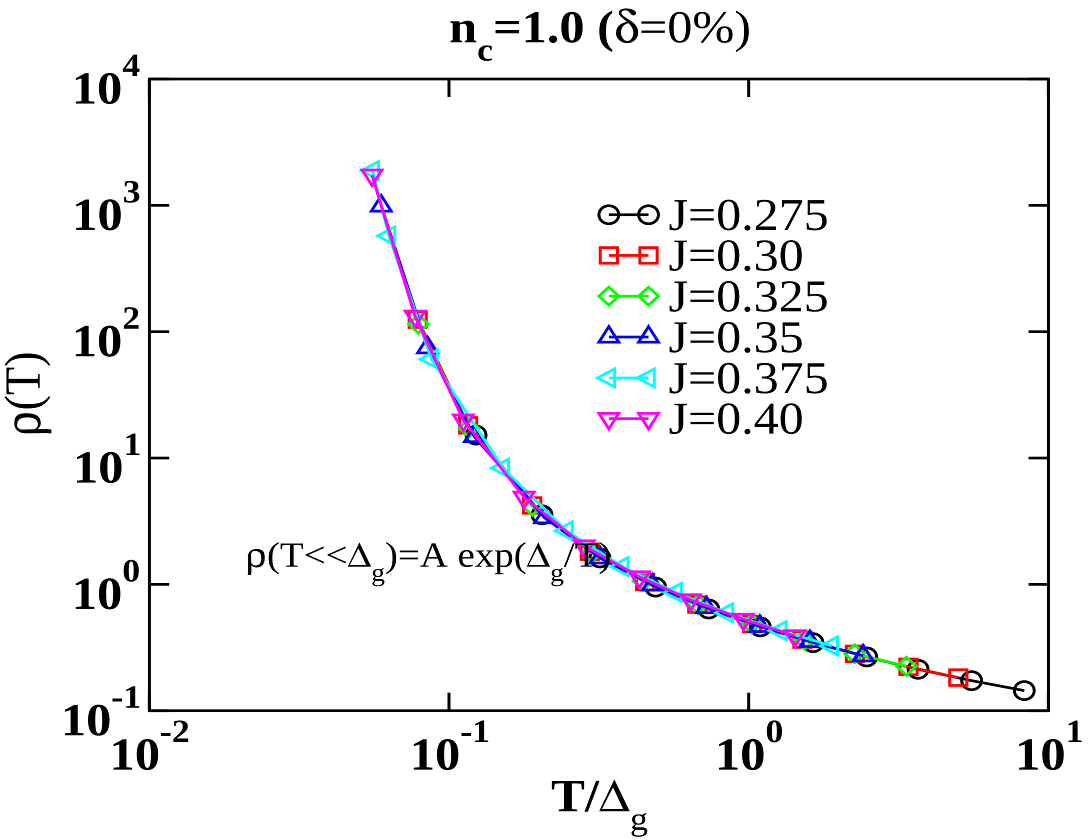


- Drude peak; transitions within E_k^-. Develops for $T < T_0$.
- Scale for T-dependence set by T_0
- mid-infrared peak; transitions across quasiparticle bands

Summary of low energy scales; scaling

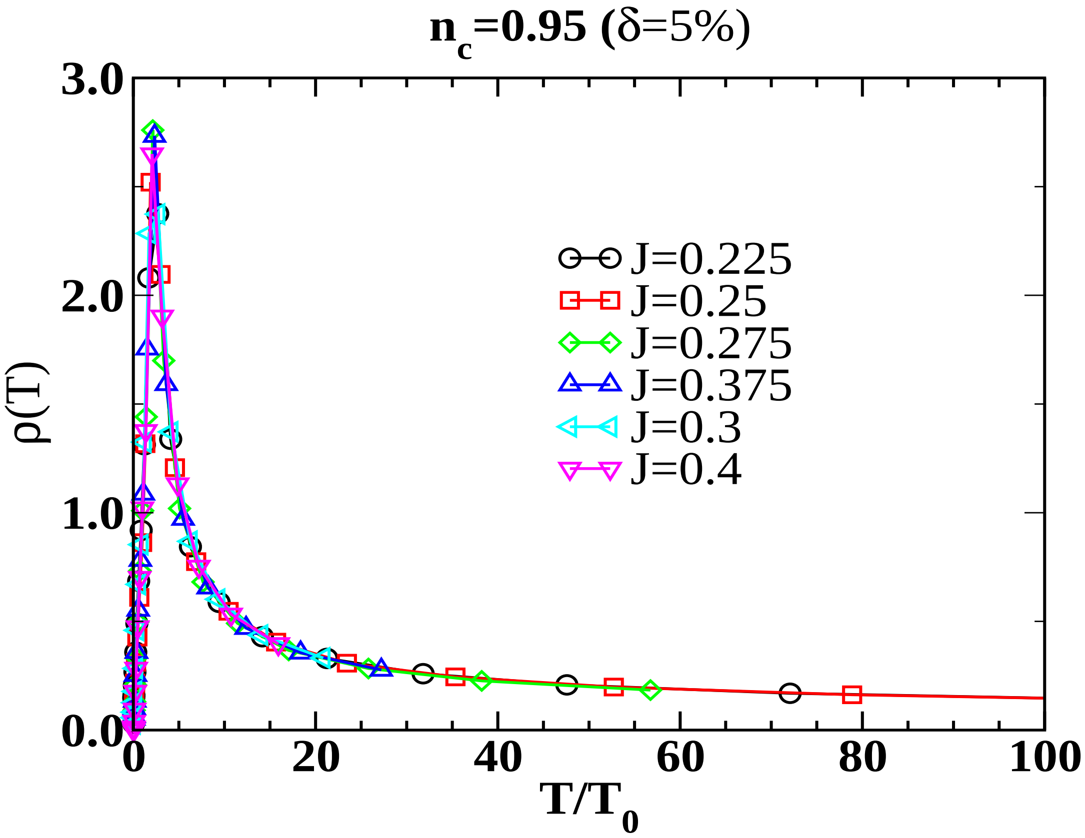
- Two low energy scales (Pruschke et al 1999, Burdin et al 2000, TAC et al 2001):
  - Fermi liquid coherence scale $T_0 = T_0(n_c)$ seen for all $\delta > 0$ in all quantities
  - single-ion Kondo scale $T_K = T_K(n_c)$ present for $\delta < 20\%$ in $\chi(\omega, T)$, $A(\omega, T)$ (and for all $\delta > 0$ in local c-electron DOS)
- universal scaling functions for fixed n_c and lattice type $(N_0(\varepsilon_k))$:
  - $\chi(T, J/D) \Rightarrow f_{\chi,n_c}(T/T_0)$
  - $\rho(T, J/D) \Rightarrow f_{\rho,n_c}(T/T_0)$
  - $A(\omega, T, J/D) \Rightarrow f_{A,n_c}(\omega/T_0, T/T_0)$
- numerically, scaling found to persist up to at least $100T_0$

Resistivity scaling: Kondo insulator



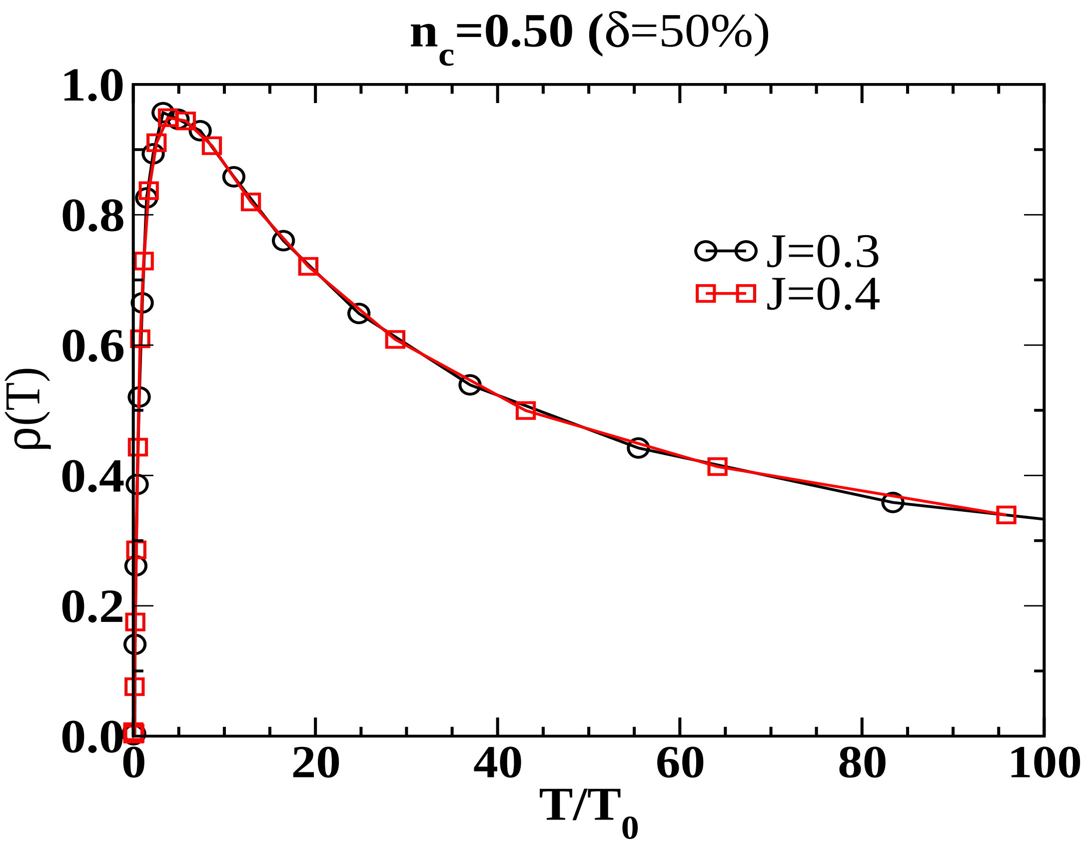
- Temperature scale: $T_K = \Delta_g = \Delta_{ind}$

Resistivity scaling: 5% doped Kondo insulator



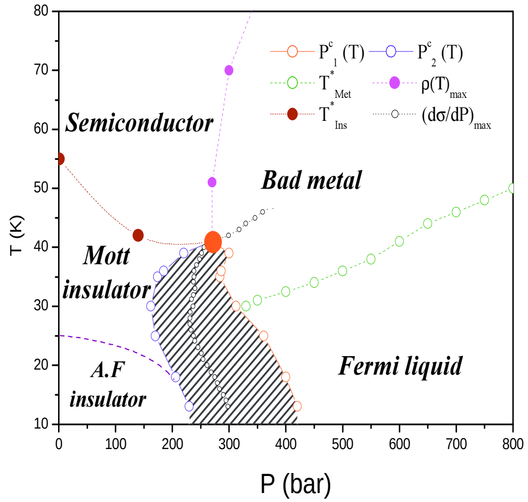
- Scaling w.r.t. T/T_0 up to $T \approx 100T_0$
- Incoherent metal region with linear T resistivity for $T \approx T_0$.

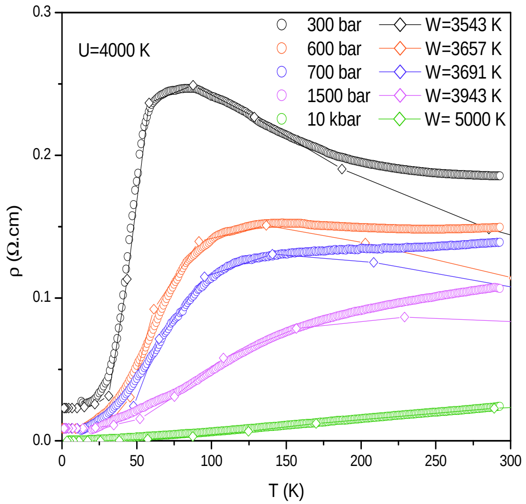
Resistivity scaling: 50% doping: heavy fermion metal

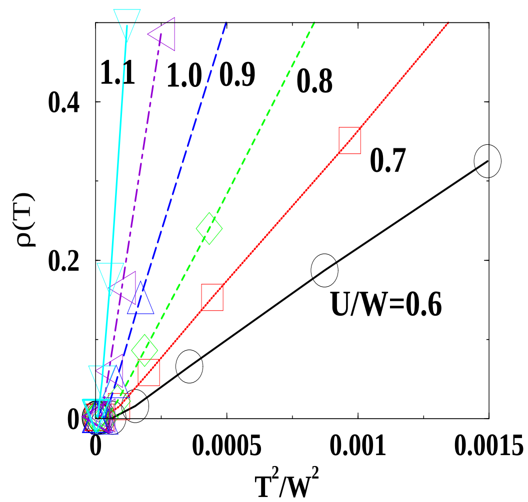


- Scaling w.r.t. T/T_0 up to $T \approx 100T_0$
- Typical paramagnetic heavy fermion metal , e.g. $CeAl_3$
- $T_{max} \approx 5 - 10T_0 \ll T_K$ is *not* a low energy scale. It is temperature at which lattice Kondo resonance vanishes on increasing T (cf. Hubbard model)

Related work: DMFT(NRG): transport crossovers in organic conductors







Experiments: Limelette et al. cond-mat/0301478.
Theory: A. Georges, S. Florens, T.A.C. cond-mat/0301478.
DMFT(NRG) results, T.A.C. cond-mat/0301478 & upublished.

- Low energy Fermi liquid scale $T_0 = zD$ (HWHM of QP peak)
- $\rho(T) \sim A\, T^2$, $A \sim 1/(T_0)^2$ for $T \ll T_0 = zD$
- Collapse of QP peak on scale $T \sim T_0$, loss of FL coherence
- Large ρ for $U > W$ and $T > T_0$ (scattering from local moments)
- Small ρ for $U \ll W$ and $T > T_0$ (no local moments)

Interpretation

- Far from Kondo insulating state, three temperature ranges:
  - $T \gg T_K \gg T_0$: single-ion Kondo behaviour
  - $T_0 \ll T \leq T_K$: lattice coherence sets in, T_K relevant scale; protracted or two-stage screening of moments (Jarrell) ?
  - $T \ll T_0$: Fermi liquid coherence sets in (lattice Kondo scale)
- For fixed n_c, scaling of $\rho(T)$ w.r.t. T/T_0 up to $T \approx 100T_0$

Conclusions and open questions

1. DMFT(NRG): allows calculation of photoemission spectra, optical conductivities, resistivities (thermodynamics ?)
2. Spectra of Kondo Lattice show two low energy scales T_0 and $T^* = T_K$
3. No clear signature of T_K in most quantities.
4. Clear signature of T_0 in all quantities (e.g. $\rho(T)$).
5. common features in $\rho(T)$ for Kondo Lattice and $U \sim W$ Hubbard models stems from similar physics: incoherent scattering from "local" moments at $T \gg T_0$ and Fermi liquid coherence resulting from formation of singlets (Kondo effect) at $T \ll T_0$.