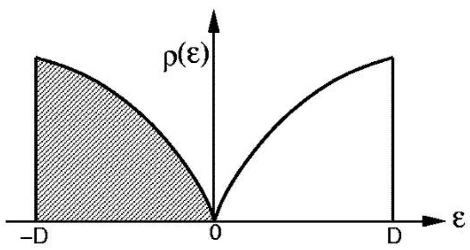
Critical Local Moments in the Pseudogap Kondo Model and the Kondo Lattice

Kevin Ingersent (U. Florida and NHMFL)

Collaborators: C. Gonzalez-Buxton (U. Florida)
Q. Si, J. L. Smith & S. Rabello (Rice U.)
R. Bulla (U. Augsberg)



Outline

- Pseudogap Kondo model
  - phase diagram
  - Kondo regime: a generalized Fermi liquid
  - interacting quantum critical point:
    - thermodynamics
    - local critical properties
- Impurities in d-wave superconductors
- Critical local moments in the Kondo lattice

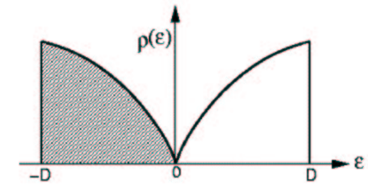
Conventional vs. Pseudogap Kondo Models

- Hamiltonian: $H_{\rm Kondo} = H_{\rm cond} + J\,\mathbf{S}_{\rm imp}\cdot\mathbf{S}_{\rm cond}(\mathbf{r}_{\rm imp})$.

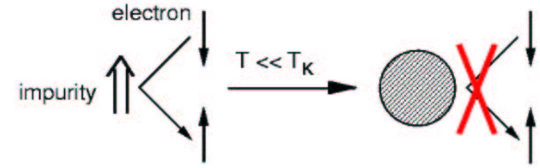
  with $s_{\rm imp} = \frac{1}{2}$ and

  $$\rho(\varepsilon) = \begin{cases} \rho_0|\varepsilon/D|^r & \text{for } |\varepsilon| < D, \\ 0 & \text{otherwise.} \end{cases}$$

  (Henceforth, absorb ρ_0 into J.)



- $r = 0$: conventional Kondo model.
  - $\mathbf{S}_{\rm imp}$ is screened for any $J > 0$ at $T \ll T_K \propto \exp(-1/J)$.



  - Scaling equation: $-dJ/d\ln D = J^2$

- $r > 0$: pseudogap (or power-law) model [Withoff & Fradkin (1990)].
  - $\mathbf{S}_{\rm imp}$ is screened only for $J > J_c$ and $T \ll T_K \propto (J - J_c)^{1/r}$.
  - Scaling equation: $-dJ/d\ln D = J(J - r)$

Pseudogap Kondo and Anderson Models: 12 Years Of Toil

- Perturbative scaling:
  - single-channel Kondo [Withoff & Fradkin (1990)].
  - n-channel Kondo [Ingersent (1996)].
  - Anderson model [Gonzalez-Buxton & Ingersent (1996)].
- Large-N (Coqblin-Schrieffer model):
  - $r \le \frac{1}{2}$, p-h symmetric [Withoff & Fradkin (1990)].
  - $r = 1$ [Cassanello & Fradkin (1996, 1997)].
  - $\chi_{\rm loc}(T)$ for $J \approx J_c$ [Ingersent & Si (1998)].
  - Effect of p-h asymmetry [Polkovnikov (2002)].
  - Overscreened large-n [Vojta (2001)].
- Numerical renormalization group:
  - Kondo thermodynamics [Chen & Jayaprakash (1995), Ingersent (1995), Gonzalez-Buxton & Ingersent (1998)].
  - Anderson thermodynamics and $A_{\rm imp}(\omega)$ [Bulla et al. (1997)].
  - Kondo $\chi_{\rm loc}(T)$ [Chen & Jayaprakash (1995), Gonzalez-Buxton & Ingersent (1998)].
  - Kondo $\chi_{\rm loc}(\omega, T)$ for $J \approx J_c$ [Ingersent & Si (1997, 1998, 2002)].
- Non-crossing approximation:
  - Anderson model thermodynamics [Borkowski (1997)].
- Perturbation theory:
  - Symmetric Anderson model [Glossop & Logan (2000)].
  - Kondo model [Ingersent & Si (2002)].
- Local-moment approximation (symmetric Anderson model):
  - Phase diagram and $A_{\rm imp}(\omega)$ [Glossop & Logan (2000)].
  - Critical properties [Glossop & Logan (2002)].

Outline of Numerical RG Approach

- Maps $H_{\rm Kondo}$ onto a chain Hamiltonian:

$$H_{\rm Kondo}(\Lambda) = J\,\mathbf{S}_{\rm imp} \cdot \sum_{\sigma,\sigma'} c_{0,\sigma}^\dagger \tfrac{1}{2}\boldsymbol{\tau}_{\sigma,\sigma'}\, c_{0,\sigma'} + \sum_{\sigma}\sum_{n=0}^{\infty} \Lambda^{-n/2}\left[\varepsilon_n c_{n,\sigma}^\dagger c_{n,\sigma} + t_n\left(c_{n,\sigma}^\dagger c_{n+1,\sigma} + \text{h.c.}\right)\right].$$

  $\Lambda = 1$ represents the continuum problem.
  $\Lambda > 1$ has artificial separation of energy scales.

- Form of density of states enters through the ε_n's and t_n's.

  For

$$\rho(\varepsilon) = \begin{cases} \rho_0|\varepsilon/D|^r & \text{for } |\varepsilon| < D, \\ 0 & \text{otherwise,} \end{cases}$$

  find

$$\varepsilon_n = 0, \qquad \lim_{k\to\infty} \frac{t_{2k+1}}{t_{2k}} = \Lambda^{-r/2}.$$

- Permits nonperturbative calculation of many-body eigenstates and matrix elements.
- Also allows algebraic analysis of weak-coupling and strong-coupling fixed points.
- Impurity properties calculated for $\Lambda > 1$ closely reproduce those of continuum problem.

Pseudogap Kondo Model: The Plot Thickens

- Simple scaling picture: Get Kondo screening for $J > J_c \approx r$.

- Three complications (revealed by numerical RG):
  1. For any $r > \frac{1}{2}$,
     - Kondo fixed point is unstable.
     - critical coupling $J_c = \infty \Rightarrow$ no Kondo effect.
     - $\mathbf{s}_{\text{imp}}$ decouples from conduction band as $T \to 0$:

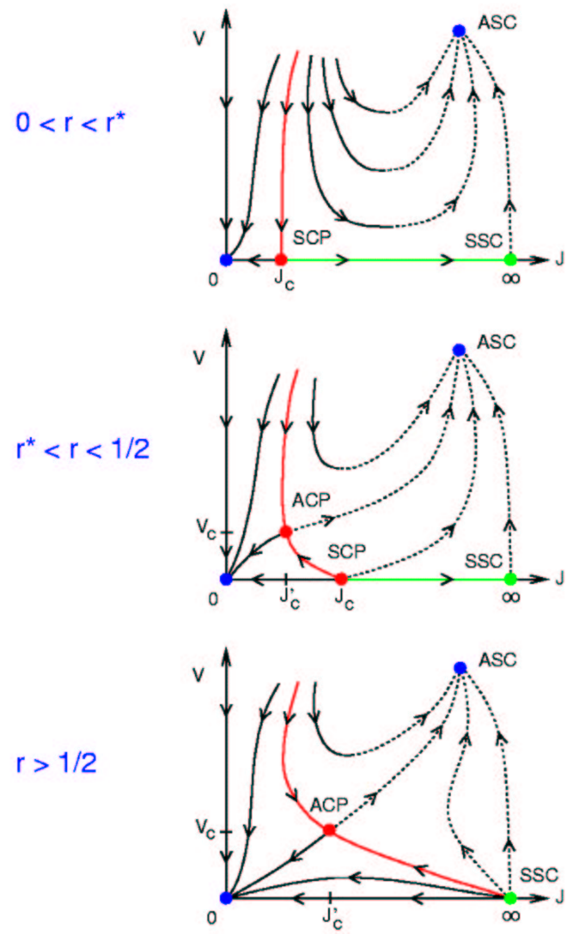
  2. P-h symmetry/asymmetry is crucial at strong coupling:
     - Can parametrize p-h asymmetry as a potential scattering:

$$H_{\text{Kondo}} \longrightarrow H_{\text{Kondo}} + V\, n_{\text{cond}}(\mathbf{r}_{\text{imp}}).$$

     - V is **irrelevant** for $J < J_c$, but **relevant** for $J > J_c$.
     - Have two distinct strong-coupling phases.
  3. P-h symmetry/asymmetry is crucial at critical coupling:
     - For $V \neq 0$, J_c is finite for all $r > 0$.
     - Can have two distinct quantum critical points:
       - symmetric ($J = J_c,\ V = 0$) for $0 < r < \frac{1}{2}$,
       - asymmetric ($J = J_c',\ V = V_c$) for $r > r^* \approx 0.375$.

Renormalization-Group Flow Diagrams

[Gonzalez-Buxton & Ingersent, PRB **57**, 14254 (1998)]

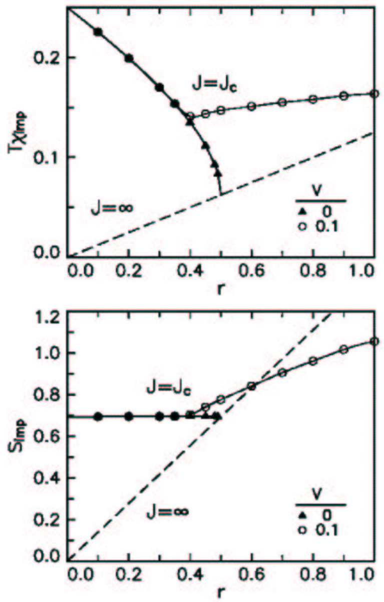


Impurity Properties $(0 < r < 1)$

- Weak coupling $(J \to 0,\ V \to 0)$
  - Free moment: $$T\chi_{imp} = 1/4 - O(T^r),$$ $$S_{imp} = \ln 2 + O(T^{2r}).$$
  - Spectral function: $A_{imp}(\omega) \propto |\omega|^r$.
  - Phase shift: $\delta_0(\varepsilon \to 0) = |\varepsilon|^r \operatorname{sgn}(-\varepsilon)$.
- Symmetric strong coupling $(J \to \infty,\ V = 0)$
  - Partially screened moment: $$T\chi_{imp} = r/8 + O(T^{1-2r}),$$ $$S_{imp} = 2r \ln 2 + O(T^{1-r}).$$
  - Spectral function: $A_{imp}(\omega) \propto |\omega|^{-r}$.
  - Phase shift: $\delta_0(\varepsilon \to 0) = (1-r)\frac{\pi}{2} \operatorname{sgn}(-\varepsilon)$.
  - Quasiparticle DOS: $\rho_{imp}(\varepsilon) = r\delta(\varepsilon) + O(|\varepsilon|^{-r})$.
  - Interpretation:
    - fraction $1 - r$ of an electron is absorbed into a resonance.
    - fraction r occupies a free level at $\varepsilon = 0$.
  - Get similar properties for a noninteracting level hybridizing with a power-law density of states.

    ⇒ This is a generalized Fermi-liquid regime.

- Asymmetric strong coupling $(J \to \infty,\ V \neq 0)$
  - Screened moment: $$T\chi_{imp} = O(T^{2r}),$$ $$S_{imp} = O(T^{2r}).$$
  - Phase shift: $\delta_0(\varepsilon \to 0) = \pi \operatorname{sgn}(-\varepsilon)$.
  - Quasiparticle DOS: $\rho_{imp}(\varepsilon) = -\delta(\varepsilon) + O(|\varepsilon|^r)$.
  - Interpretation: impurity freezes out first **two** Wilson shells.
- Symmetric and asymmetric quantum critical points (QCPs)
  - Exhibit non-Fermi-liquid impurity properties:



Static Critical Properties

[Ingersent & Si, PRL **89**, 076403 (2002)]

- Critical properties show up in the **local** magnetic susceptibility:

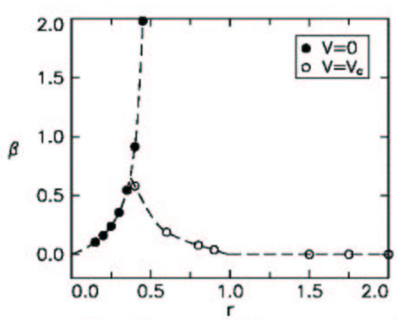
$$M_{\rm loc}(T) = -\partial F/\partial h \equiv \langle s^z_{\rm imp}\rangle,$$
$$\chi_{\rm loc}(T) = -\partial^2 F/\partial h^2 \equiv \partial M_{\rm loc}/\partial h,$$

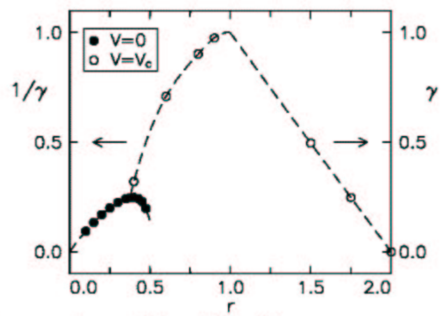
where $F(T)$ = free energy at temperature T,
h = static magnetic field acting only on $\mathbf{s}_{\rm imp}$.

- Using numerical RG, find for all $0 < r < 2$

$$M_{\rm loc}(J < J_c, T = 0) \propto (J_c - J)^{\beta},$$
$$\chi_{\rm loc}(J > J_c, T = 0) \propto (J - J_c)^{-\gamma},$$
$$M_{\rm loc}(J = J_c, T = 0) \propto |h|^{1/\delta},$$
$$\chi_{\rm loc}(J = J_c, T > 0) \propto T^{-x}.$$

  - These exponents have nontrivial r dependence:

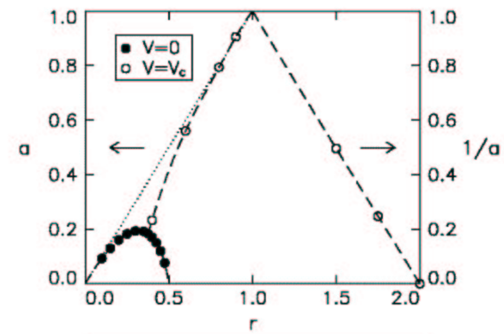


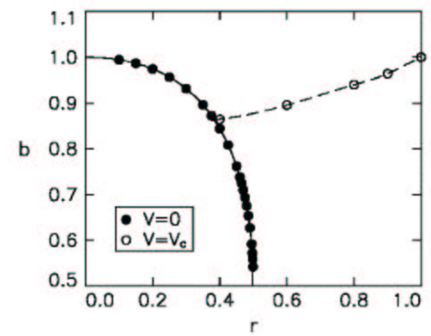


  - For $0 < r < 1$, have a continuous transition ($\beta > 0$).
    For $0 < r < 1$, $M_{\rm loc}$ undergoes jump at transition.

- NRG exponents β, γ, δ and x are consistent with a free energy

$$F = T\mathcal{F}\left(\frac{|J - J_c|}{T^a}, \frac{|h|}{T^b}\right).$$





- Other methods:
  - Scaling and LMA: $a = r$.
  - Large-N: Directly calculates only γ.
    With scaling ansatz $\Rightarrow$ $a = \min[r, (1-r)/2r]$, $b = 1$.

Dynamical Critical Properties

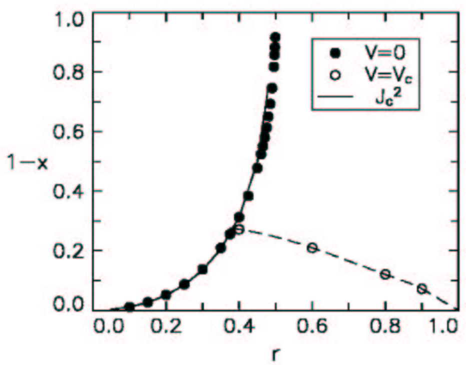
[Ingersent & Si, PRL **89**, 076403 (2002)]

- At $J = J_c$, dynamical local susceptibility is found to satisfy

$$\chi_{\rm loc}(J = J_c, T > 0) \propto T^{-x},$$
$$\mathrm{Im}\,\chi_{\rm loc}(J = J_c, \omega > 0, T = 0) \propto |\omega|^{-y}.$$

where

$$y = \begin{cases} x & \text{for } 0 < r < 1, \\ \gamma & \text{for } 1 < r < 2. \end{cases}$$



- For $0 < r < 1$, $y = x$ is suggestive of ω/T scaling, i.e.,

$$\chi(J = J_c, \omega, T) = T^{-x} X(\omega/T).$$

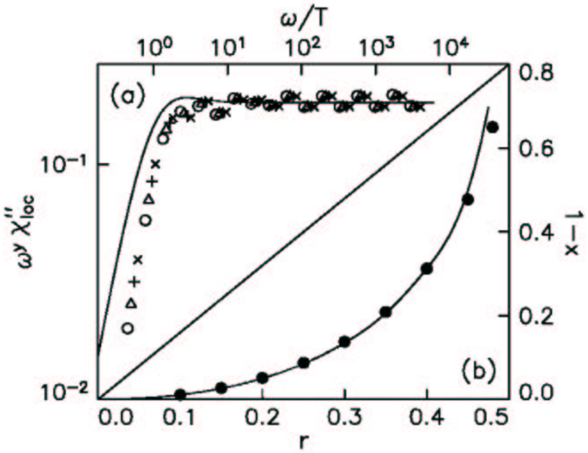
ω/T scaling $\Rightarrow$ relaxation rate $\propto T$ $\Rightarrow$ fully interacting QCP.

- For $r > 1$, have a superlinear relaxation rate $\propto T^{x/y}$.
This is consistent with a noninteracting (Gaussian) QCP.

- Can calculate full $\chi_{\rm loc}(J = J_c, \omega, T)$ in the limit $r \ll 1$:
  - Perturbative expansion in J gives

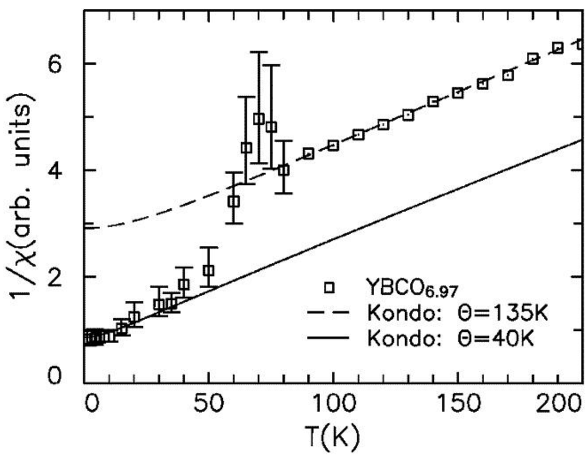
$$\chi_{\rm loc}(\tau) \approx \frac{1}{4}\left(\frac{\pi T \tau_0}{\sin(\pi T \tau)}\right)^{J_c^2}.$$

  - Predicts $x = y = 1 - J_c^2$, in agreement with NRG.
  - Furthermore, demonstrates complete ω/T scaling.



Nonmagnetic Impurities in High-T_c Cuprates

- Non-magnetic impurities (e.g., Zn, Li) induce localized moments, which can be probed via NMR/ESR.
- NMR on Li-doped YBCO [Bobroff et al. (1999–2001)]:
  - At $T > T_c$, can fit $\quad {}^7K(T) = {}^7K_0 + \dfrac{C}{T+\Theta}$.
  - Form is reminiscent of Kondo systems, where $\Theta \sim T_K$ $\Rightarrow$ interpreted as signature of local moment.
  - Signal persists into superconducting state:

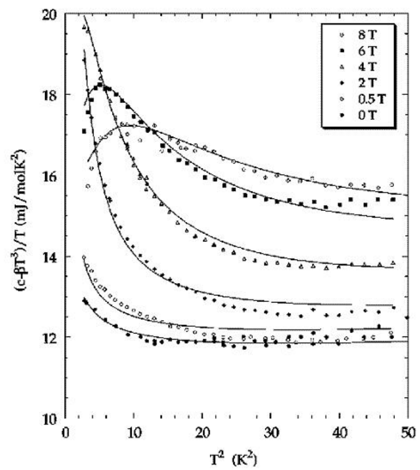


  - Within conventional Kondo picture, would expect
$$\Theta_{\text{super}}/\Theta_{\text{normal}} \ll 10^{-2},$$
c.f. experimental ratio ≈ 0.3.
  - Need to account for d-wave pseudogap.

Impurities in d-Wave Superconductors

- Theoretical connection to pseudogap Kondo model?
  - Start with $\quad H = H_{d\text{-wave}} + J\mathbf{S}_{\text{imp}} \cdot \mathbf{s}_{d\text{-wave}}(\mathbf{r}_{\text{imp}})$.
  - Can map problem onto pseudogap Kondo model with $r = 1$ [Cassanello & Fradkin (1997)].
  - Can also solve problem directly:
    - large-N [Polkovnikov et al. (2001), Zhu & Ting (2001), Zhang et al. (2001), Polkovnikov (2002)].
    - variational approach [Simon & Varma (1999)].

    With careful treatment of particle-hole (a)symmetry, find good agreement with pseudogap Kondo model [Polkovnikov (2002)].
- Specific heat of Zn-substituted YBCO (optimally doped):

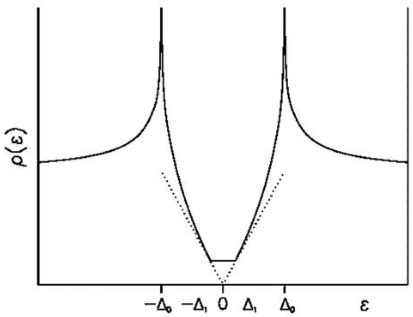


Sisson et al., PRB **61**, 3604 (1997)

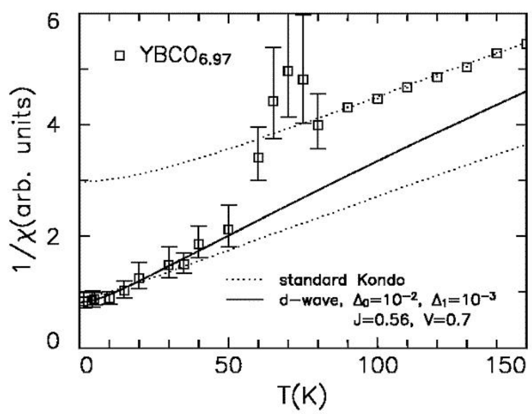
  - Shows no Schottky anomaly due to free Zn moments.
  - Fits pseudogap Kondo model for $r = 1$ [Cassanello & Fradkin (1997)].

Fitting ^{7}Li NMR Data to Kondo Model

- For $T < T_c$, can fit Knight shift using Kondo model with d-wave density of states (with partial infilling):

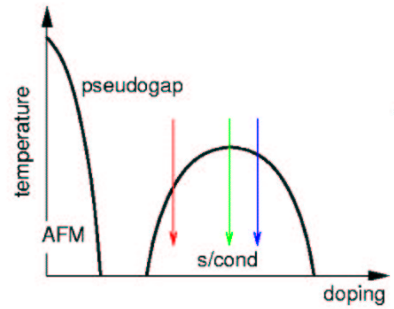


- Fit bandwidth D and Curie constant C using normal-state data.



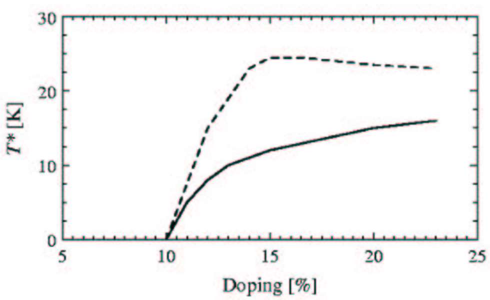
- Best fits have: strong particle-hole asymmetry,
  J within a few % of J_c.

- Since $J \sim J_c$, can one find the J_c QCP?
  - Recall that can fit $\quad {}^7K(T) = {}^7K_0 + \dfrac{C}{T+\Theta}$.
  - Θ varies dramatically with hole doping:



	doping	Θ_{normal}	Θ_{super}
● (red)	$O_{6.6}$	3 K	3 K
● (green)	$O_{6.96}$	135 K	40 K
● (blue)	Ca 20%	226 K	110 K

  - Near optimal doping, Θ_{super} changes faster than Θ_{normal}. Hints that Θ_{super} may vanish on slightly underdoped side.
  - T_K calculated using doping-dependent gap values changes rapidly with doping:



Vojta & Bulla, PRB **65**, 014511 (2002)

  - Further experiments between $O_{6.6}$ and $O_{6.96}$ are desirable.

Critical Local Moments in Lattice Problems

- Effective impurity models with nontrivial baths arise in the dynamical mean-field theory (DMFT) and extensions thereof.
- Pseudogap Kondo model is not realized in DMFT.
- However, a similar model is found in an extended DMFT treatment of the Kondo lattice [Si et al., Nature **413**, 804 (2001)]:
  - Impurity spin couples to a fermionic bath **and** a vector-bosonic bath.
  - Densities of states are chosen self-consistently to simulate the lattice.
- Two self-consistent solutions have been found, each corresponding to
  - a constant fermionic density of states,
  - a sub-ohmic bosonic density of states $\propto |\omega|^\gamma$, where $0 \le \gamma < 1$.
- The Kondo lattice has a locally critical quantum critical point:
  - Effective T_K vanishes at QCP.
  - Critical local-moment fluctuations coexist with long-wavelength SDW fluctuations.
  - Reproduces many of the salient properties of $CeCu_{6-x}Au_x$, particularly the ω/T scaling with a fractional exponent.

Summary

- Magnetic impurities coupled to strongly correlated hosts can exhibit exotic Kondo physics arising from the presence of a pseudogap in the quasiparticle density of states.
- Nontrivial critical behavior arises when the pseudogap drives the effective Kondo temperature to zero.
- The critical behavior is (presumably) associated with a new universality class of interacting critical points.
- Much works remains to be done to understand the fundamental the nature of these critical points.
- This physics may be directly relevant to impurities in high-T_c cuprates; it may also serve as a proving ground for ideas related to novel critical behavior in correlated lattices.