

## Quantum Criticality in the Bose-Fermi Kondo Model

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### Bose-Fermi Kondo model (BFKM):

- Couples an impurity spin to both Fermi and Bose baths.
- Enters extended dynamical mean-field theory of the Kondo lattice.
- Previous impurity solutions have produced conflicting results.

### New numerical renormalization-group treatment:

- Novel bath discretization and iterative solution procedure.
- Initial application to the Ising-symmetry BFKM—has interacting QCP in same universality class as the spin-boson model.
- Opens the way for decisive EDMFT studies of the Kondo lattice.

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## Impurity Quantum Phase Transitions

[Recent review: M. Vojta, cond-mat/0412208]

- Impurities can undergo continuous (boundary) quantum phase transitions when coupled to noninteracting baths.
- Fermionic baths:
  - **suppression of the Kondo effect** due to ...
    - a pseudogap in the density of states;
    - competition between multiple conduction bands;
    - magnetic correlation between multiple impurities.
- Bosonic baths:
  - **(de)localization transition** in a two-level system.
- Fermionic and bosonic baths:
  - **competition** between Kondo screening and bosonic localization.

## Bose-Fermi Kondo Model

- Describes a local spin-half  $\mathbf{S}$  coupled both to a **conduction band** and to three **dissipative baths**.

- Isotropic model has the Hamiltonian

$$H = \underbrace{JS \cdot \mathbf{s} + H_{\text{band}}}_{H_{\text{Kondo}}} + \underbrace{g\mathbf{S} \cdot \mathbf{u} + H_{\text{bath}}}_{H_{\text{spin-boson}}}$$

where (for  $\alpha = x, y, z$ )

$$S_\alpha = \frac{1}{2} \sum_{\sigma, \sigma'} c_{0\sigma}^\dagger \sigma_{\sigma\sigma'}^\alpha c_{0\sigma'}$$

$$u_\alpha = a_{0\alpha} + a_{0\alpha}^\dagger$$

$$H_{\text{band}} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$$

$$H_{\text{bath}} = \sum_{\mathbf{q}, \alpha} \omega_{\mathbf{q}} a_{\mathbf{q}\alpha}^\dagger a_{\mathbf{q}\alpha}$$

- Anisotropic versions distinguish between

$$J_z \text{ and } J_x = J_y = J_\perp$$

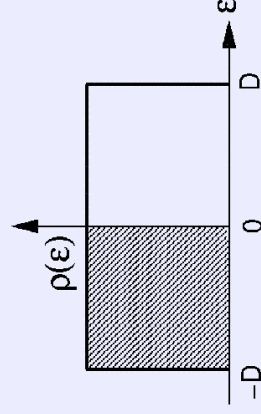
$$g_z \text{ and } g_x = g_y = g_\perp$$

## Bose-Fermi Kondo Model: Bath Spectra

$$H = JS \cdot \mathbf{s} + H_{\text{band}} + g\mathbf{S} \cdot \mathbf{u} + H_{\text{bath}}$$

- Take a **flat conduction** band density of states:

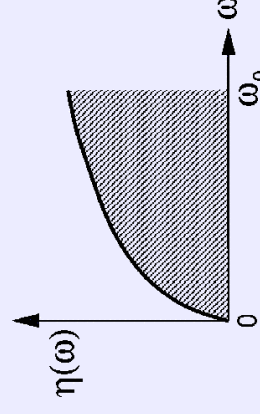
$$\rho(\epsilon) = \rho_0 \text{ for } |\epsilon| < D$$



- Assume a **power-law** bosonic spectrum:

$$\eta(\omega) = K_0^2 \omega_0 (\omega / \omega_c)^s$$

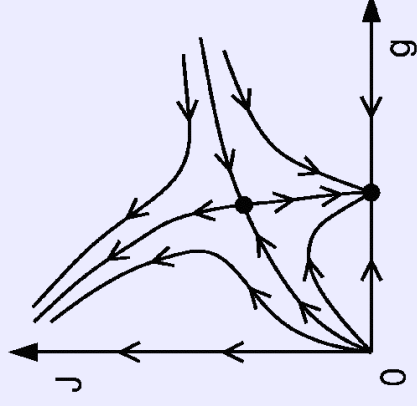
$$\text{for } 0 \leq \omega < \omega_0$$



- Dimensionless parameters:  $\rho_0 J$  and  $K_0 g$ .

## Perturbative Solutions of the BFKM

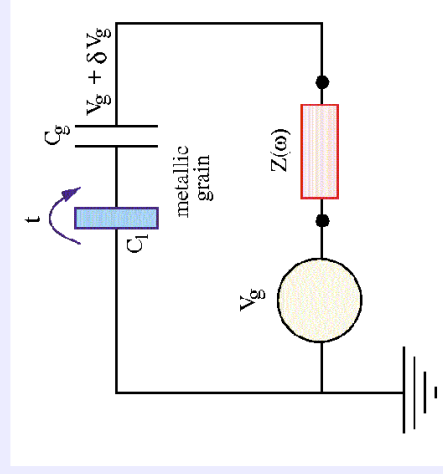
- Model has been solved via expansion in  $\epsilon = 1 - s$  [Si & Smith '99, Sengupta '00, Zhu & Si '02, Zaránd & Demler '02].
- A quantum critical point separates Kondo and bosonic regimes.
- Critical point couplings  $\rho_0 J_c$  and  $K_0 g_c$  are of order  $\epsilon$ .  
Exception: Ising symmetry ( $g_{\perp} = 0$ ), for which  $\rho_0 J, K_0 g_c \sim O(1)$ .
- At the QCP,  $\chi_{\text{loc}}$  shows power laws in  $\omega$  and  $T$  with  $\epsilon$ -dependent exponents.
- Large- $N$  multichannel BFKM has also been studied [Zhu et al. '04].



## Application I: Coulomb Blockade in a Noisy Dot

[K. Le Hur, PRL 92, 196804 (2004)]

- Consider a metallic box ...  
... in a strong magnetic field,  
... grounded via a point contact,  
... subject to a noisy gate voltage.
- Can map charge fluctuations onto an anisotropic BFKM with ...  
... an Ohmic bath ( $s = 1$ );  
...  $J_{\perp} \propto t$ ;  
...  $g_z \propto R = Z(\omega = 0)$ .
- Predicts a Kosterlitz-Thouless transition at  $R = R_c$ .



## Application II: EDMFT Treatment of the Kondo Lattice

- Extended dynamical mean-field theory includes some spatial fluctuations [Si and Smith '96, Kajueter & Kotliar].

- Fermionic band accounts for local dynamical correlations.

- Dissipative baths represent

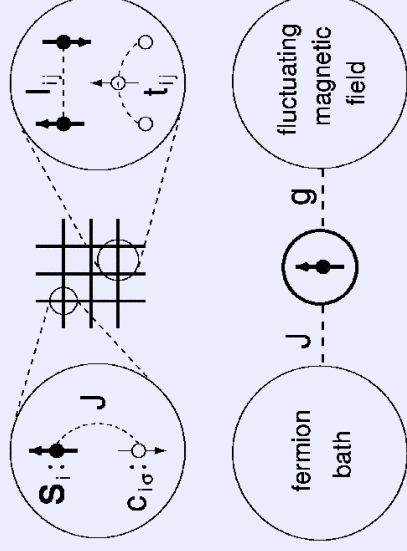
a **fluctuating magnetic field**

due to other local moments.

- Band and bath densities

of states must be found

**self-consistently.**



## What is the Nature of the QPT in EDMFT?

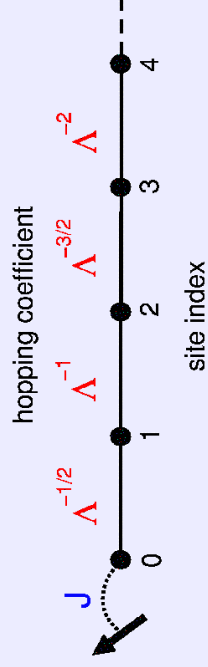
- EDMFT equations have been solved using various impurity solvers.
- $\epsilon$ -expansion [Si et al. '01, '03] finds two types of QCP:
  - conventional **spin-density-wave** type;
  - **locally critical QCP**—reproduces some features of  $\text{CeCu}_{6-x}\text{Au}_x$  and  $\text{YbRh}_2\text{Si}_2$ , but corresponds to  $\epsilon = 1$ .
- Quantum Monte Carlo yields conflicting results:
  - Anderson lattice has no locally critical QPT; transition is 1<sup>st</sup> order [Sun & Kotliar '03].
  - Kondo lattice has 1<sup>st</sup> order transition at  $T > 0$ , but a locally critical QCP at  $T = 0$  [Grepel & Si, '03, Zhu et al. '04].
- To resolve this discrepancy, **need nonperturbative  $T = 0$  solutions.**

## Numerical Renormalization-Group Method [Wilson '74]

- NRG replaces a **continuum** of fermionic states by a **discrete set** having energies  $\epsilon = \pm D, \pm D\Lambda^{-1}, \pm D\Lambda^{-2}, \dots$  ( $\Lambda > 1$ ).
- Then the kinetic energy is converted to a tight-binding form:

$$H_{\text{band}} = \sum_{\sigma} \sum_{n=0}^{\infty} \Lambda^{-n/2} (c_{n\sigma}^{\dagger} c_{n-1,\sigma} + \text{h.c.}),$$

where only  $c_{0\sigma}$  couples to the impurity.

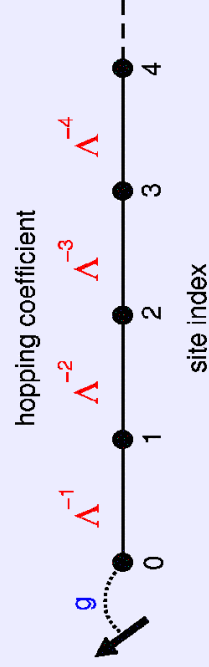


- The **exponential decay** of the hopping permits **iterative solution** via diagonalization of progressively longer chains.

## Discretizing a Bosonic Bath

- Can use the **same energy discretization** as for fermions.
- No negative- $\omega$  states  $\Rightarrow$  **hopping decays faster**:

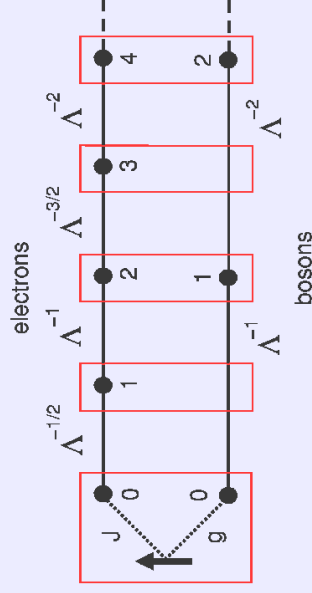
$$H_{\text{bath}} = \sum_{\alpha} \sum_{n=0}^{\infty} \Lambda^{-n} [t(a_{n\alpha}^{\dagger} a_{n-1,\alpha} + \text{h.c.}) + e a_{n\alpha}^{\dagger} a_{n\alpha}]$$



- This discretization has been used to study the **spin-boson model** [Bulla et al., '03, '04].

## Combining Fermionic and Bosonic Baths

- Seek an iterative procedure that treats simultaneously fermionic and bosonic degrees of freedom of the same energy.
- One method—**add a bosonic site every other iteration:**



- Iterate until reach a scale-invariant fixed point describing the ground state.

## NRG Results: Bose-Fermi Kondo and Anderson Models

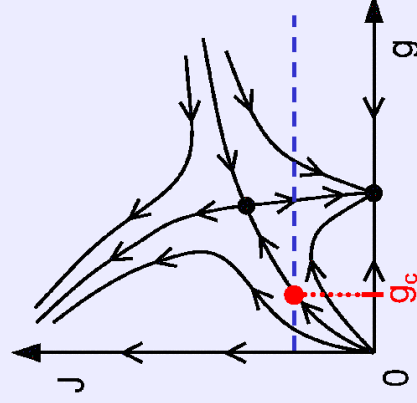
- Have first studied the **Ising-symmetry BFKM** ( $g_{\perp} = 0$ ):

$$H_{\text{imp}} = JS \cdot s + g S_z u_z.$$

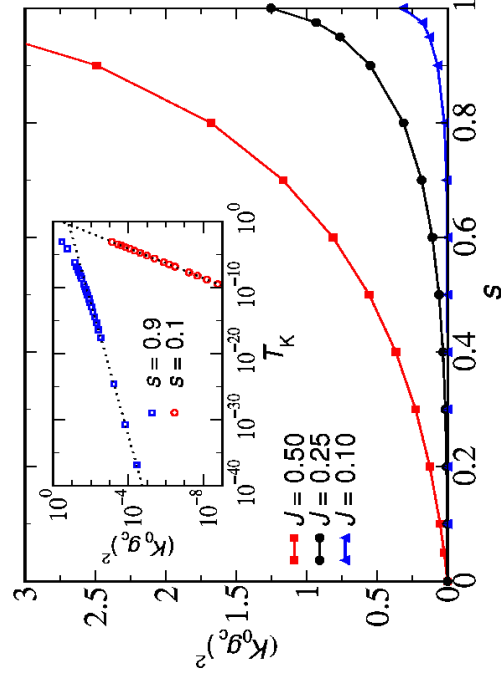
- Only one bosonic bath  
⇒ computationally most tractable.
- Probably most relevant to

CeCu<sub>6-x</sub>Au<sub>x</sub>.

- For convenience, take  $\omega_0 = D = 1$ .
- Results will be presented at **fixed  $J$**  ⇒ QPT is located at  $g = g_c$ .

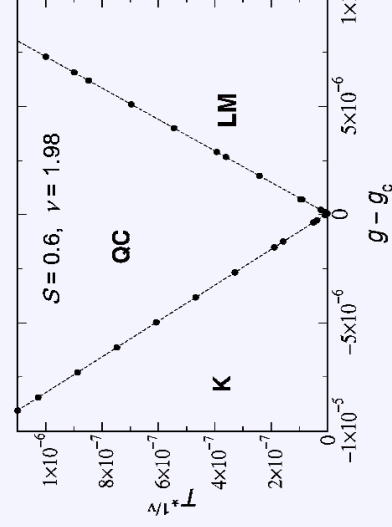


## Critical Coupling $g_c$



$$(K_0 g_c)^2 T_K^s \sim T_K \approx \exp(-1/\rho_0 J)$$

## Crossover Temperature Scale $T^*$



Exponent  $\nu$  diverges as

$$s \rightarrow 0^+ \text{ and } s \rightarrow 1^-.$$

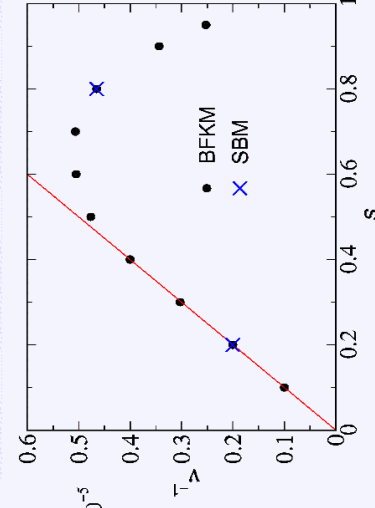
Have interacting QCP only

for  $0 < s < 1$ .

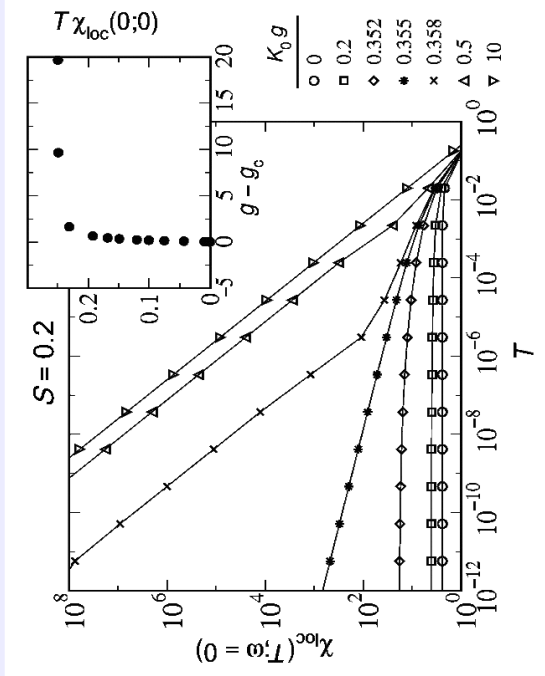
Identify a crossover scale

$$T^* \sim |g - g_c|^\nu$$

from many-body spectrum or physical properties.



## Response $\chi_{\text{loc}}$ to a Local Magnetic Field



$\chi_{\text{loc}}(\omega=0, g = g_c) \sim T^{-x}$  with  $x = s$  (agrees with  $\epsilon$ -expansion)

## Response to a Local Magnetic Field (continued)

- All critical exponents agree with those for the spin-boson model.  
 $\Rightarrow$  Ising BFKM and SBM belong to same universality class.
- Static exponents are consistent with a critical free energy

$$F_{\text{imp}} = T f\left(\frac{g - g_c}{T^{1/\nu}}, \frac{h}{T^b}\right)$$

$h$  = local magnetic field

i.e., exponents obey hyperscaling  $\Rightarrow$  QCP is interacting.

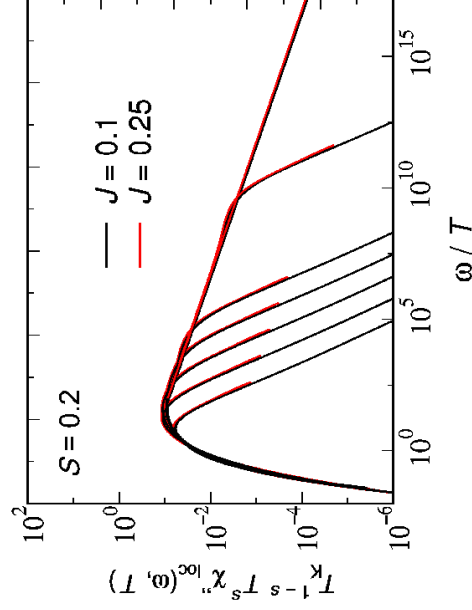
- Local spin dynamics obey

$$\chi''_{\text{loc}}(\omega, T = 0, g = g_c) \sim |\omega|^{-y} \text{sgn } \omega \quad \text{with} \quad y = x = s$$

consistent with  $\omega T$  scaling.



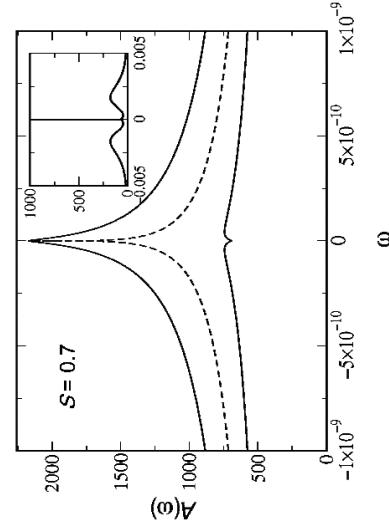
## $\omega T$ Scaling



For  $|\omega| \ll T_K$ ,

$$T_K \chi''_{loc}(\omega, T, g = g_c) = \left( \frac{T}{T_K} \right)^{-x} \Phi_x \left( \frac{\omega}{T} \right)$$

## Bose-Fermi Anderson Model: Impurity Spectral Function

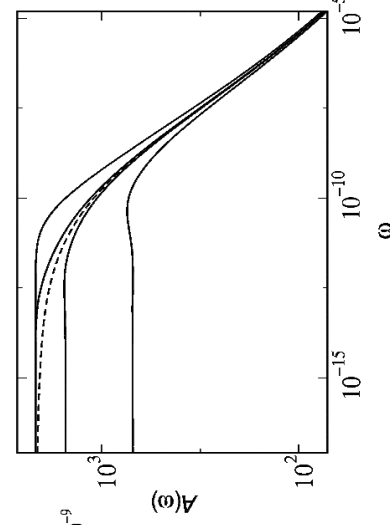


Throughout bosonic regime,  
have maximum at  $\omega = \pm \omega^*$ ,  
and

$$A(\omega = 0) < 1/\pi\Gamma_0.$$

Throughout Kondo regime,  
resonance width  $\approx T_K$ , and

$$A(\omega = 0) = 1/\pi\Gamma_0.$$



## Summary

- We have developed a new nonperturbative numerical method for Bose-Fermi quantum impurity models at  $T = 0$  and  $T > 0$ .
- Initial application to the Ising-symmetry BFKM:
  - Continuous QPT exists for power-law bosonic baths with exponents  $0 < s < 1$ .
  - Critical exponents coincide with those of the spin-boson model.
  - QCP exhibits hyperscaling and  $\omega T$  scaling.
  - Destruction of the Kondo resonance at the QCP is directly seen in the impurity spectral function.
- Opens the way to resolve controversy surrounding the EDMFT treatment of the Kondo lattice.