Quantum Phase Transitions in Magnetic Impurity Problems

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Project Goals

Physics Goals: Explore quantum phase transitions in strongly correlated electron systems in order to

- elucidate non-Fermi-liquid properties;
- understand “local criticality” in heavy fermions.

IT Goals: Advance the numerical RG method by providing

- new algorithms (e.g., for Bose-Fermi problems);
- efficient, adaptable codes for “complex” impurity problems (e.g., orbital degeneracy, coupled quantum dots, DMFT & beyond).

“Classic” Quantum Impurity Models

- Describe local, dynamical degree of freedom coupled to dispersive bath(s) of noninteracting (quasi)particles.
- E.g., Kondo model for a spin $\mathbf{S}$ coupled to a conduction band

$$H = J\,\mathbf{S}\cdot\mathbf{s} + H_{\text{cond}},$$

where

$$\mathbf{s} = \tfrac{1}{2}\textstyle\sum_{\sigma,\sigma'} c^{\dagger}_{0\sigma}\,\boldsymbol{\sigma}_{\sigma\sigma'}\,c_{0\sigma'}, \quad H_{\text{cond}} = \textstyle\sum_{\mathbf{k},\sigma}\epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \quad |\epsilon_{\mathbf{k}}| \le D.$$

- Breakdown of perturbative expansion in J/D prompted development of many techniques.
  - Approximate: perturbative scaling/RG, large-degeneracy.
  - Exact (but limited): Bethe ansatz, bosonization.
  - Numerical (controlled): numerical RG, Quantum Monte Carlo.

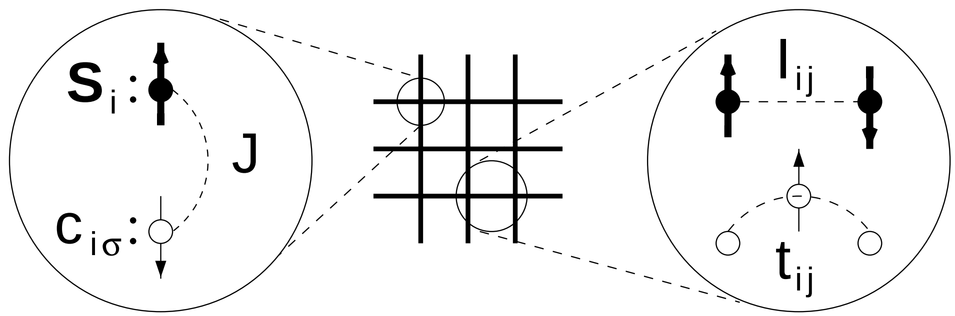
“Modern” Quantum Impurity Models

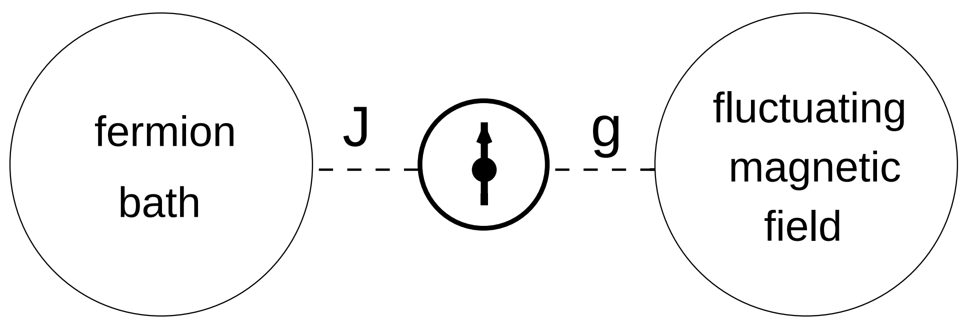
- Feature some or all of the following:
  - complex impurities with many internal degrees of freedom;
  - multiple impurities and/or multiple conduction bands;
  - coupling to bosonic baths.
- Topical examples include . . .
  - Magnetic clusters on metallic surfaces [Crommie; Manoharan; . . .]
  - Coupled quantum dots
  - Cluster corrections to the dynamical mean-field theory of correlated lattice fermions [Jarrell et al. (1998); Kotliar et al. (2001)]
  - Bose-Fermi impurity models:
    - Enter the extended dynamical mean-field treatment of heavy fermions [Si et al. (2001)].
    - Describe quantum dots coupled to noisy leads [Le Hur (2004)].

Critical Local Moments in Lattice Problems

The Bose-Fermi Kondo model arises in the extended DMFT treatment of the Kondo lattice [Si et al. (2001, 2003)]:

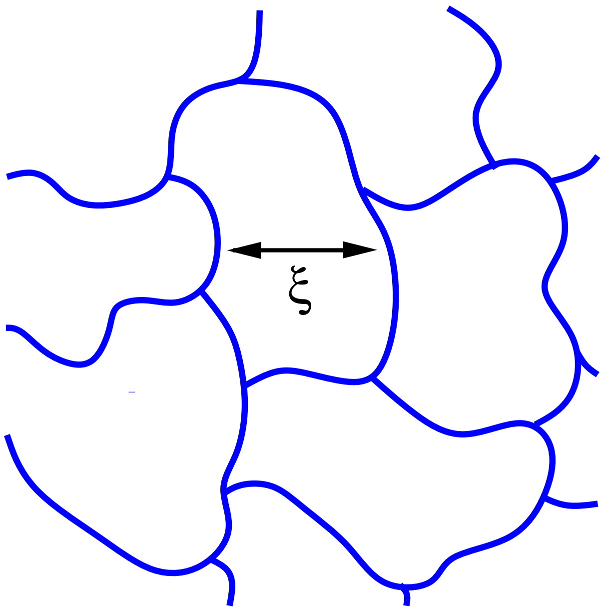
- Extended DMFT includes some spatial fluctuations [Smith & Si (2000); Chitra & Kotliar (2000)].
- Effective impurity model couples a local spin to a fermionic bath **and** a vector-bosonic bath.
- Bath densities of states must be determined self-consistently.





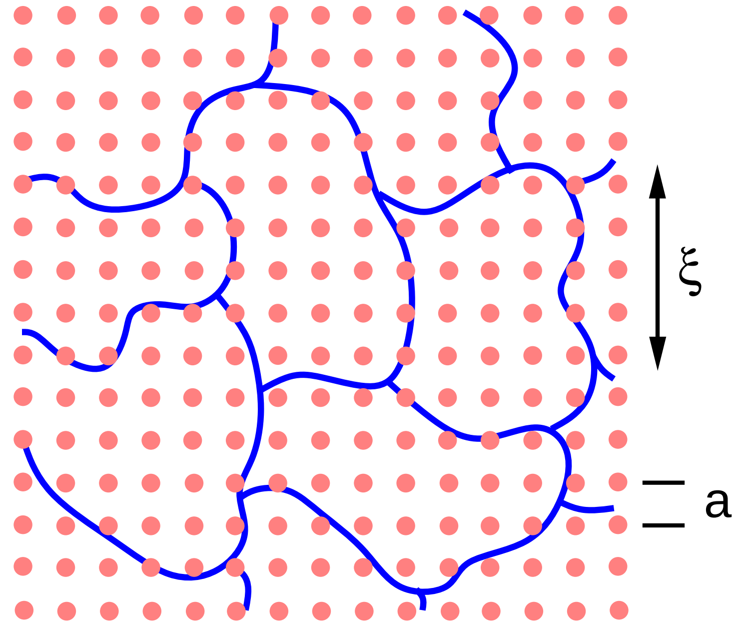
EDMFT Prediction: Two Types of Quantum Criticality

conventional criticality



only long-wavelength fluctuations are important

"local criticality"



long-wavelength and spatially local (dynamical) fluctuations play central roles

The locally critical QCP reproduces some anomalous properties of $CeCu_{6-x}Au_x$ and $YbRh_2Si_2$.

The Bose-Fermi Kondo Model

- Describes a local spin $\mathbf{S}$ coupled both to delocalized fermions (e.g., a conduction band) and bosons (e.g., phonons).

- Isotropic version has a Hamiltonian

$$H = J\,\mathbf{S}\cdot\mathbf{s} + H_{\text{Fermi}} + g\,\mathbf{S}\cdot\mathbf{u} + H_{\text{Bose}},$$

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

$$s_\alpha = \tfrac{1}{2}\sum_{\sigma,\sigma'} c_{0\sigma}^\dagger\,\sigma_{\sigma\sigma'}^\alpha\,c_{0\sigma'} \qquad u_\alpha = a_{0\alpha} + a_{0\alpha}^\dagger,$$

$$H_{\text{Fermi}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \qquad H_{\text{Bose}} = \sum_{\mathbf{q},\alpha} \omega_{\mathbf{q}} a_{\mathbf{q}\alpha}^\dagger a_{\mathbf{q}\alpha}.$$

- Anisotropic versions distinguish between

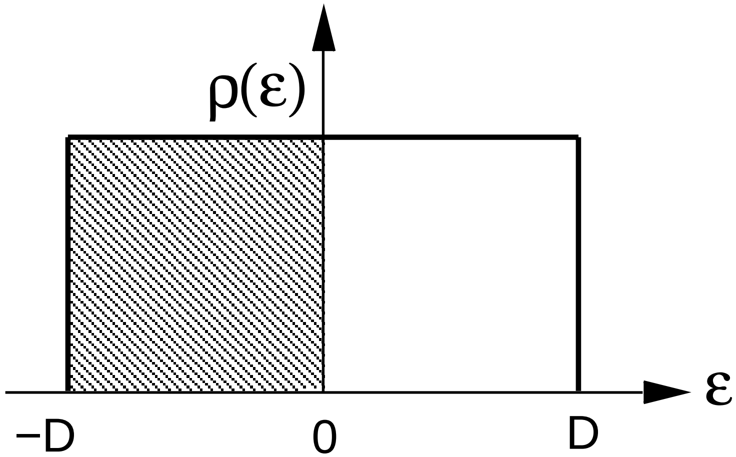
$$J_z \quad \text{and} \quad J_x = J_y = J_\perp,$$

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

The Bose-Fermi Kondo Model (continued)

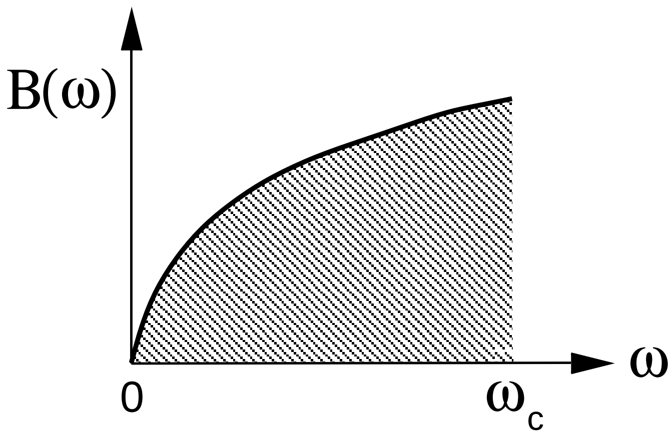
$$H = J\,\mathbf{S}\cdot\mathbf{s} + H_{\text{Fermi}} + g\,\mathbf{S}\cdot\mathbf{u} + H_{\text{Bose}}.$$

- Take a flat fermionic density of states:



$$\rho(\varepsilon) = \rho_0 \quad \text{for } |\varepsilon| \leq D.$$

- Assume a power-law bosonic spectral function:



$$B(\omega) = K_0^2\,\omega_c(\omega/\omega_c)^s.$$

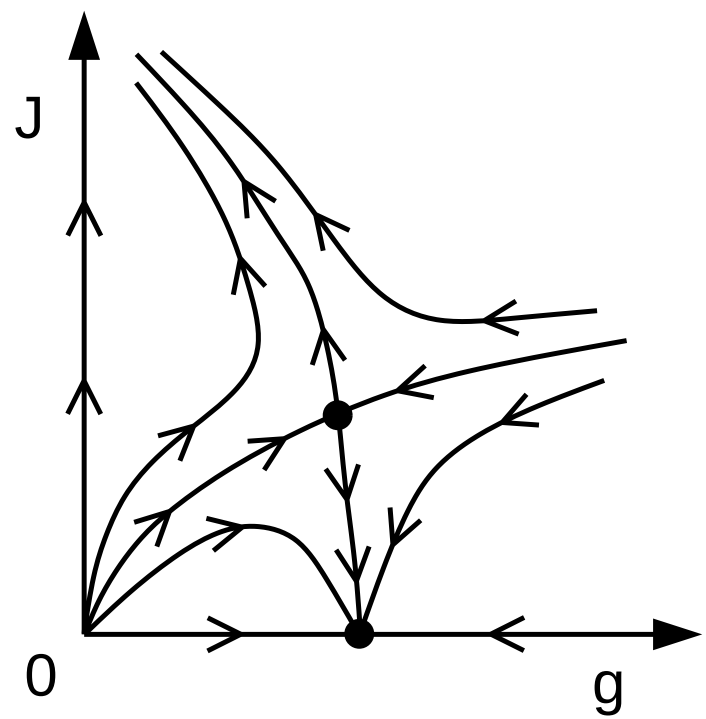
Perturbative Solutions of the Bose-Fermi Kondo Model

- The model has been solved by expansion in $\epsilon = 1 - s$ [Si & Smith (1999), Sengupta (2000), Zhu & Si (2002), Zaránd & Demler (2002)].

- A QCP separates Kondo and bosonic regimes.

- Critical point couplings $\rho_0 J^*$ and $K_0 g^*$ are of order ϵ (except for $g_\perp = 0$).

- At QCP, $\chi_{\rm loc}$ shows power laws in ω and T with ϵ-dependent exponents.



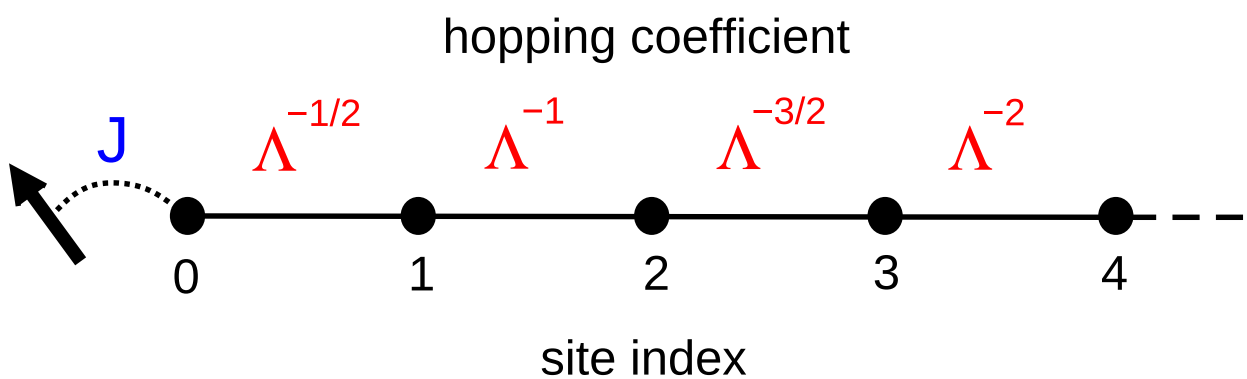
- Locally critical EDMFT solution corresponds to $\epsilon = 1^-$.
  $\Rightarrow$ Seek non-perturbative solutions.

Numerical Renormalization Group Method [Wilson (1974)]

- Replaces a continuum of fermionic states ($|\varepsilon| \leq D$) by a discrete set having energies $\varepsilon = \pm D$, $\pm D\Lambda^{-1}$, $\pm D\Lambda^{-2}$, $\ldots$ ($\Lambda > 1$).
- Then the kinetic energy is converted to a tight-binding form:

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

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

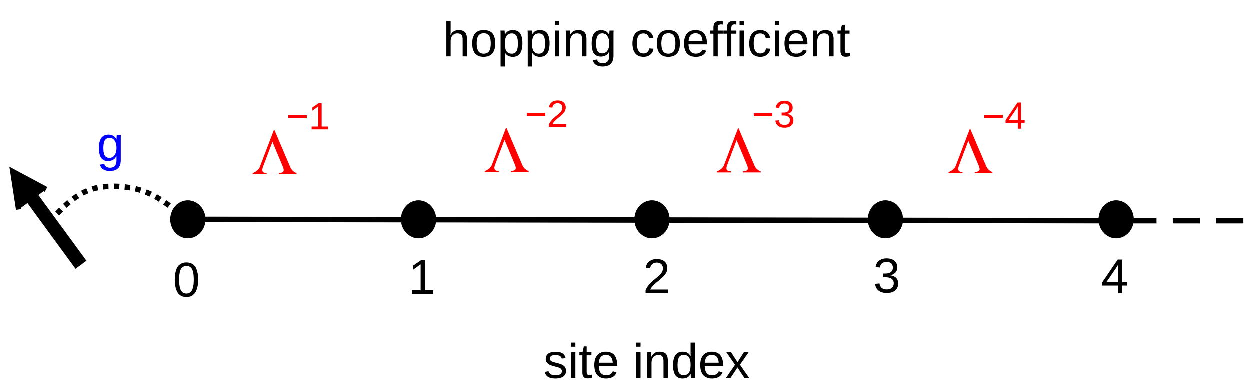


- The exponential decay of the hopping permits iterative solution via diagonalization of progressively longer chains.

Discretizing a Bosonic Bath

- Can use the same energy discretization as for fermions.
- No negative-ω states $\Rightarrow$ hopping coefficients decay faster:

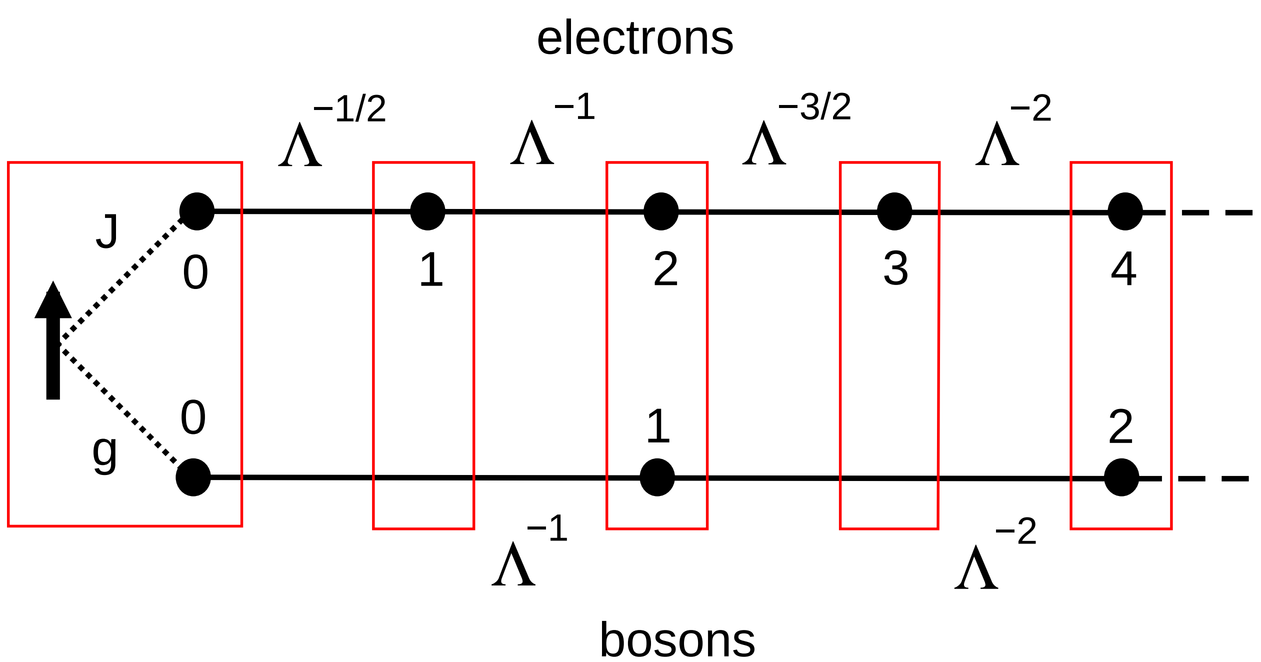
$$H_{\text{Bose}} = D \sum_\alpha \sum_{n=0}^{\infty} \left[t\, \Lambda^{-n} \left(a^\dagger_{n,\alpha} a_{n-1,\alpha} + \text{h.c.} \right) + e\, \Lambda^{-n} a^\dagger_{n,\alpha} a_{n,\alpha} \right]$$



- This discretization has been used to study the spin-boson model [Bulla et al. (2003)].

Combining Fermionic and Bosonic Baths

- Seek an iterative procedure that treats simultaneously fermionic and bosonic degrees of freedom having the same energy scale.
- One method: add a bosonic site at every second iteration:



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

Adding Bosons = More CPU Time!

- Add a fermionic site $\Rightarrow$ basis increases by a factor $N_F = 4$.
- Number of bosons on each site is unlimited, but restrict it to no more than N_b per bath. $4 \leq N_b \leq 8$ seems to suffice.
- Add both fermionic and bosonic sites $\Rightarrow$ basis increases by $N_F = 4(N_b+1)^n$ for n Bose baths.
- After a few iterations, basis is so large that can retain only the M states of lowest-energy. Typically, $500 \leq M \leq 2000$.
- As in other “modern” impurity problems, large N_F and M lead to long CPU times $\sim O\left[(N_F M)^3\right]$.
- To tackle these problems, we are developing parallelized NRG codes (using MPI, ScaLAPACK).

Initial Results: Bose-Fermi Kondo and Anderson Models

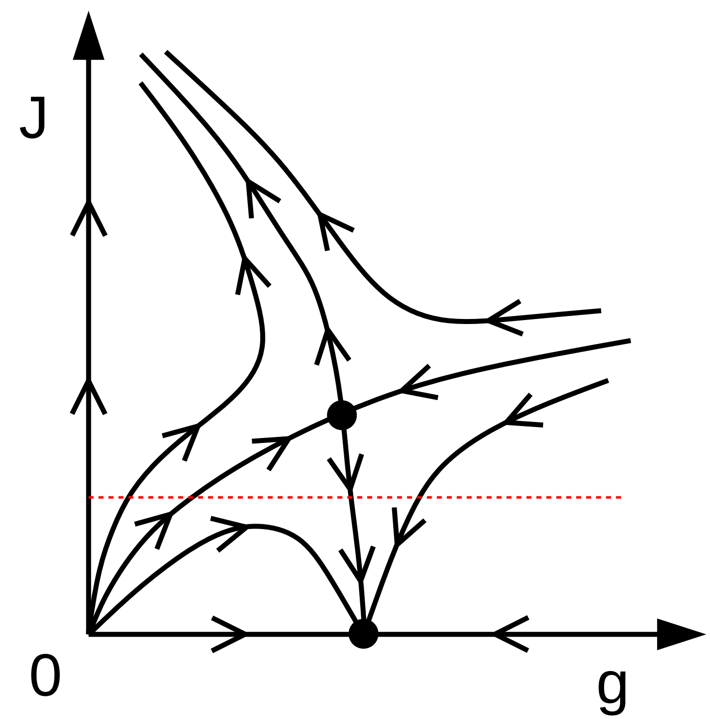
- Have started with the Ising-symmetry ($g_\perp = 0$) model:

$$H_{\mathrm{imp}} = J\mathbf{S}\cdot\mathbf{s} + gS_z(a_0 + a_0^\dagger).$$

  Has smallest N_F, and is possibly the most relevant for $CeCu_{6-x}Au_x$.

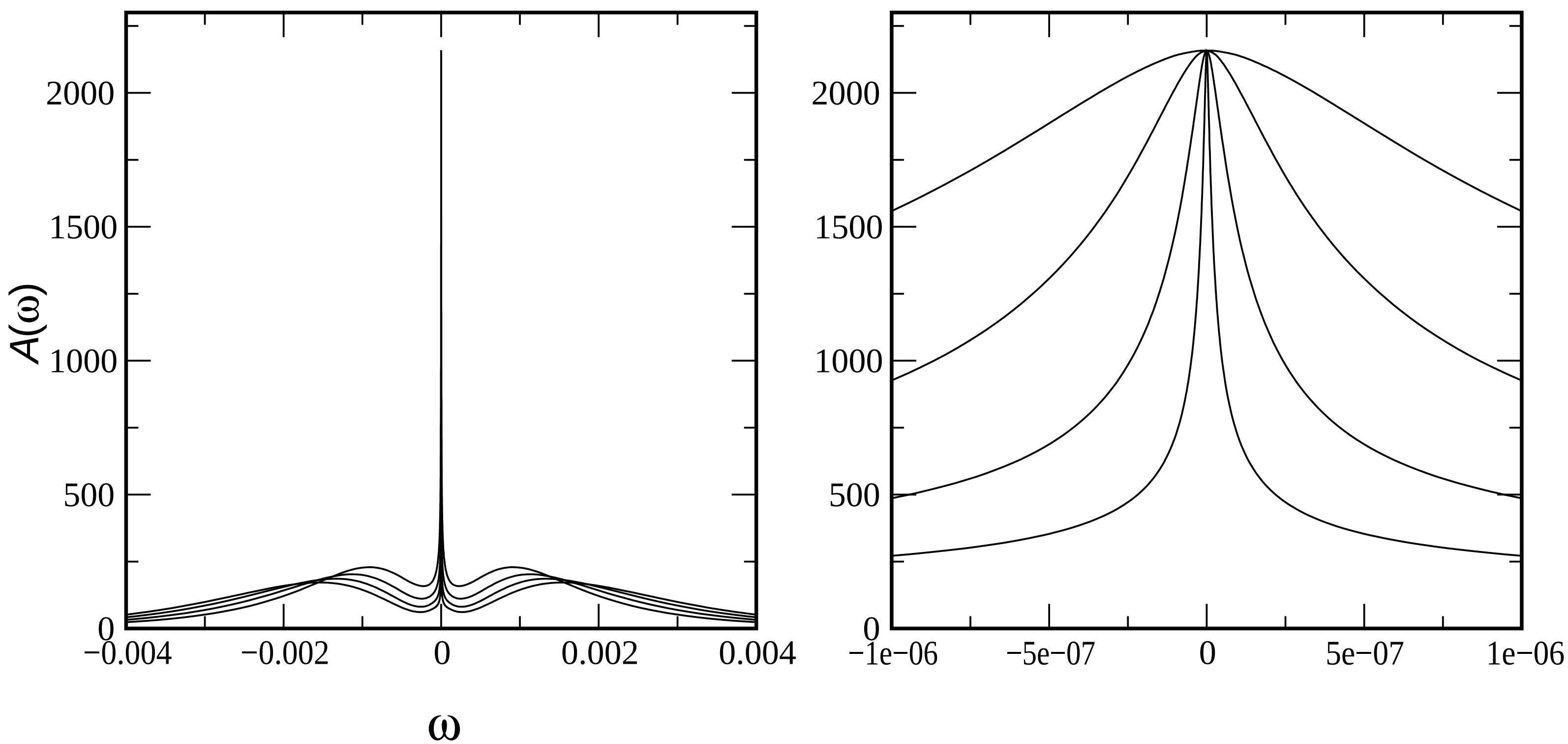
- Have calculated phase diagram, $T = 0$ impurity dynamics, and static magnetic response.

- Will show results along constant-J cuts through the parameter space.



Impurity Spectral Function $[\Delta = (K_0 g)^2]$

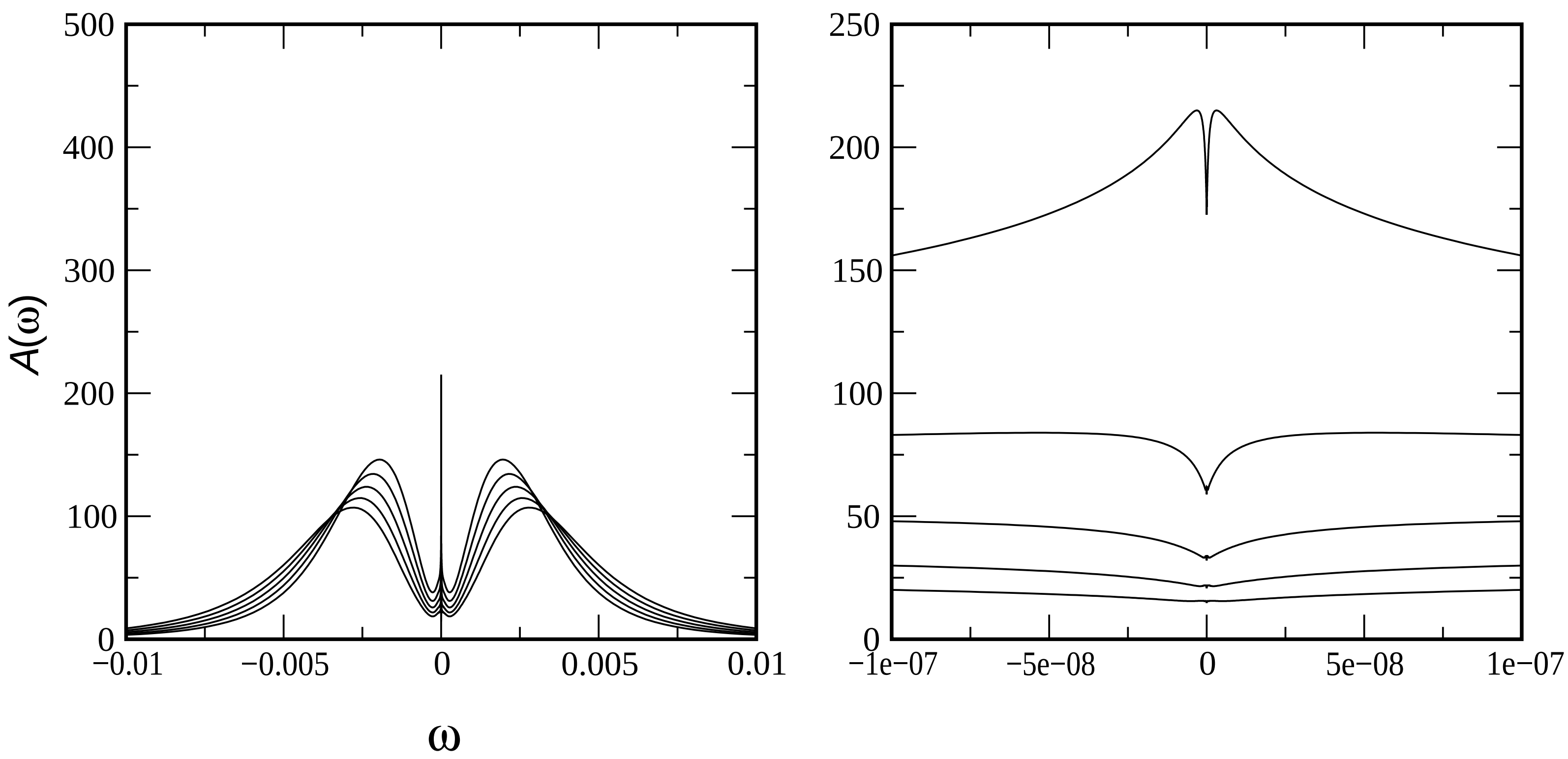
Increasing $\Delta < \Delta_c$ for $s = 0.7$



Kondo regime: $A(0)$ is pinned, but the Abrikosov-Suhl resonance narrows as $\Delta \to \Delta_c$, signaling suppression of the Kondo effect.

Impurity Spectral Function $[\Delta = (K_0 g)^2]$

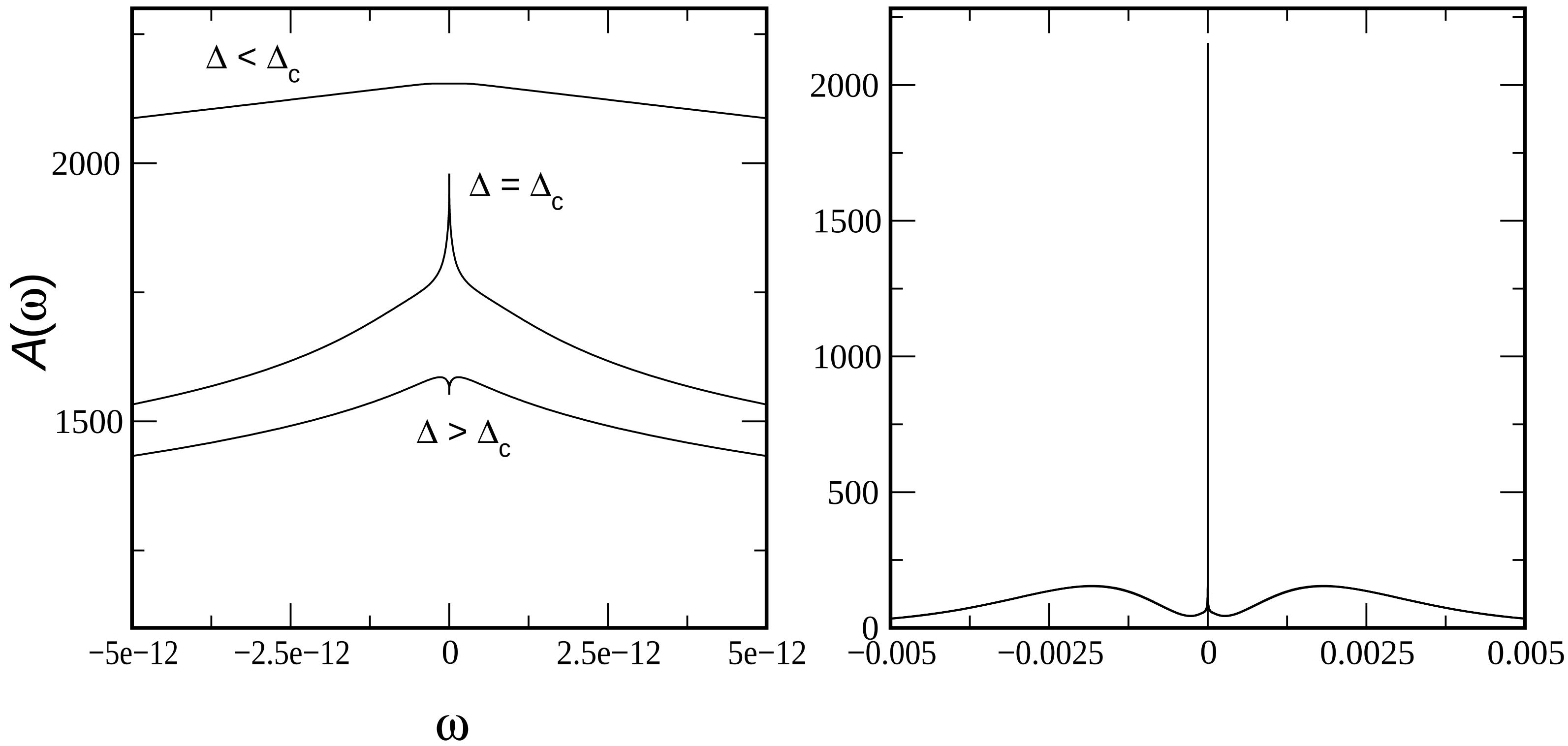
Decreasing $\Delta > \Delta_c$ for $s = 0.7$



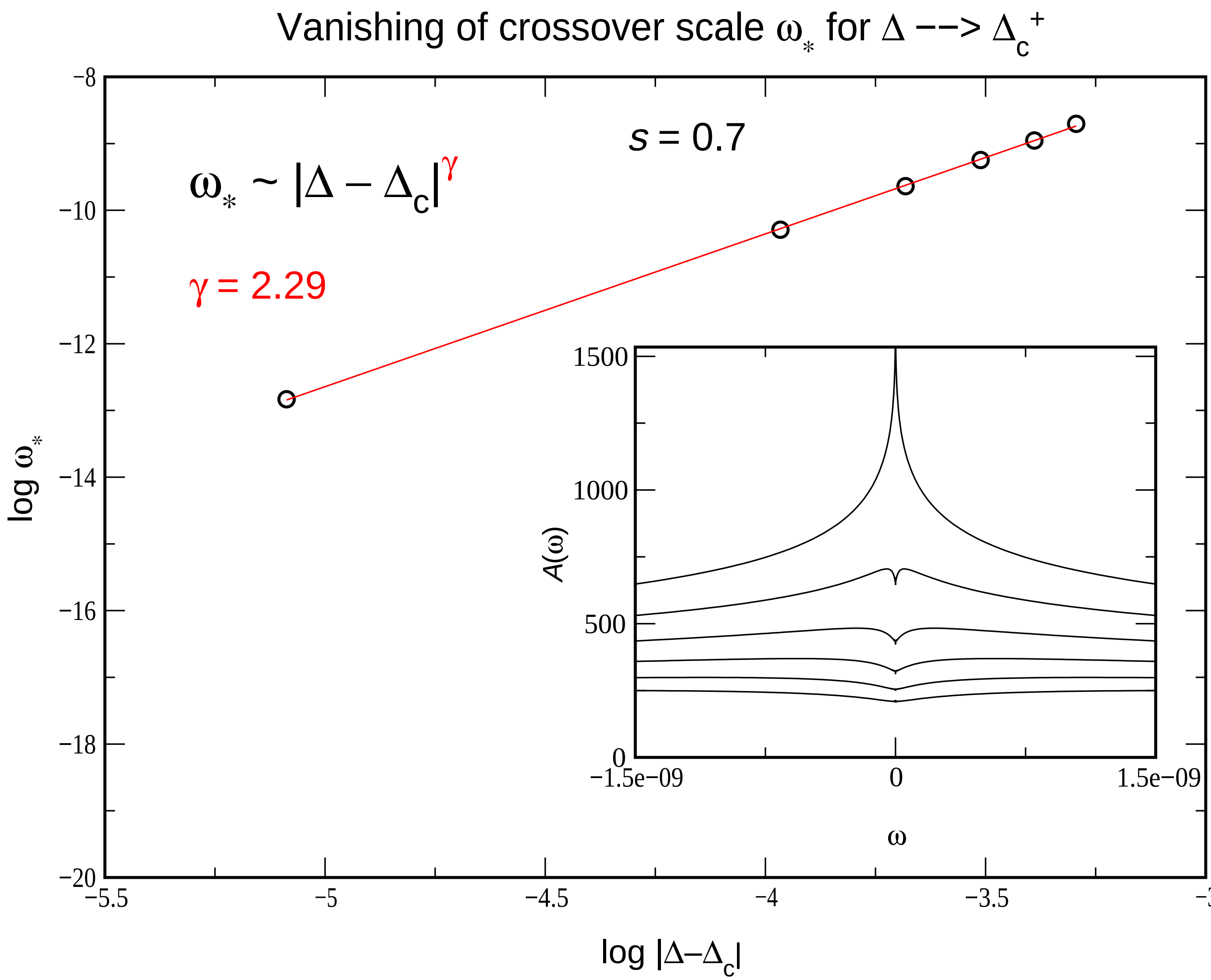
Bosonic regime: A low-energy feature grows as $\Delta \to \Delta_c$.

Impurity Spectral Function $[\Delta = (K_0 g)^2]$

$s = 0.7$

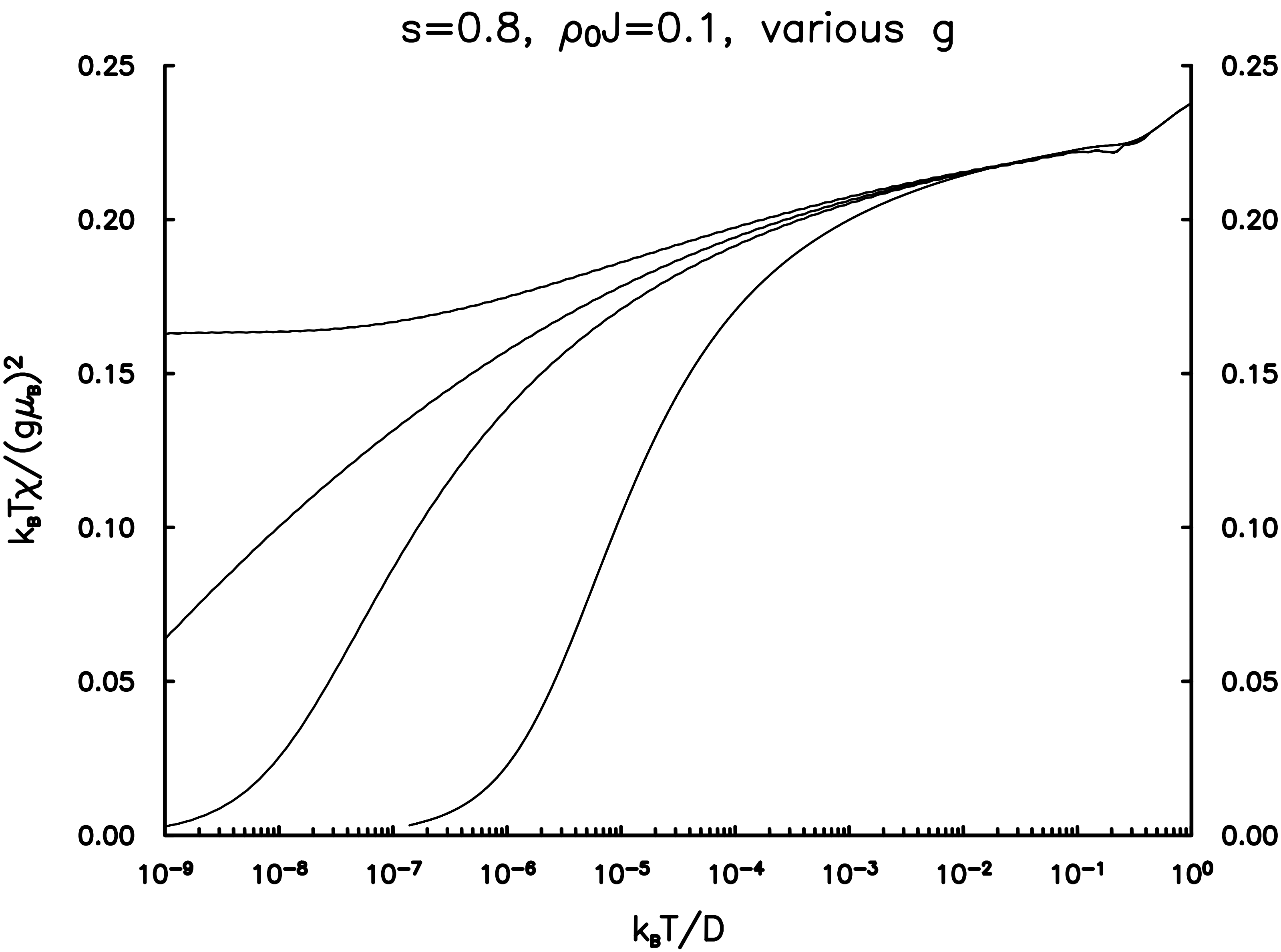


Passing through the quantum critical point, $A(0)$ undergoes a jump.



Can extract the same critical exponent from the width of the Abrikosov-Suhl resonance and from the many-body eigenspectrum.

Static Susceptibility



Summary

- Have implemented the first numerical renormalization group treatment of a quantum impurity coupled to both fermionic and bosonic baths.
- As an initial application, are studying the Ising-symmetry Bose-Fermi Kondo model.
- The method should permit study of critical properties beyond the range of perturbative methods.
- The method will extend to other models and can serve as an impurity solver in extended DMFT treatments of lattice fermion problems.
- Parallelized, readily-adaptable NRG codes will be available for a wide range of quantum impurity problems.