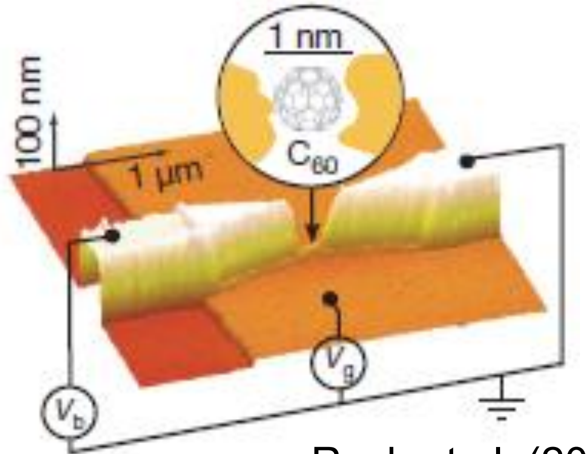
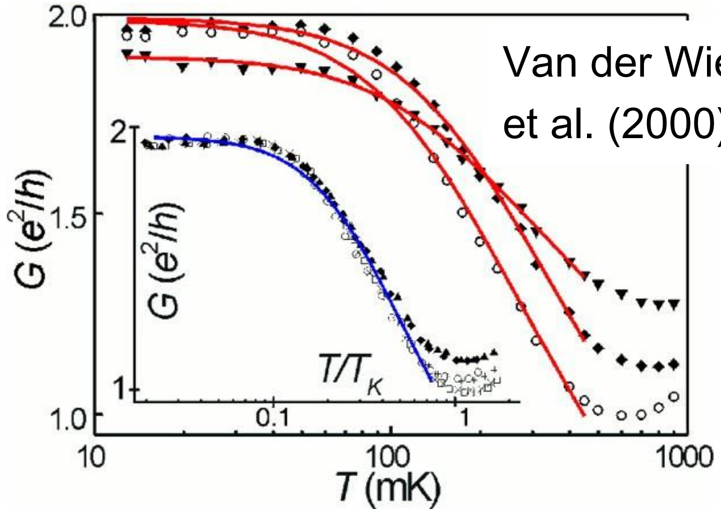
# NRG methods and applications

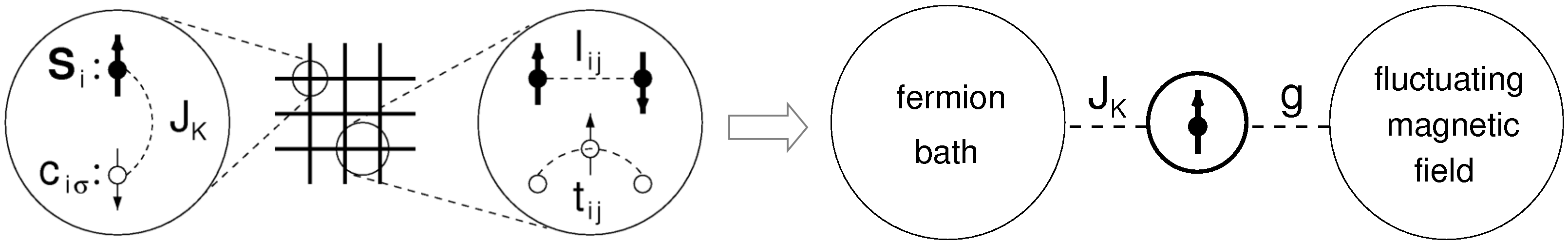
Kevin Ingersent (U. of Florida)




Roch et al. (2008)




Van der Wiel et al. (2000)




Si et al. (2001)

Supported by NSF DMR-1508122

# Before we begin …

UF UNIVERSITY of FLORIDA

# It looks beautiful …

Physics Department

Lake Alice

# … but beware of the natives

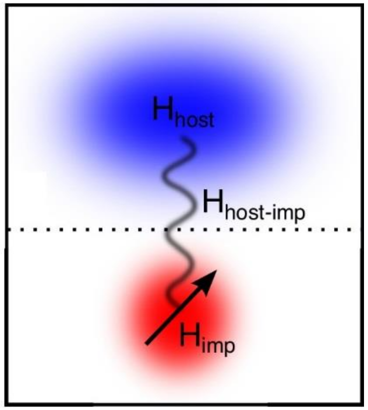
A resident of Lake Alice


Residents of “The Swamp”

# Outline

- Quantum impurity problems couple a local degree of freedom to a gapless, noninteracting host:

$$H = H_{\text{host}} + H_{\text{host-imp}} + H_{\text{imp}}$$




- Ken Wilson devised the numerical renormalization group for controlled nonperturbative evaluation of equilibrium thermodynamics of impurity models with fermionic hosts.
- The original NRG has been extended to …
  - dynamical properties
  - multi-orbital impurities, multiple impurities, bosonic hosts
  - impurity solution in dynamical mean-field methods
  - non-equilibrium properties.

# NRG Strengths and Weaknesses

- NRG methods are non-perturbative in model parameters
  - Can often map out the full phase diagram.
- Can accurately calculate properties over many decades of temperature/frequency
  - **Important** where there is a very small many-body scale, e.g., in Kondo physics.
  - **Essential** for studying quantum criticality.
- Not as flexible as QMC methods
  - Cannot treat bulk interactions.
  - Laborious to calculate higher-order correlation functions or finite bias.
- NRG does not scale well with increasing number or impurities and/or bands

# Some References and Public Domain Codes

- Background on quantum-impurity problems:
  Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge Univ. Press, 1997).

- NRG reviews:
  - Wilson, Rev. Mod. Phys. **44**, 773 (1975)
  - Krishna-murthy et al., PRB 21, 1003, 1044 (1980)
  - Bulla et al., Rev. Mod. Phys. **80**, 395 (2008)

- Public-domain codes:
  - *NRG Ljubljana* code (http://nrgljubljana.ijs.si)
    A flexible implementation of "traditional" NRG
  - *Flexible DM-NRG* (http://www.phy.bme.hu/~dmnrg)
    Implements density-matrix NRG method described in Toth et al., PRB **78**, 245109 (2008).

# Motivation for the NRG

- The NRG was developed for problems with fermionic hosts, e.g.,

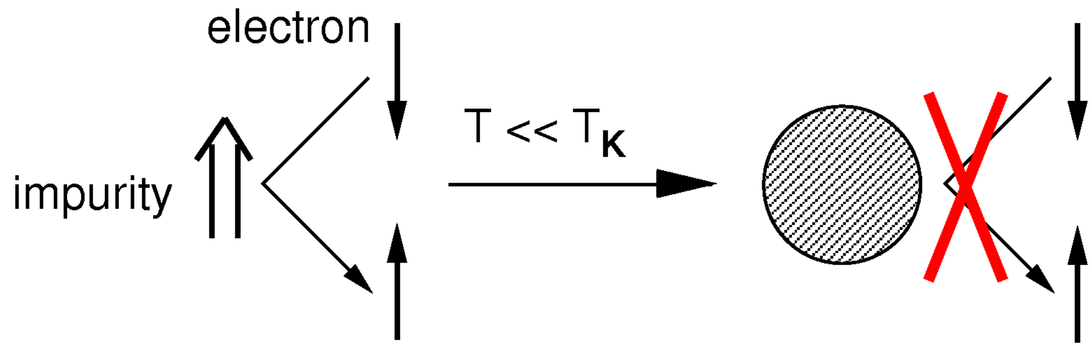
$$H_{\text{Kondo}} = H_{\text{host}} + J\,\mathbf{S}_{\text{imp}} \cdot \mathbf{s}_{\text{host}}(\mathbf{r}_{\text{imp}}),$$

where

$$H_{\text{host}} = \sum_{k,\sigma} \varepsilon_k\, c_{k\sigma}^{\dagger}\, c_{k\sigma}\,.$$

- With decreasing $T$, the impurity spin-½ is progressively screened with a characteristic many-body scale

$$T_K = D \exp(-1/\rho_0 J).$$



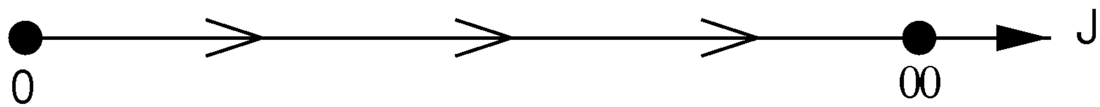
# What makes the Kondo model hard?

- The fundamental challenge of the Kondo model

$$H_{\mathrm{Kondo}} = H_{\mathrm{host}} + J\,\mathbf{S}_{\mathrm{imp}} \cdot \mathbf{s}_{\mathrm{host}}\left(\mathbf{r}_{\mathrm{imp}}\right),$$

  is the equal importance of spin-flip scattering of band electrons on every energy scale $\varepsilon$ on the range $-D \le \varepsilon \le D$.

- Poor man's scaling (Anderson, 1970): Each decade of band energies about the Fermi level contributes equally to the renormalization of $J$ toward $J^{*} = \infty$:



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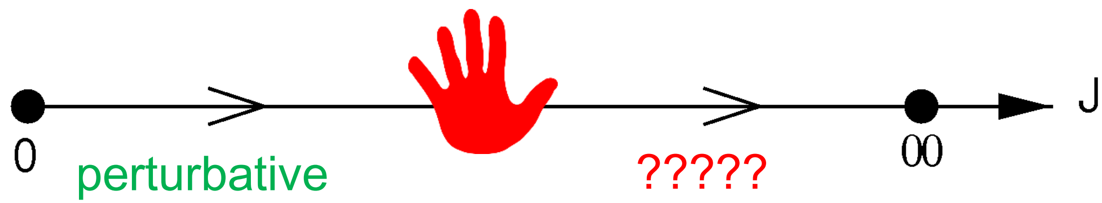
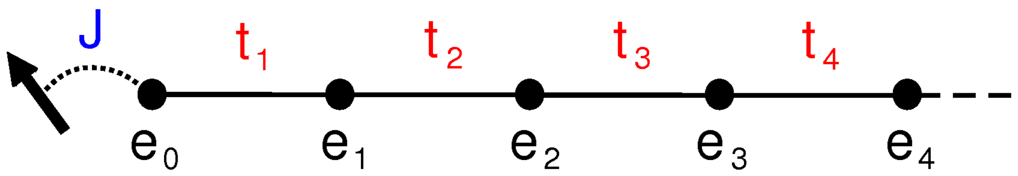



- Scaling is perturbative in the renormalized value of $\rho_0 J$ and thus limited to temperatures $T > T_K = D \exp\left(-1/\rho_0 J\right)$.

- The NRG was conceived to reliably reach down to $T = 0$.

# Chain mapping of any host

- Any noninteracting host can be mapped exactly to a tight-binding form on one or more semi-infinite chains:




  - Start with $|f_0\rangle =$ host state entering $H_{\text{host-imp}}$
  - Since $i\hbar \frac{d}{dt}|\Psi\rangle = H|\Psi\rangle,$

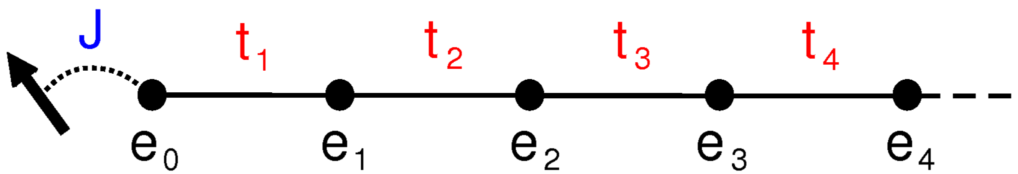
    reach only host states given by repeated action of $H_{\text{host}}$
  - Lanczos (1950): $H_{\text{host}}|f_0\rangle = e_0|f_0\rangle + t_1|f_1\rangle$

$$H_{\text{host}}|f_1\rangle = e_1|f_1\rangle + t_1|f_0\rangle + t_2|f_2\rangle$$

$$H_{\text{host}}|f_2\rangle = e_2|f_2\rangle + t_2|f_1\rangle + t_3|f_3\rangle \qquad \text{etc}$$

# Chain mapping of a conduction band

- Any noninteracting host can be mapped exactly to a tight-binding form on one or more semi-infinite chains:




- The conduction band in the Kondo model maps to

$$H_{\text{host}} = \sum_{\sigma} \sum_{n=0}^{\infty} \left[ e_n f_{n\sigma}^{\dagger} f_{n\sigma} + t_n \left( f_{n\sigma}^{\dagger} f_{n-1,\sigma} + \text{H.c.} \right) \right]$$

- Since the basis grows by a factor of 4 for each chain site, we would like to diagonalize $H$ on finite chains. **But …**
  - Coefficients $e_n$, $t_n$ are all of order the half-bandwidth.
  - No useful truncations: Ground state for chain length $L$ is not built just from low-lying states for chain length $L-1$.

# NRG's key feature: Band discretization

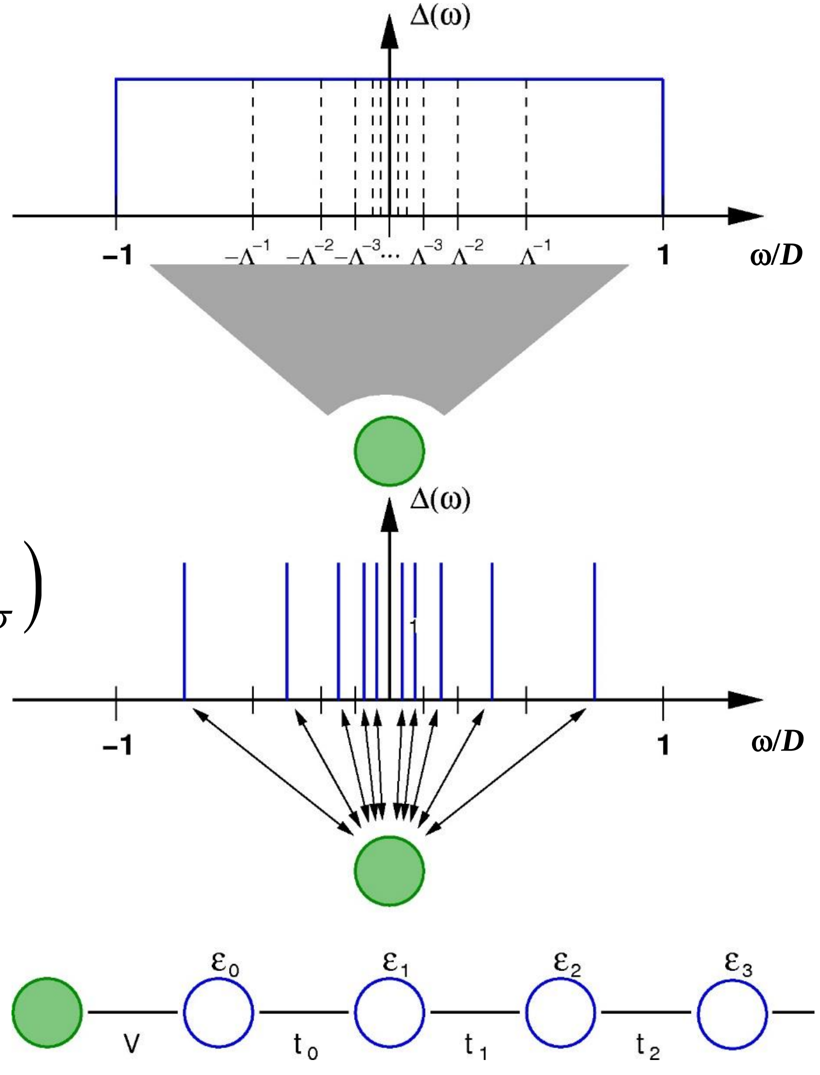
- Wilson (~1974) logarithmically discretized the conduction band via a parameter $\Lambda > 1$.

- The impurity couples to just one state per bin:

$$H_{\text{host},\Lambda} = \sum_{\sigma} \sum_{m=0}^{\infty} \omega_m \left( a_{m\sigma}^{\dagger} a_{m\sigma} - b_{m\sigma}^{\dagger} b_{m\sigma} \right)$$

$$\omega_m = \tfrac{1}{2}\left(1 + \Lambda^{-1}\right)\Lambda^{-m} D$$

- Now apply Lanczos to the discretized band:



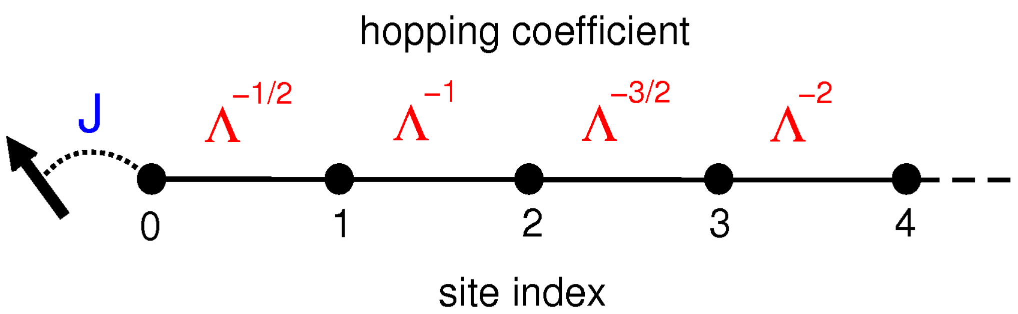

Bulla et al. (2008)

# NRG iterative solution

- Wilson's artificial separation of bin energy scales $\propto \Lambda^{-m}$ gives exponentially decaying tight-binding coefficients:

$$H_{\text{host},\Lambda} = \sum_{\sigma} \sum_{n=0}^{\infty} \left[ e_n f_{n\sigma}^{\dagger} f_{n\sigma} + t_n \left( f_{n\sigma}^{\dagger} f_{n-1,\sigma} + \text{H.c.} \right) \right] \quad |e_n|, t_n \le cD\Lambda^{-n/2}$$

(not a $\Lambda^{-n}$ decay!)

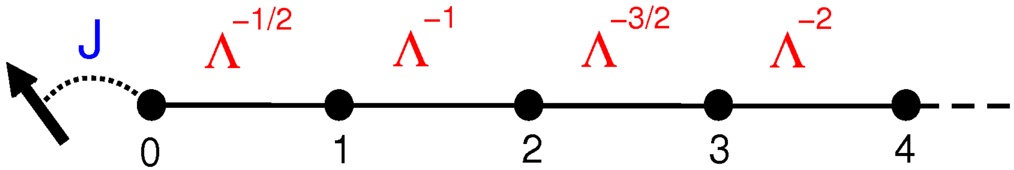



- Allows iterative solution on chains of length $L = 1, 2, 3, \ldots$
  - Ground state for chain length $L$ is mainly built from low-lying states for chain length $L-1$.
  - Thus, can truncate the Fock space after each iteration to cap the computational time.

# NRG iterative solution

- Start with $H_0 = H_{\text{imp}} + H_{\text{host-imp}}\left(f^\dagger_{0\sigma}, f_{0\sigma'}\right) + e_0 f^\dagger_{0\sigma} f_{0\sigma}$.

  e.g., Kondo: $H_{\text{imp}} = 0$; $H_{\text{host-imp}} = 2J\,\mathbf{S}_{imp} \cdot \sum_{\sigma,\sigma'} f^\dagger_{0\sigma} \tfrac{1}{2}\tau_{\sigma\sigma'} f_{0\sigma}$; $e_0 = 0$ (p-h symm.)




- Then $H_N = \Lambda^{1/2} H_{N-1} + \Lambda^{N/2} \sum_\sigma \left[ e_N f^\dagger_{N\sigma} f_{N\sigma} + t_N \left( f^\dagger_{N\sigma} f_{N-1,\sigma} + \text{H.c.} \right) \right]$

  Diagonalize in a basis $\left|E_{N-1,r}\right\rangle \otimes \left|b\left(f^\dagger_{N\sigma}, f_{N\sigma'}\right)\right\rangle$ to find $\left\{\left|E_{Ns}\right\rangle\right\}$.

- Keep states $1 \le s \le N_s$ of lowest energy $E_{Ns}$, discard the rest. Computational time $\sim N_s^3$.

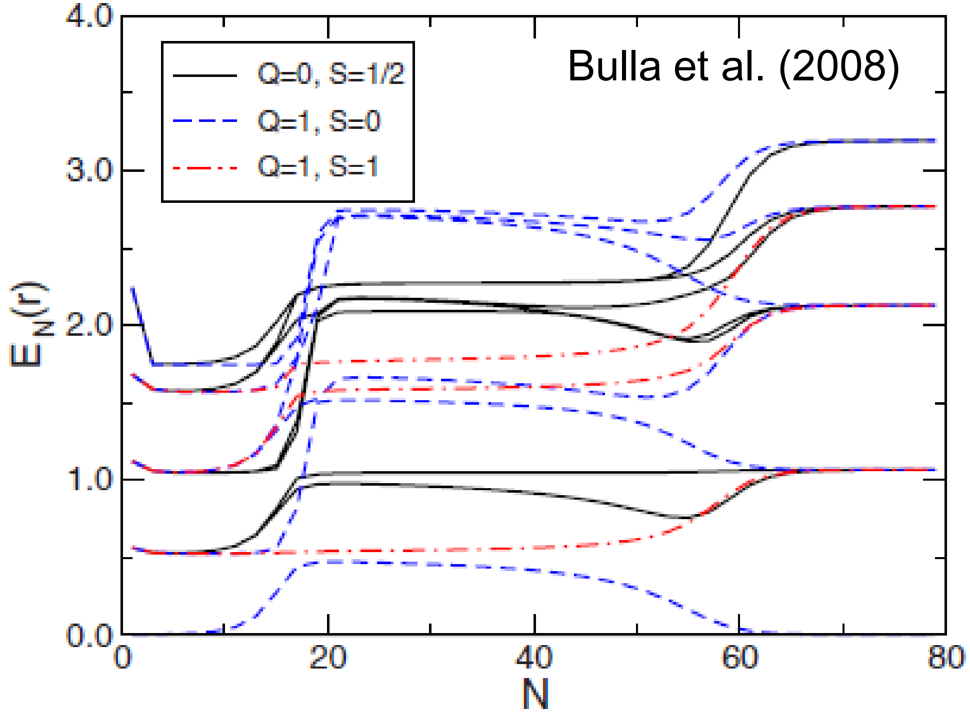
# NRG level flow

- Iterate $H_N \rightarrow \{|E_{Nr}\rangle\} \rightarrow H_{N+1} \rightarrow \ldots$

  until reach a scale-invariant RG fixed point where

  low-lying solution of $H_N$ = low-lying solution of $H_{N\text{-}2}$

- E.g., Anderson model




With
  - increasing $N$,
  - decreasing energy $\approx D\Lambda^{-N/2}$,

observe two crossovers

free orbital → local moment → strong coupling (Kondo)

# What does NRG give?

- The solutions of $H_{\text{host},\Lambda}$ give the value $X_{\text{host}}$ of a bulk thermodynamic property in the pure host (no impurity).
- Solutions of $H_{\text{Kondo}} = H_{\text{host},\Lambda} + J\,\mathbf{S}_{\text{imp}} \cdot \mathbf{s}_{\text{host}}(\mathbf{r}_{\text{imp}})$

  give the value $X_{\text{total}}$ in the full system with the impurity:

$$X_{\text{total}}(T) = Z_N^{-1} \sum_r \langle E_{Nr} | \hat{X} | E_{Nr} \rangle e^{-E_{Nr}/T} \quad \text{where} \quad T \approx D\Lambda^{-N/2}$$

- Both $X_{\text{host}}$ and $X_{\text{total}}$ vary strongly with the discretization $\Lambda$.
- But the value of

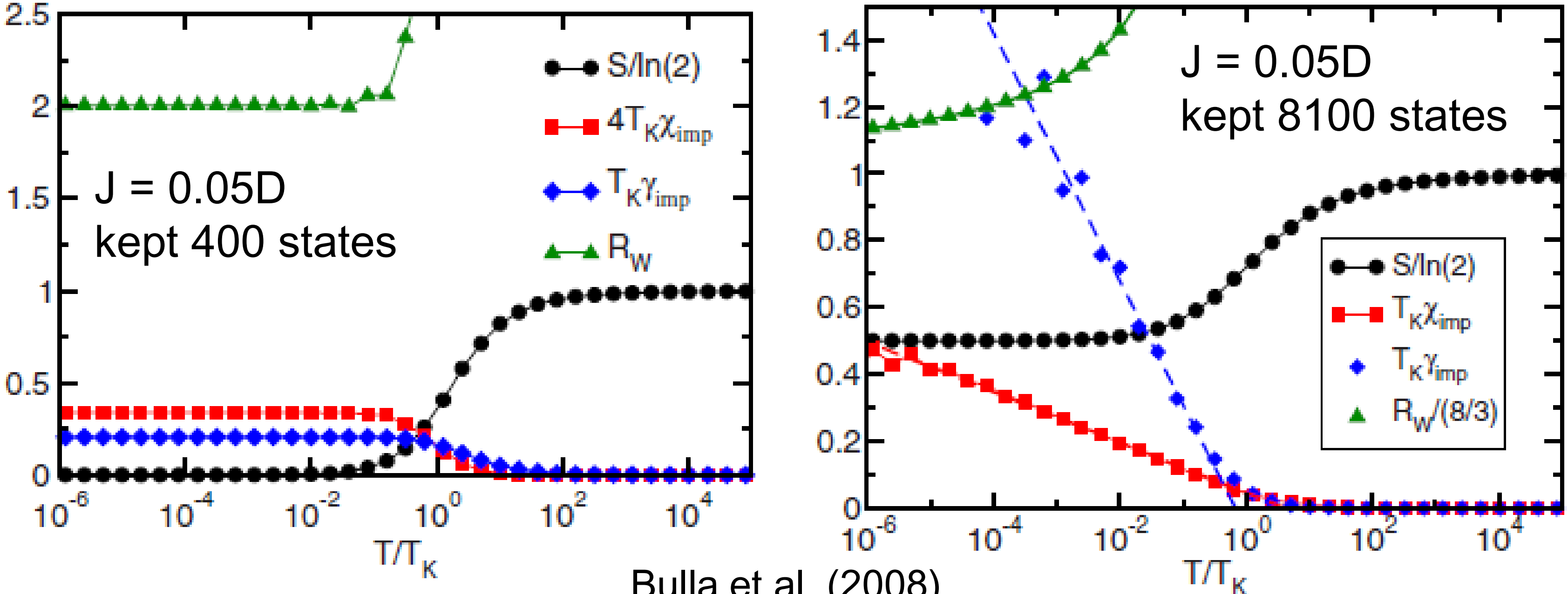
$$X_{\text{imp}} = X_{\text{total}} - X_{\text{host}}$$

  varies remarkably weakly with $\Lambda$.

- Can use $2 \le \Lambda \le 10$ to estimate the physical ($\Lambda = 1$) value.

# Examples of impurity thermodynamics

- Can reliably distinguish Fermi liquids & non-Fermi-liquids:




Bulla et al. (2008)

| conventional (1-channel) Kondo model | overscreened (2-channel) Kondo model |
| --- | --- |
| $\chi_{\text{imp}}, C_{\text{imp}}/T \to \text{const.}$ | $\chi_{\text{imp}}, C_{\text{imp}}/T \propto \ln(1/T)$ |
| $S_{\text{imp}} \to 0$ | $S_{\text{imp}} \to \ln 2$ |

# Dynamical properties

- Consider the Anderson impurity model

$$H = \varepsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + V \sum_{\sigma} \left( d_{\sigma}^{\dagger} c_{0\sigma} + \text{H.c.} \right) + H_{\text{host}}$$

- Interested in the impurity Green's function

$$G_{\sigma}(t) = -i\theta(t) \left\langle \left\{ d_{\sigma}(t), d_{\sigma}^{\dagger}(0) \right\} \right\rangle \quad \leftrightarrow \quad A_{\sigma}(\omega) = -\tfrac{1}{\pi} \operatorname{Im} G_{\sigma}(\omega)$$

- NRG solutions tracking $M_{Nrr'} = \left\langle E_{Nr} \middle| d_{\sigma}^{\dagger} \middle| E_{Nr'} \right\rangle$ yield a discrete approximation

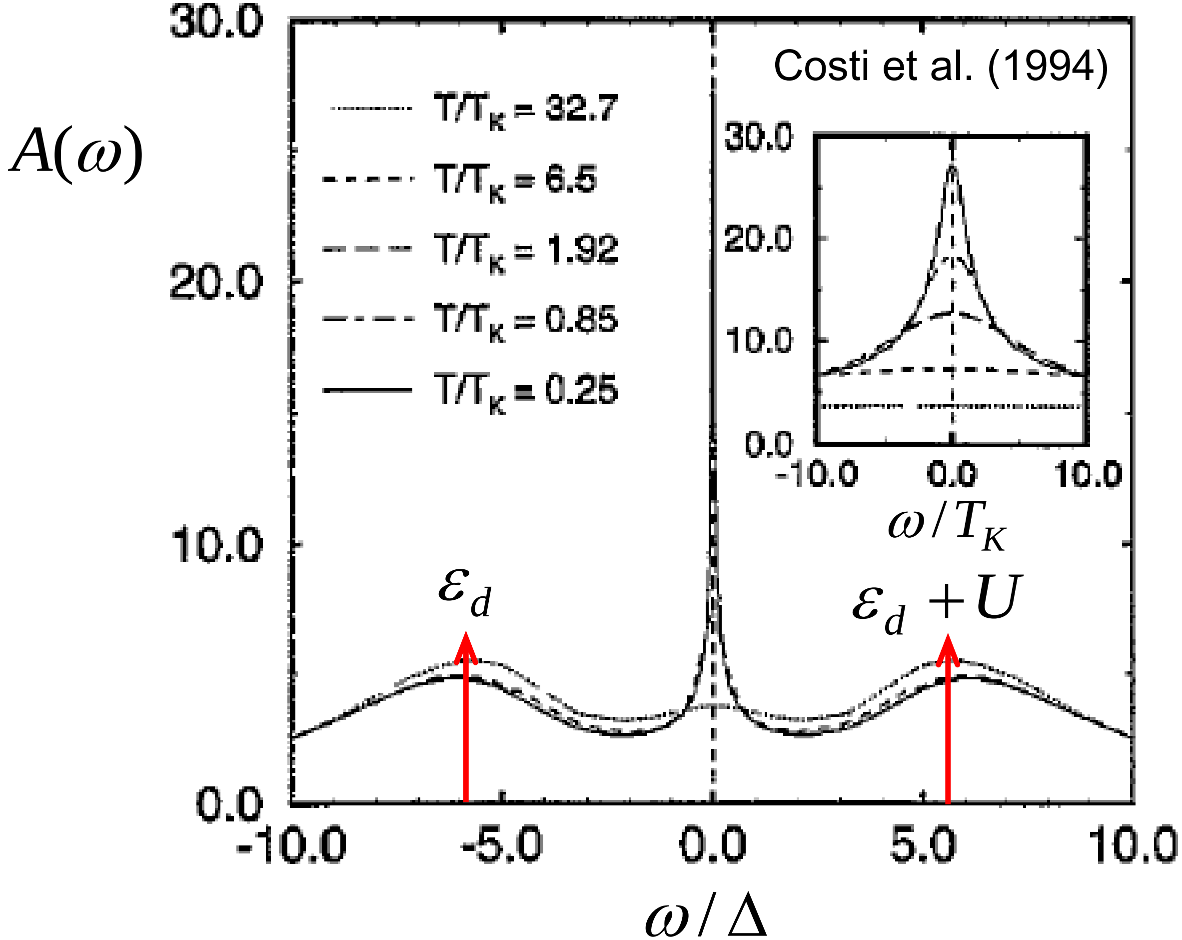
$$A_{\sigma}(\omega, T) = Z_N^{-1} \sum_{r,r'} \left| M_{Nrr'} \right|^2 \left( e^{-E_{Nr}/T} + e^{-E_{Nr'}/T} \right) \delta\left(\omega - E_{Nr} + E_{Nr'}\right)$$

where $|\omega| \approx D\Lambda^{-N/2}$.

- Obtain a smooth $A_{\sigma}(\omega, T)$ by replacing $\delta(\omega - \omega_{rr'})$ by a broadening function of width proportional to $\max(|\omega_{rr'}|, T)$.

# Calculation of transport properties

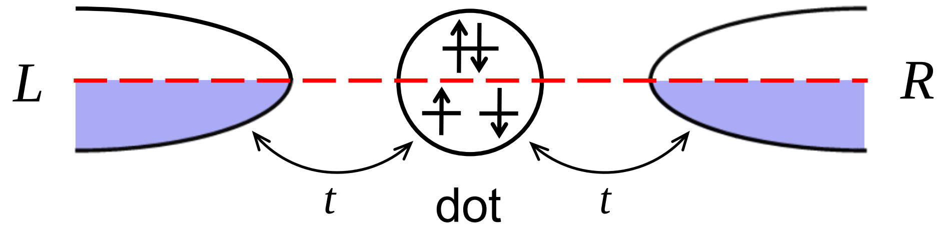
- Smoothed spectral function reveals the Kondo resonance:




$$\Delta = \pi \rho_0 V^2$$

# Calculation of transport properties

- Smoothed spectral function can be used to calculate linear-response transport properties.
- E.g., for a quantum-dot setup

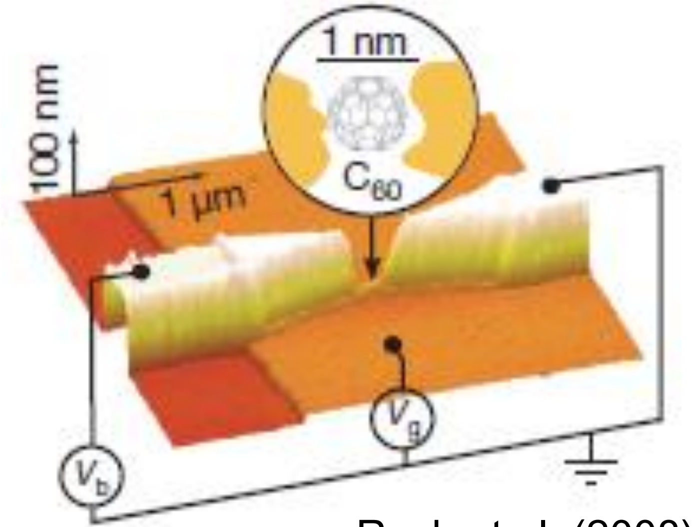



zero-bias conductance is

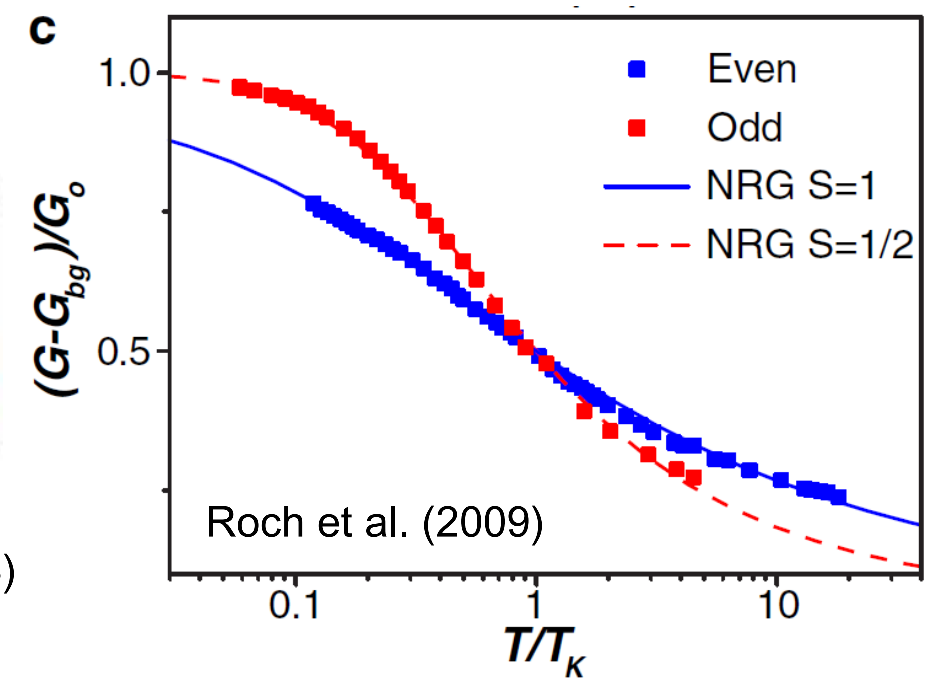
$$G(T) = \frac{e^2}{h} \pi \Delta \sum_{\sigma} \int (-\partial f / \partial \omega) A_{\sigma}(\omega, T)\, d\omega$$

where $\Delta = \pi \rho_{\text{lead}} t^2$ is the noninteracting level width.

# Application: Conductance of $C_{60}$ quantum dot



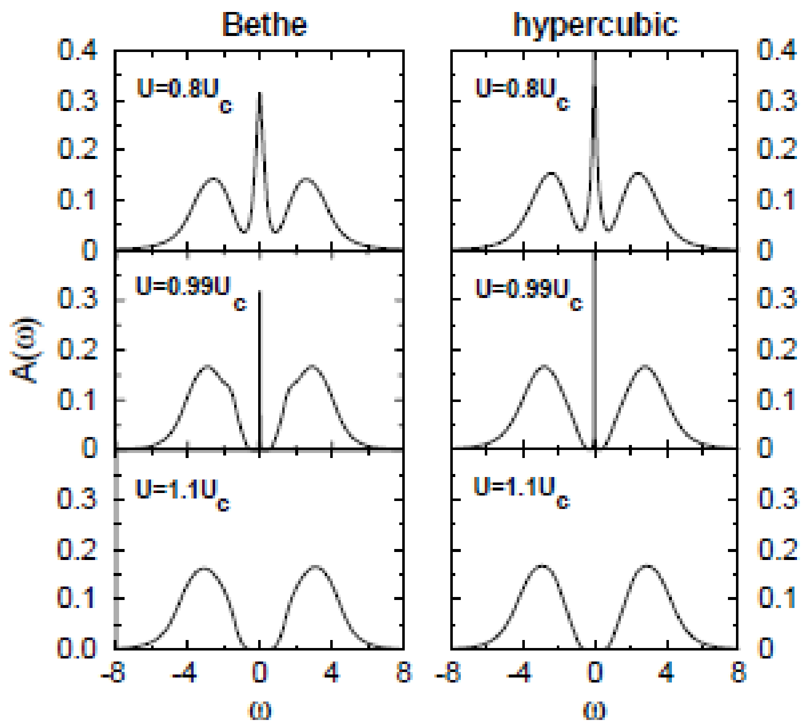

Roch et al. (2008)




- $V_g$ can drive $C_{60}$ electron occupancy from odd to even.
- Comparison of measured $G(T)$ with NRG suggests
  - spin-½ Kondo for odd occupancy ($T_K = 4.4$ K)
  - underscreened spin-1 Kondo for even ($T_K = 1.1$ K)

# Application: Dynamical mean-field theory

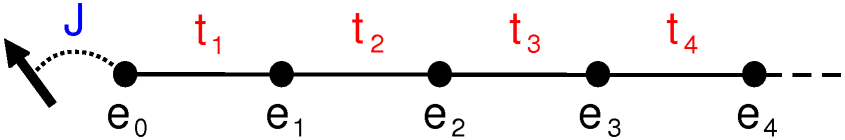
- NRG has been used as the impurity solver in the DMFT treatment of many lattice Hamiltonians.
- It is especially useful if there is a vanishing energy scale, e.g., the Mott transition in the Hubbard model.




Bulla (1999)

# Application: Dynamical mean-field theory

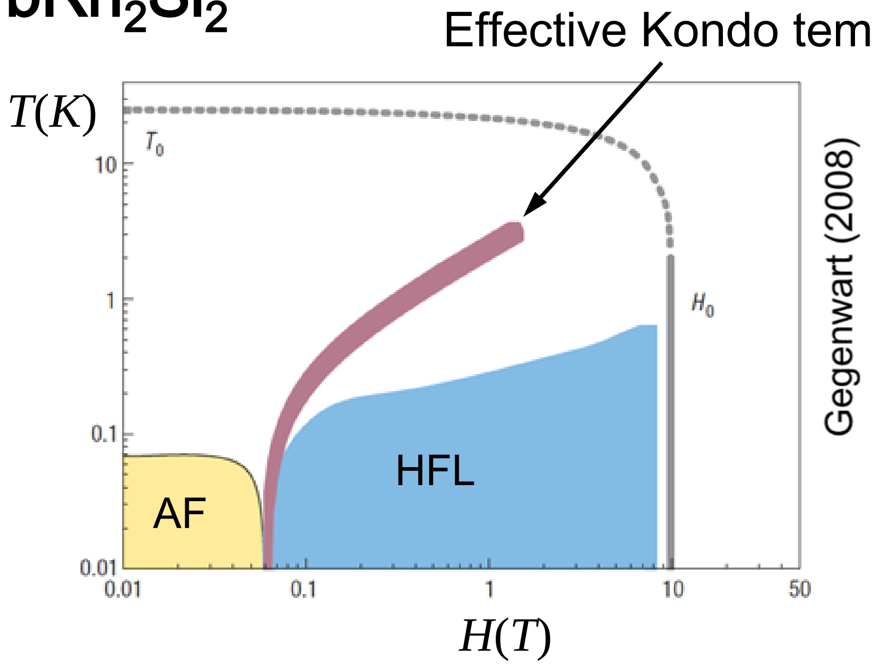
- NRG has been used as the impurity solver in the DMFT treatment of many lattice Hamiltonians.
- However, the NRG does not scale well for the multiband models and cluster DMFT extensions that are of interest for many correlated materials (cuprates, pnictides, …).
  - NRG basis grows at each iteration by a factor of $2^{n_f}$, where $n_f$ is the num. of distinct bulk fermionic species.

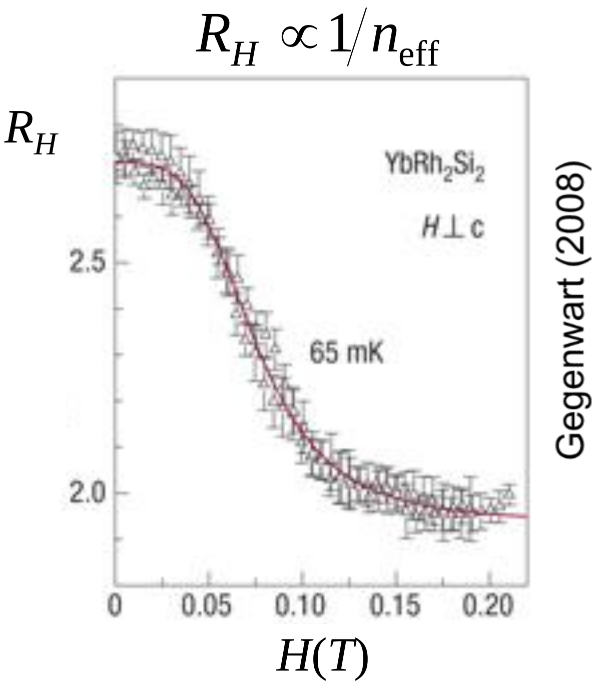



  - Usually, $n_f = (2s+1)$ x (num. impurities) x (num. bands).
  - As $n_f$ increases, so too must $N_s$, the number of retained many-body states.
  - Computational time per NRG iteration $\propto \left(2^{n_f} N_s\right)^3$.

# Application: Kondo-destruction QPTs

$YbRh_2Si_2$



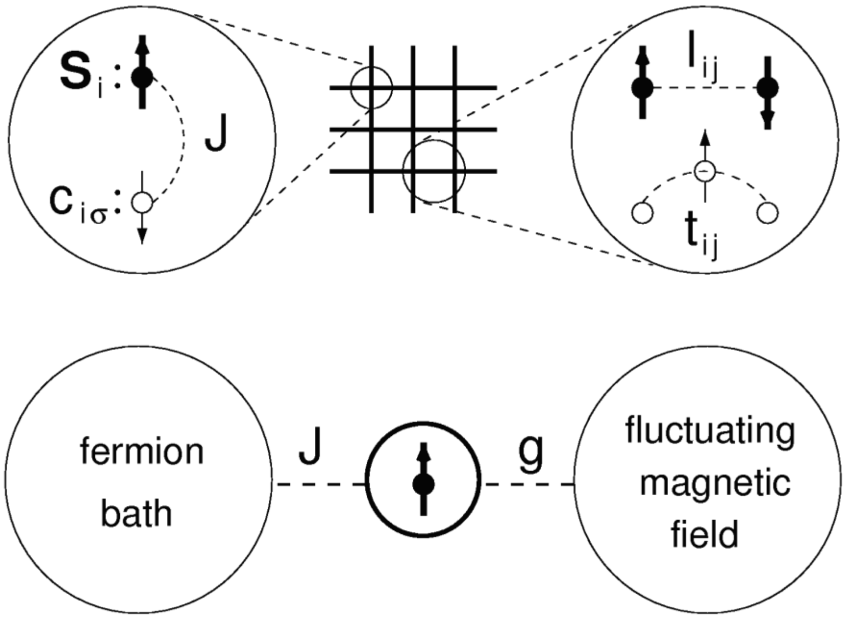

- At the QPT, Kondo scale vanishes, Fermi surface jumps.
- Neutron scattering on **$CeCu_{1-x}Au_x$** shows **quasi-2D** magnetic critical fluctuations with $\omega/T$ scaling **at generic q**.
- Points to a local QPT outside the Landau framework.

# Extended dynamical mean-field theory

- EDMFT includes some spatial fluctuations (unlike DMFT).
- Lattice Kondo model maps to a Bose-Fermi Kondo impurity model:

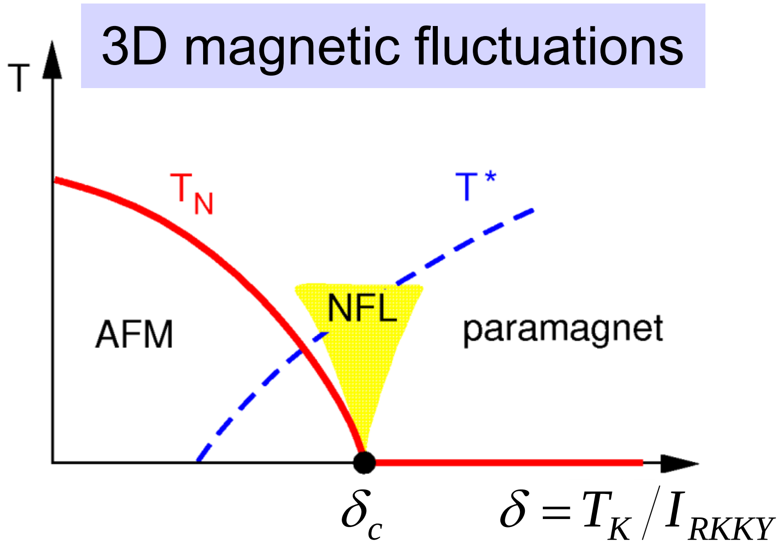
$$H = J\mathbf{S}\cdot\mathbf{s} + H_{\text{band}} + \sum_{\alpha=x,y,z}\left[g_\alpha S_\alpha \sum_{\mathbf{q}}\left(a_{\mathbf{q}\alpha} + a_{\mathbf{q}\alpha}^\dagger\right) + \sum_{\mathbf{q}}\omega_{\mathbf{q}} a_{\mathbf{q}\alpha}^\dagger a_{\mathbf{q}\alpha}\right]$$

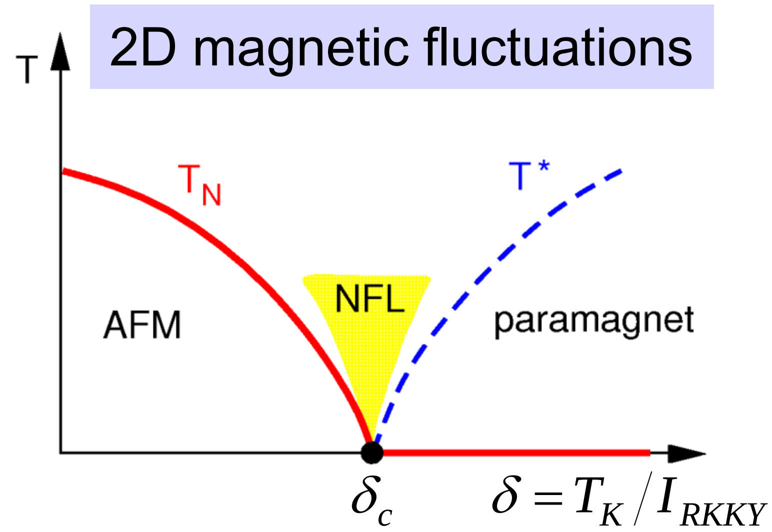
- Fermionic band accounts for local dynamical correlations.
- Dissipative baths represent a fluctuating magnetic field due to other local moments.
- Band and bath densities of states must be found **self-consistently.**



# EDMFT for Ising-symmetry Kondo lattice

- Two types of solution [Si + collaborators (2001,2003,2007)]:



# EDMFT for Ising-symmetry Kondo lattice

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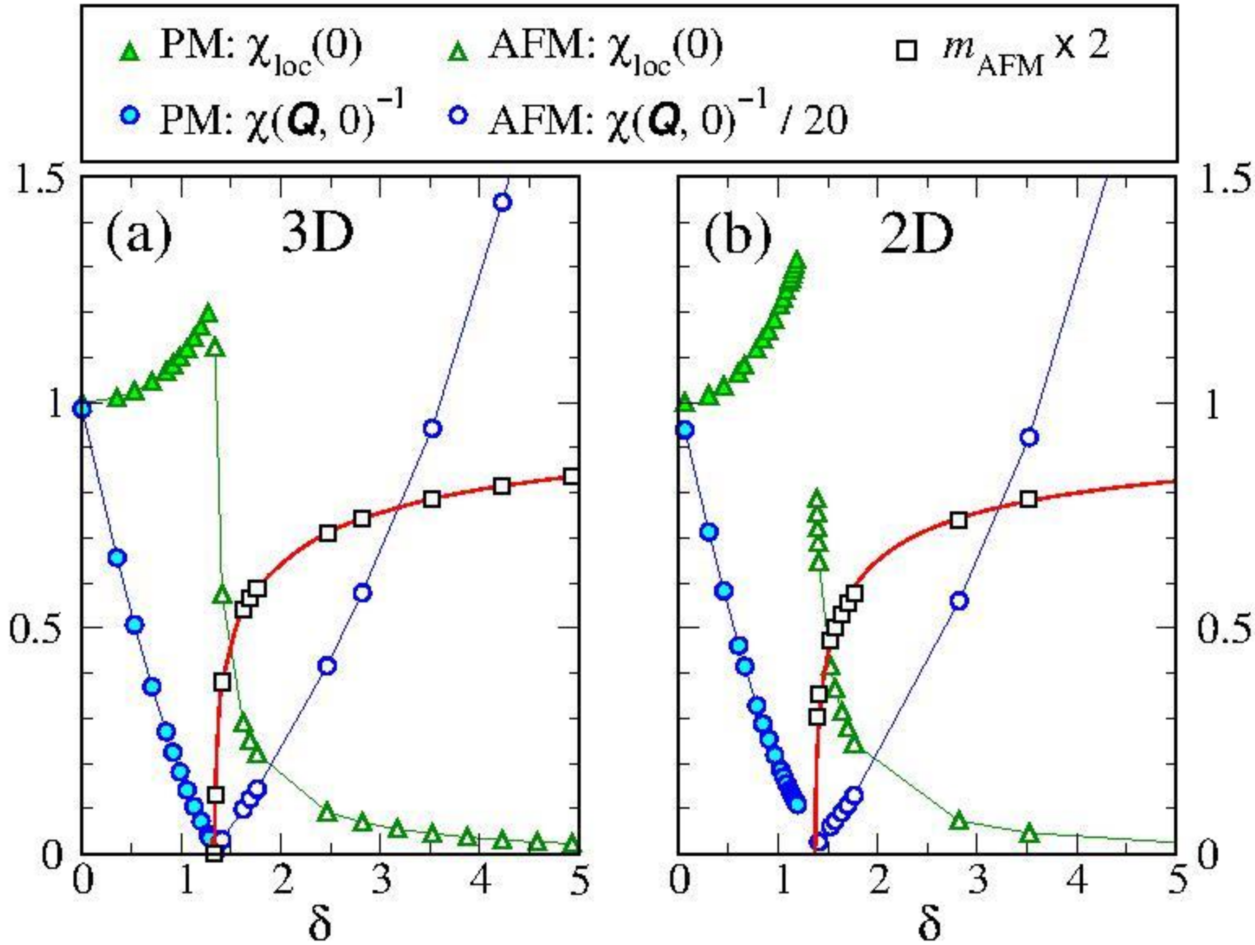
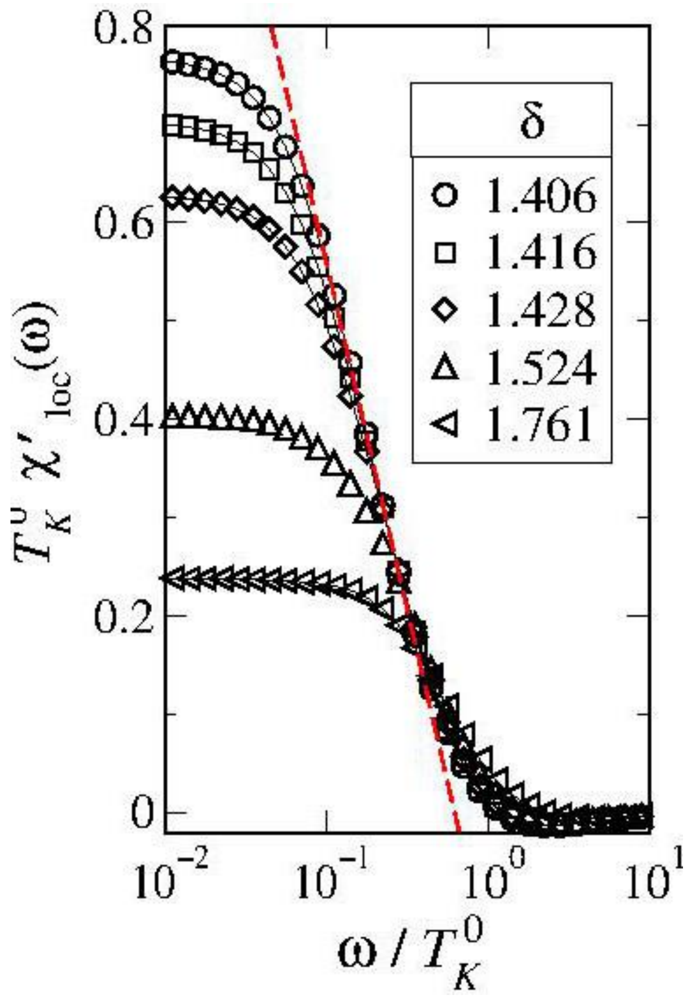



$$\delta = T_K / I_{RKKY}$$

# EDMFT for Ising-symmetry Kondo lattice

• Locally critical NRG solution [Glossop and KI (2007)]:

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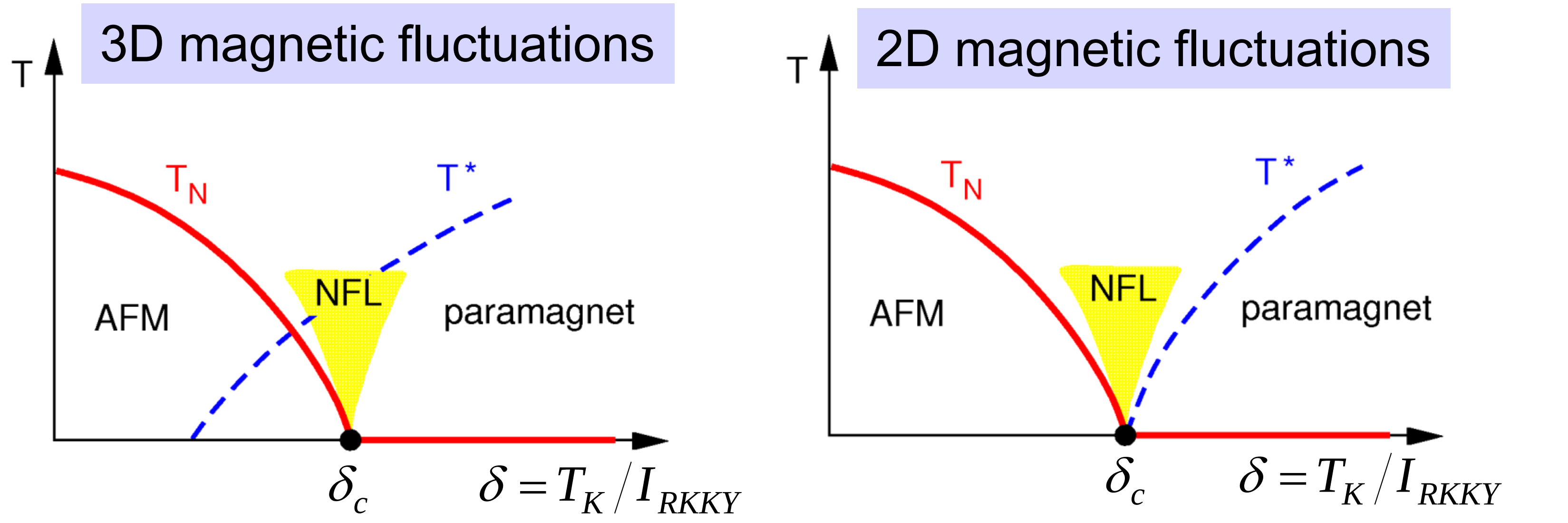



- Locally critical QPT in the 2D case is consistent with …
  - Jumps in the Fermi-surface volume, carrier conc'n.
  - A divergence of the Gruneisen ratio $\beta / C_p$.
  - Anomalous $\omega/T$ scaling of dynamical spin susceptibility.

# Locally critical EDMFT solutions

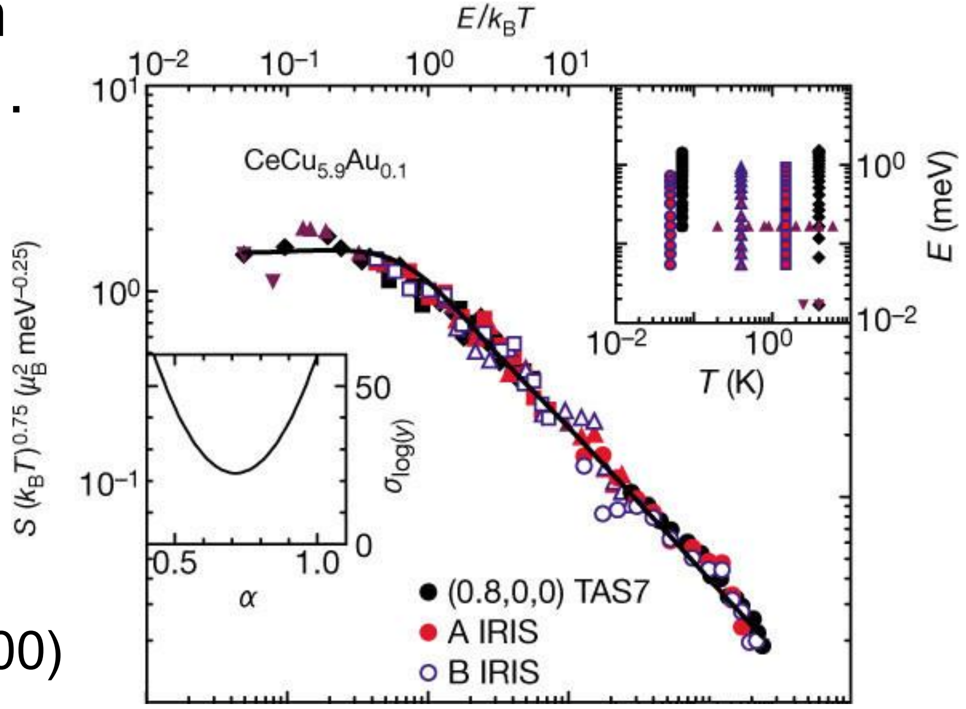
- Dynamical spin susceptibility takes the form

$$\chi(\mathbf{q},\omega) = \frac{1}{(I_{\mathbf{q}} - I_{\mathbf{Q}}) + A\,(-i\omega)^{\alpha} W(\omega/T)}$$

where $0.72 \le \alpha \le 0.78$ from numerics compares with …

$\alpha \approx 0.75$ from neutrons

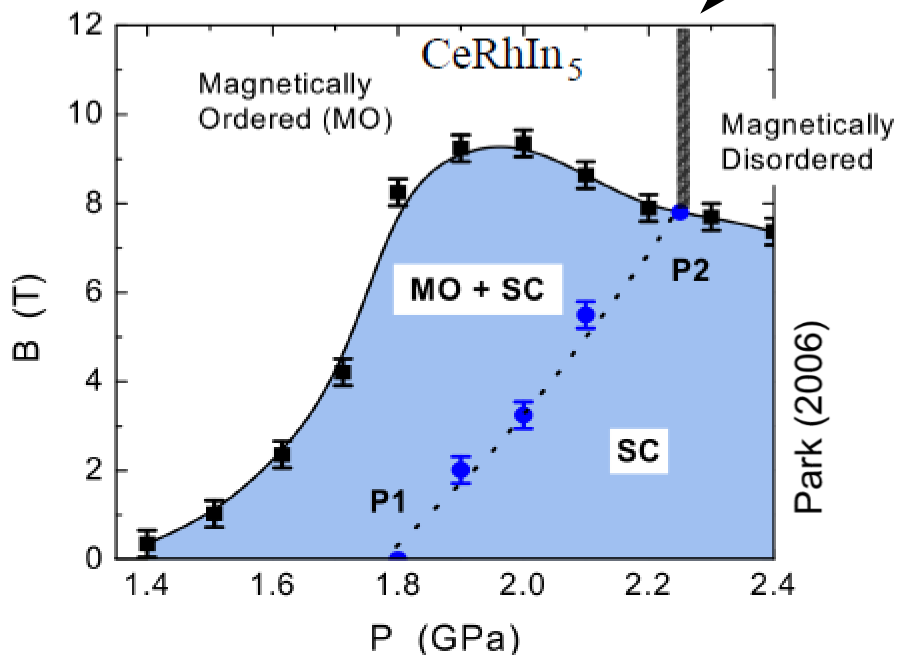
Schröder et al (2000)

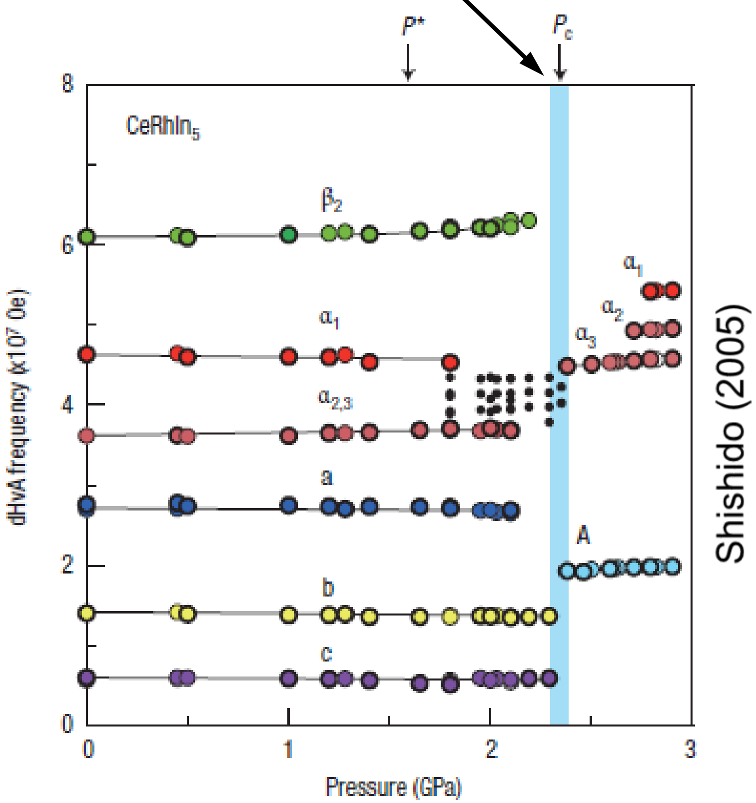


# Superconductivity near a Kondo-destruction QPT

## $CeRhIn_5$

Jump in Fermi surface



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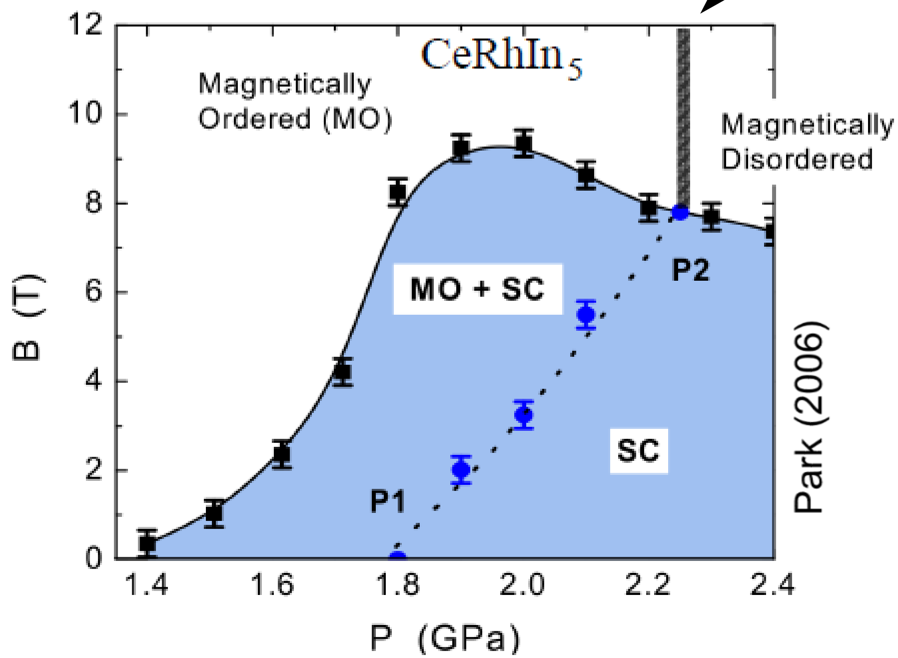
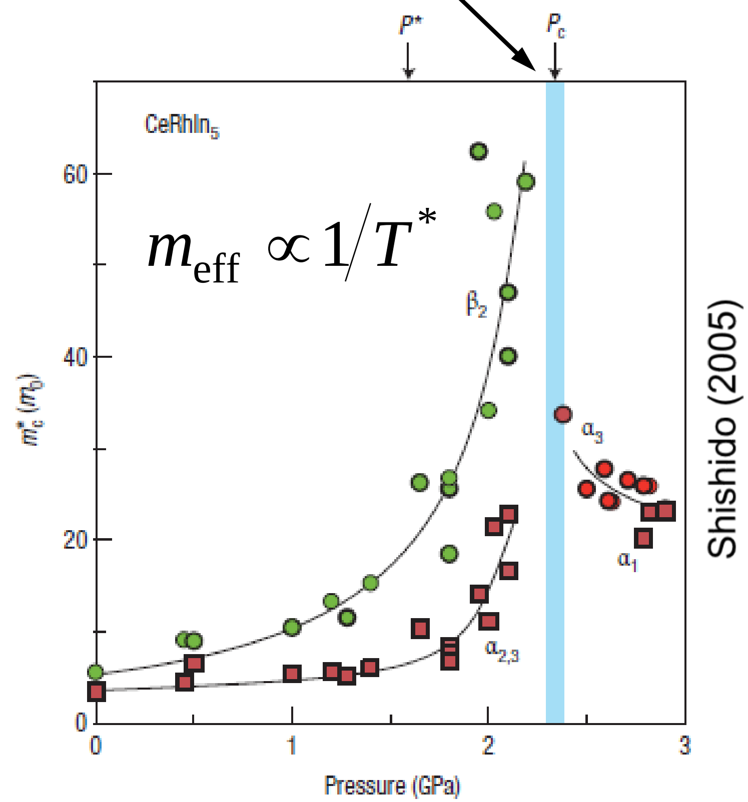


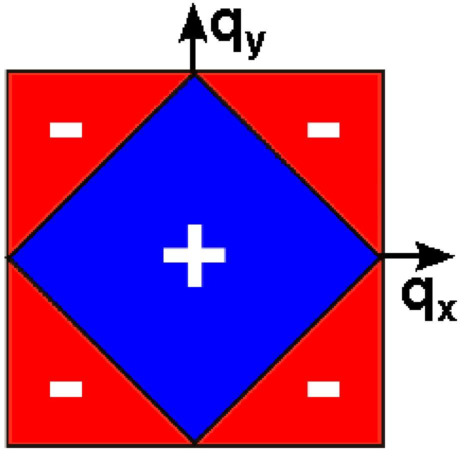

How does Kondo destruction affect superconductivity?

# Cluster EDMFT approach

- EDMFT cannot describe non-s-wave superconductivity.
- For this, we apply a cluster extension of EDMFT [Pixley et al. (2015)] to the Anderson lattice model:

$$H = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_i (\epsilon_f n_{fi} + U n_{fi\uparrow} n_{fi\downarrow}) + \sum_{i,\sigma} \left( V c^\dagger_{i\sigma} f_{i\sigma} + \text{h.c.} \right) + \sum_{\langle i,j \rangle} I_{ij} S^z_{fi} S^z_{fj}$$

- Simplest approximation divides the Brillouin zone into two patches: one FM ('+') and one AFM ('–').

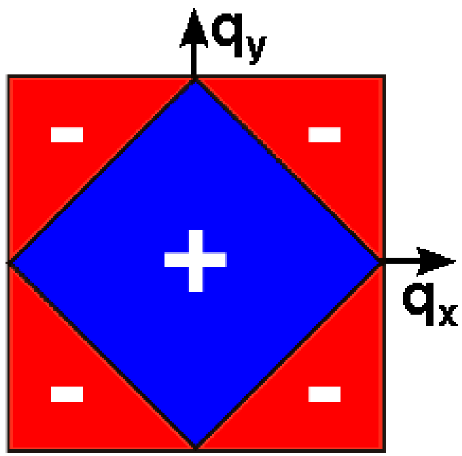


# Cluster EDMFT (cont.)

- Assume that

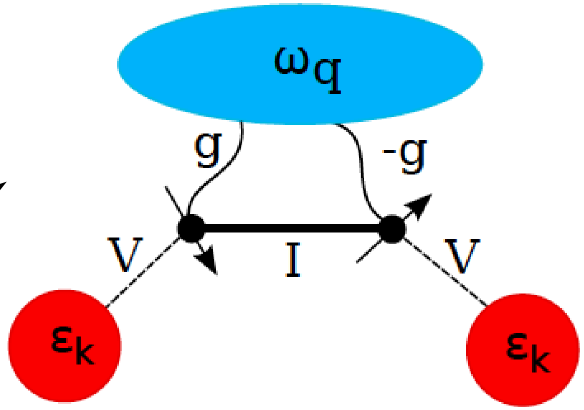
$$G(\mathbf{k},\omega)=\frac{1}{\omega-\varepsilon_{\mathbf{k}}-\Sigma(\mathbf{K}_{\mathbf{k}},\omega)}$$

$$\chi(\mathbf{q},\omega)=\frac{1}{I_{\mathbf{q}}+M(\mathbf{Q}_{\mathbf{q}},\omega)}$$



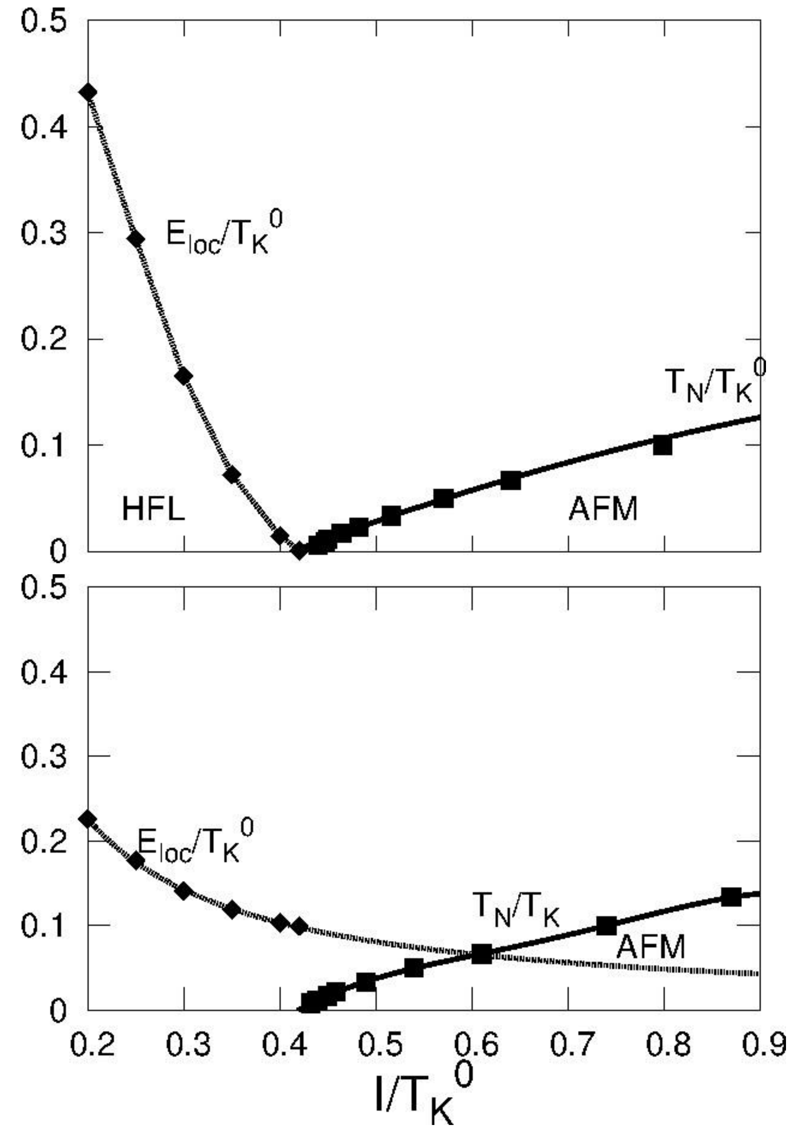

- This leaves an effective two-impurity Bose-Fermi Anderson model with two bosonic baths.

- Coupling $g\,(S_{1z}-S_{2z})\cdot u_{-}$ to the '–' bosonic bath should dominate near QTP.



# Cluster EDMFT solutions

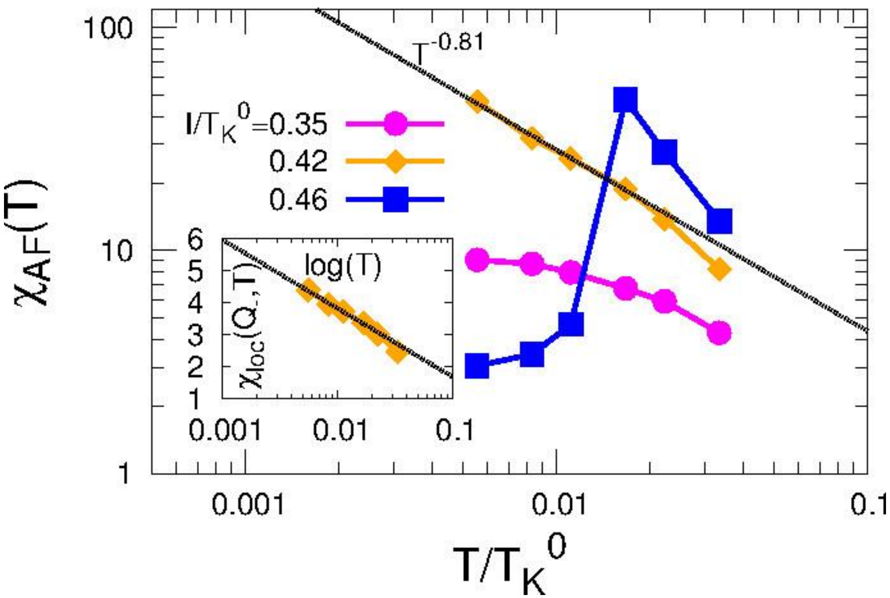
- Solve using
  - Numerical RG at $T = 0$.
  - Continuous time QMC at $T > 0$.
- Again find two types of solution:
  - 2D spin fluctuations lead to local criticality
  - 3D spin fluctuations yield a spin-density-wave (conventional) QPT

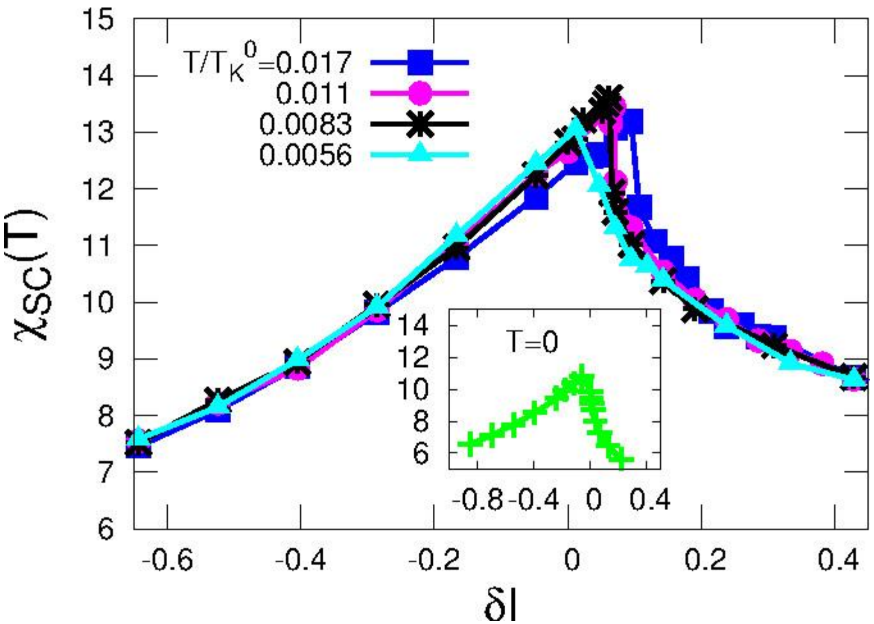


# Cluster EDMFT solutions

Focus on locally critical case:

- Spin susceptibility again has anomalous exponent, here $\alpha \approx 0.81$ cf. $\alpha \approx 0.75$ from neutrons.



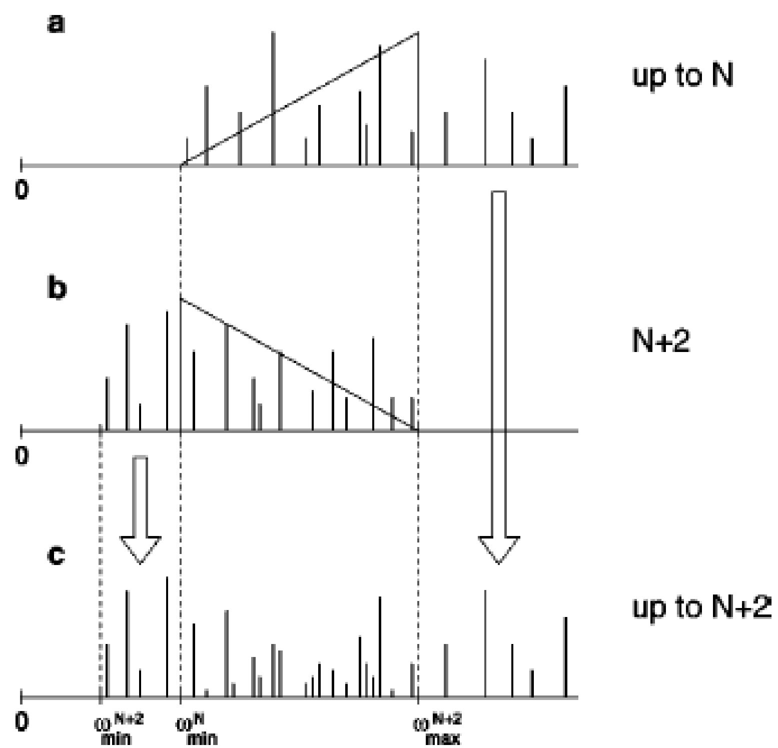

Singlet pairing correlations are strongly enhanced near a Kondo-destruction QPT.

$$\Delta_d^\dagger = \frac{1}{\sqrt{2}}(d_{1\uparrow}^\dagger d_{2\downarrow}^\dagger - d_{1\downarrow}^\dagger d_{2\uparrow}^\dagger)$$

# Correcting a technical flaw of Wilson's NRG

- Having to calculate a property using the iteration $N$ where $T \approx D\Lambda^{-N/2}$ and/or $|\omega| \approx D\Lambda^{-N/2}$ creates problems:
  - edge effects where switch from using $N$ to $N+1$ (or $N+2$)
  - or overcounting if blend information from multiple iterations.
- Leads to NRG violations of exact relations, e.g.,

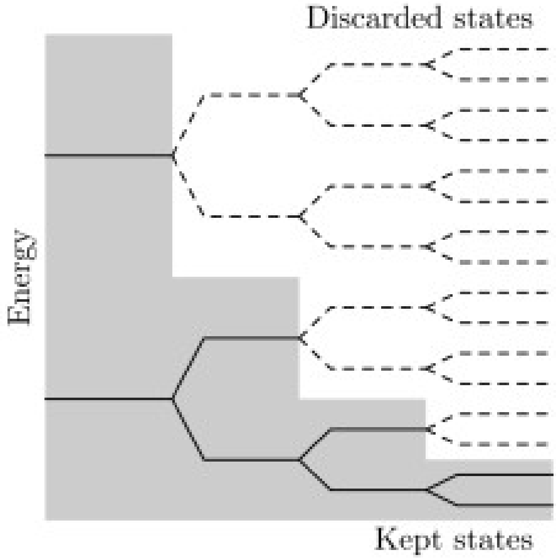
$$\int A_\sigma(\omega,T)\, d\omega \neq 1$$




Bulla et al. (2001)

# Complete basis (or density matrix) NRG

- These problems are fixed in the complete-basis NRG (Anders & Schiller, 2005):




Szalay et al. (2015)

  - NRG uses the kept states at one or a few iterations $N$.

# Complete basis (or density matrix) NRG

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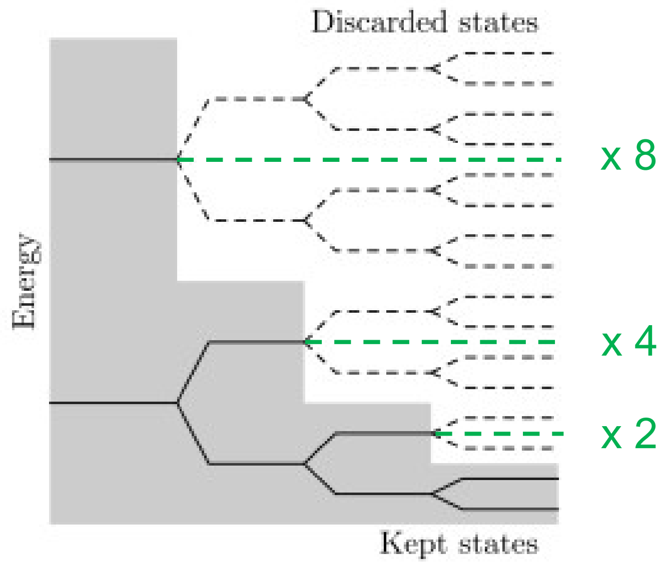


Szalay et al. (2015)

- NRG uses the kept states at one or a few iterations $N$.
- CB-NRG also accounts for every state at the largest $N$, although it has to approximate discarded state energies.

# Complete basis (or density matrix) NRG

- CB-NRG yields exact conservation of spectral weight:

$$\int A_\sigma(\omega,T)\,d\omega = 1$$

- Also opens the way for treatment of non-equilibrium problems:
  - Time evolution after a sudden perturbation (quantum quench) – reasonably successful.
  - Steady state – still in its infancy.

# Summary: NRG Strengths and Weaknesses

- NRG methods are non-perturbative in model parameters
- Can accurately calculate properties over many decades of temperature/frequency
- Not as flexible as QMC methods
- NRG does not scale well with increasing number or impurities and/or bands
- Some of the weaknesses can be overcome using matrix product state methods to be described in the next talk.