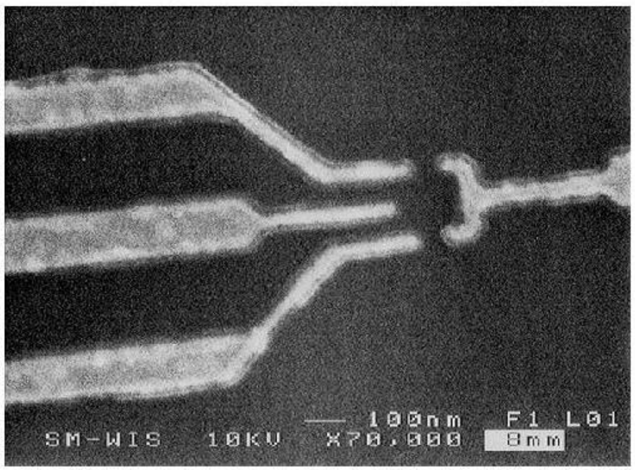
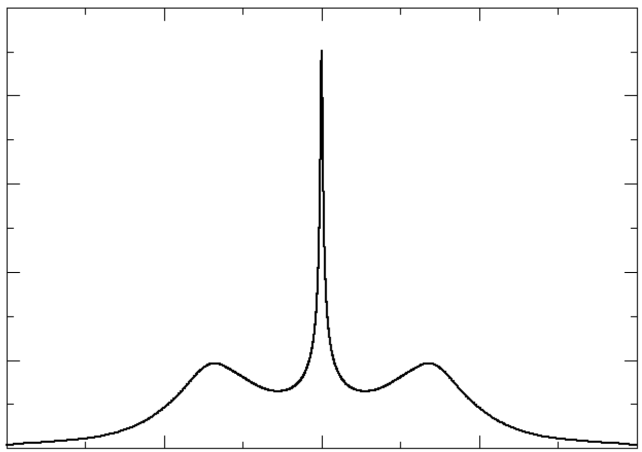
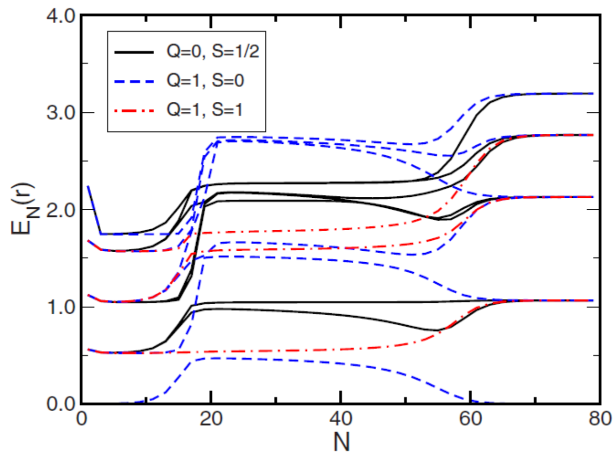
NUMERICAL METHODS FOR QUANTUM IMPURITY MODELS







http://www.staff.science.uu.nl/~mitch003/nrg.html

March 2015

Andrew Mitchell, Utrecht University

Quantum impurity problems

- Part 1: Quantum impurity problems and theoretical background
- Part 2: Kondo effect and RG. 1d chain formulation and iterative diagonalization
- Part 3: Logarithmic discretization and truncation. The RG in NRG
- Part 4: Physical quantities. Results and discussion.

NUMERICAL METHODS FOR QUANTUM IMPURITY MODELS

Part 4: Results and Applications

March 2015

Andrew Mitchell, Utrecht University

Overview: Part 4

- RG flow in physical quantities

- Calculation of thermodynamics
- Evolution of the Kondo temperature
- Scaling and universality

- Calculation of dynamics, t matrix

- Conclusion

NRG: recap

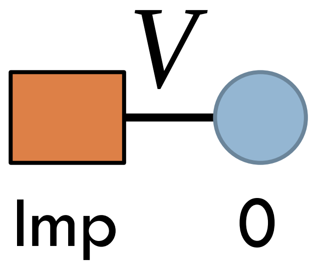
- Logarithmic discretization of conduction band
- Mapping to 1d Wilson chain
- Iterative diagonalization
- Successive Hilbert space truncation

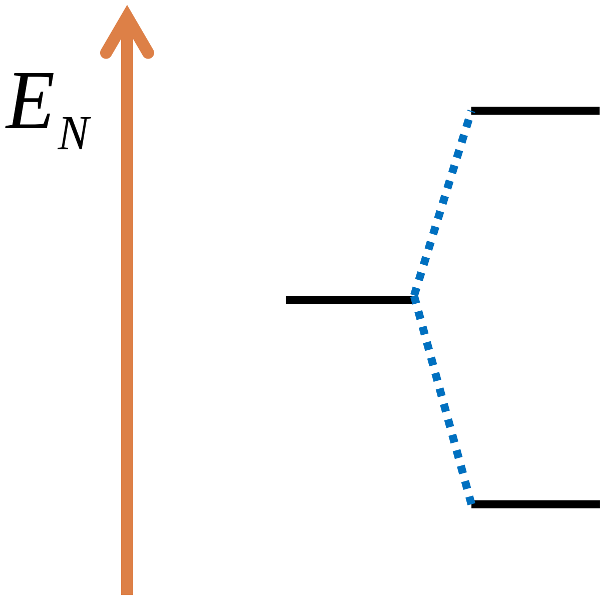
- Keep a large but finite number of states at each iteration (discard the high-energy states):
  - Access ground state information
    (in a finite number of steps)

- BUT: what about physical quantities?!

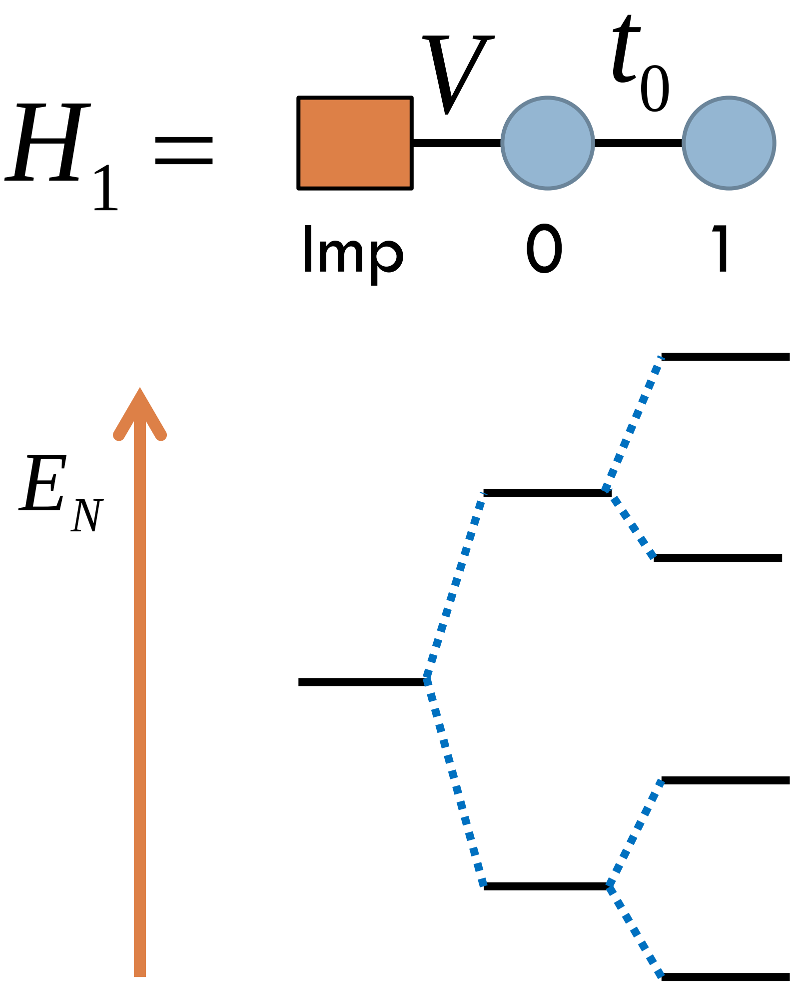
Iterative diagonalization / truncation

$H_0 =$

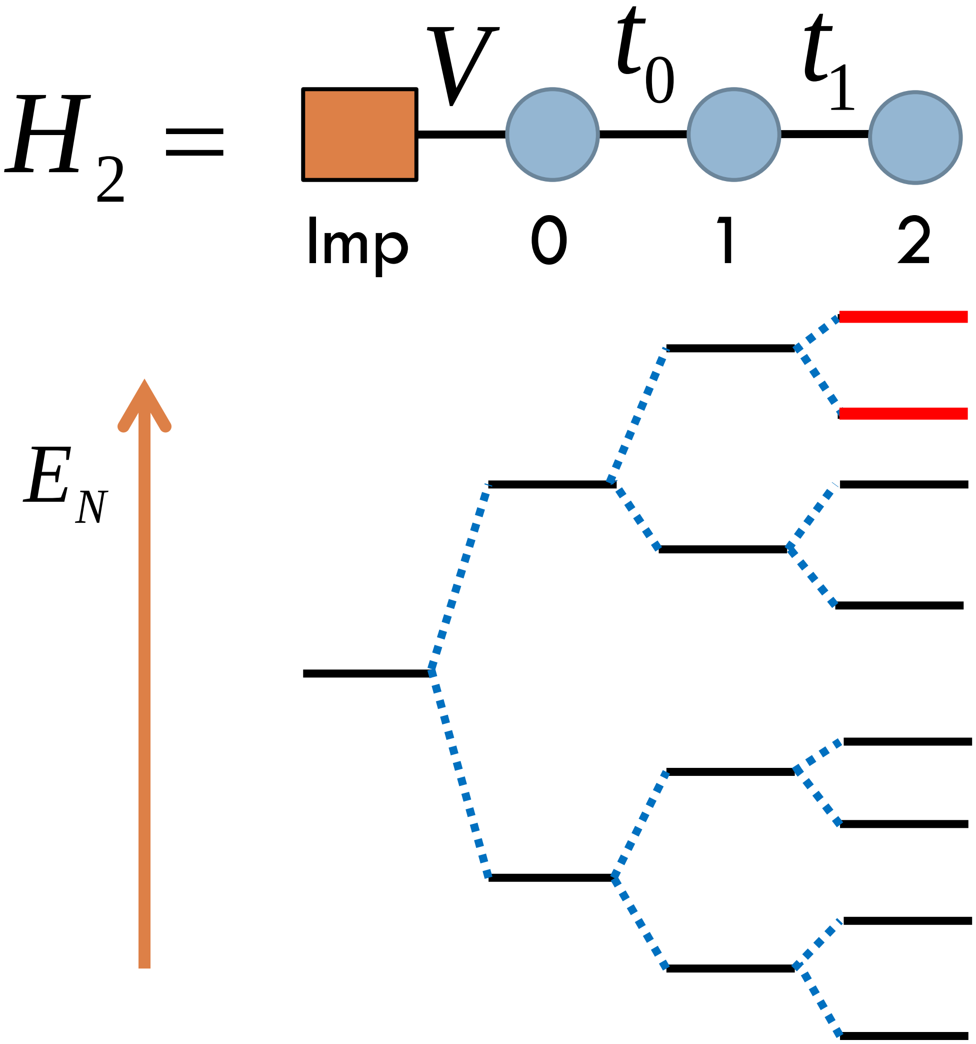




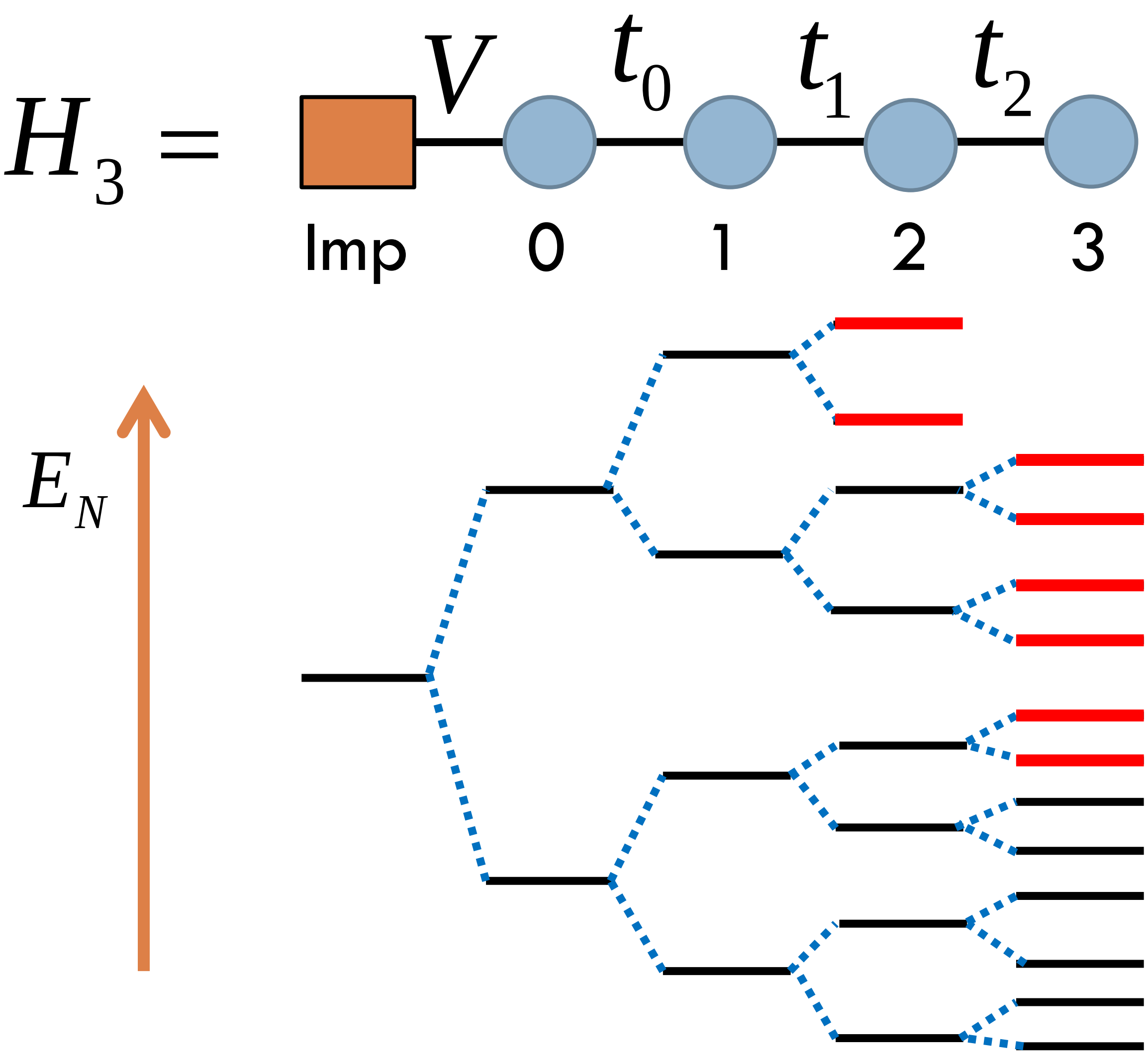
Iterative diagonalization / truncation

$H_1 =$ 

Iterative diagonalization / truncation

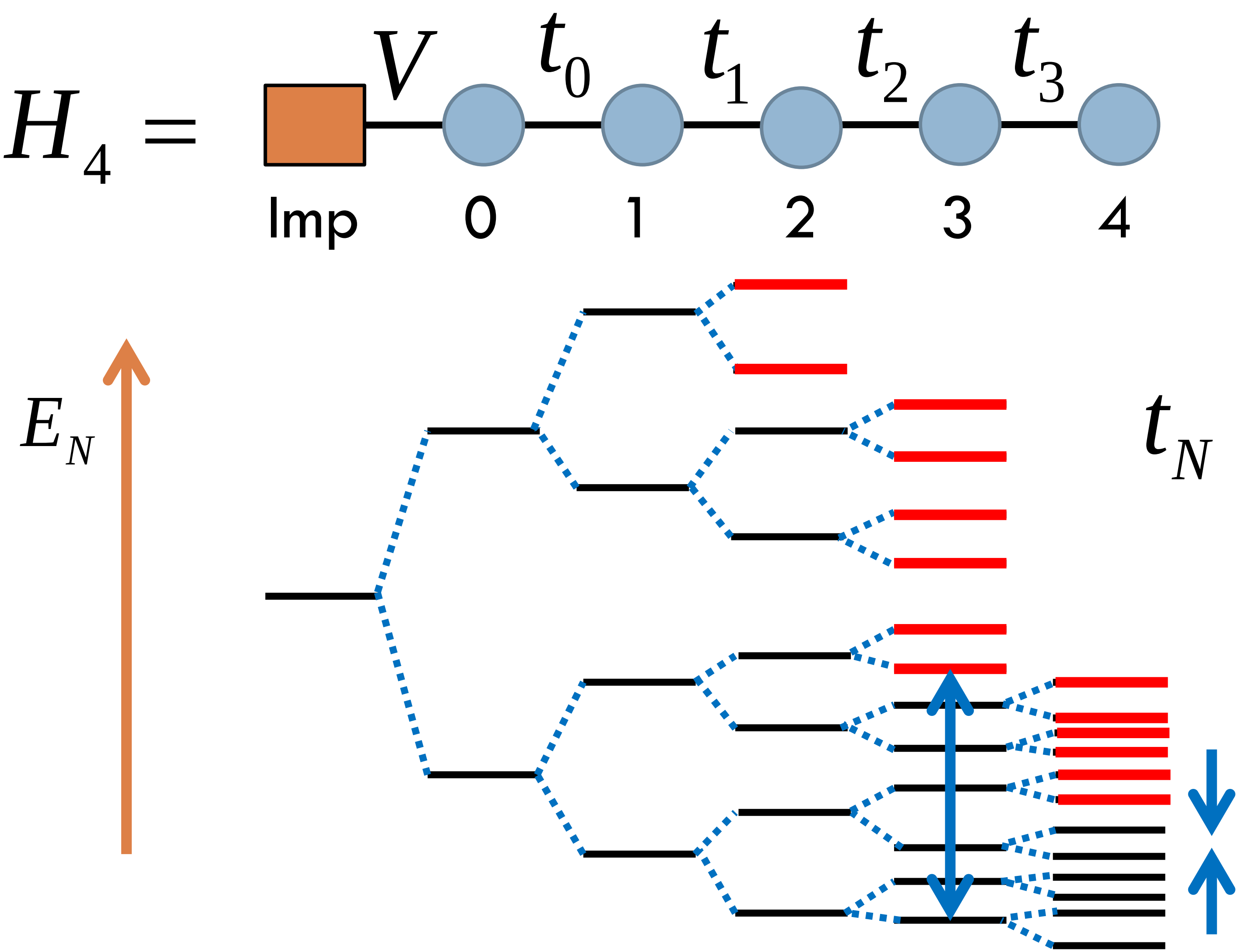


Iterative diagonalization / truncation



Iterative diagonalization / truncation

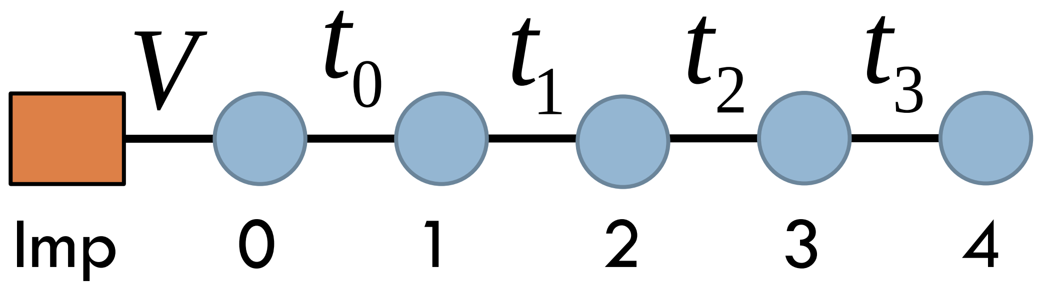
$$H_4 = $$

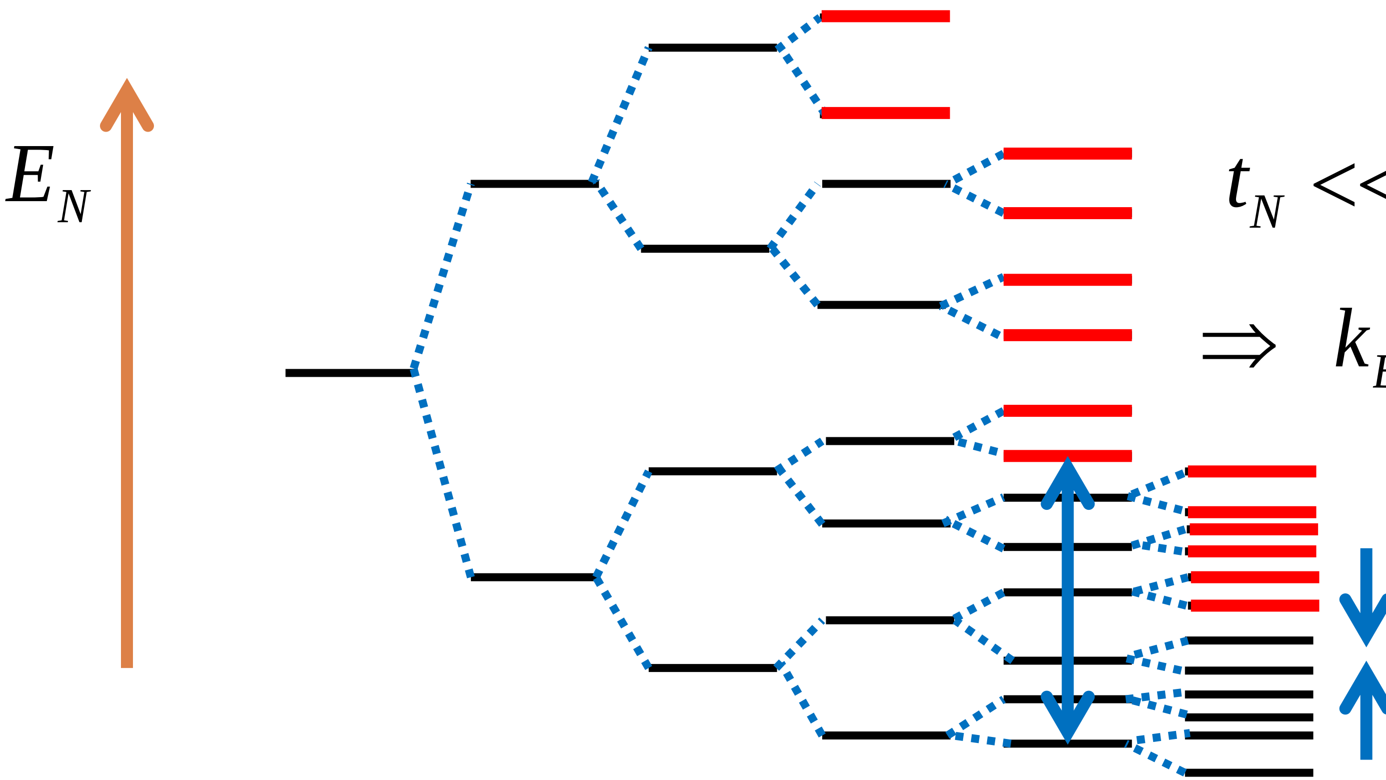


$$t_N \ll E_{cut}$$

Iterative diagonalization / truncation

$H_4 =$





$$t_N << k_B T_N << E_{cut}$$

$$\Rightarrow \quad k_B T_N \propto D\Lambda^{-N/2}$$

Effective temperature

- We recover the full (discretized) Hamiltonian only in the limit $H = \lim_{N\to\infty} \Lambda^{-(N-1)/2} H_N$

- BUT: the sequence of **approximate Hamiltonians** H_N for finite *N=0, 1, 2, 3*, … accurately describe the full system at an **effective temperature** $k_B T_N \propto D\Lambda^{-N/2}$

- Useful information can be extracted **at each iteration!**

- **Thermodynamics** can be calculated from the finite set of NRG energy levels at a given iteration for this temperature

Thermodynamics

- Entropy: $S_N / k_B = \beta \langle H_N \rangle + \ln(Z_N)$
- Magnetic susceptibility: $\chi_N / \left(g^2 \mu_B^2 k_B^{-1}\right) = \beta \left[\left\langle \left(S_N^z\right)^2 \right\rangle - \left\langle S_N^z \right\rangle^2 \right]$
- Specific heat: $C_N / k_B = \beta^2 \left[\left\langle \left(H_N\right)^2 \right\rangle - \left\langle H_N \right\rangle^2 \right]$
  - Evaluated at effective temperature $k_B T_N \propto D\Lambda^{-N/2}$ from finite set of NRG levels at iteration N via,

$$\left\langle \hat{\Omega}_N \right\rangle = \frac{1}{Z_N} \sum_r \langle r | \hat{\Omega}_N | r \rangle_N \times \exp\left[-\beta E_N(r) \right]$$

- Impurity contributions defined as: $\left\langle \hat{\Omega} \right\rangle_{imp} = \left\langle \hat{\Omega} \right\rangle_{full} - \left\langle \hat{\Omega} \right\rangle_{host}$

Fixed point thermodynamics

- For the Anderson impurity model:
  - **FO fixed point: decoupled free impurity site**

    Expect entropy: $S_{imp} = \ln(4)$

    magnetic susceptibility: $T\chi_{imp} = \frac{1}{8}$

  - **LM fixed point: decoupled free impurity spin-1/2**

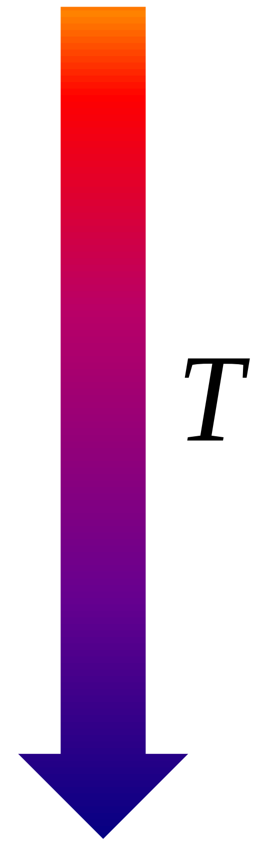
    Expect entropy: $S_{imp} = \ln(2)$

    magnetic susceptibility: $T\chi_{imp} = \frac{1}{4}$

  - **SC fixed point: Kondo singlet ground state**

    Expect entropy: $S_{imp} = 0$

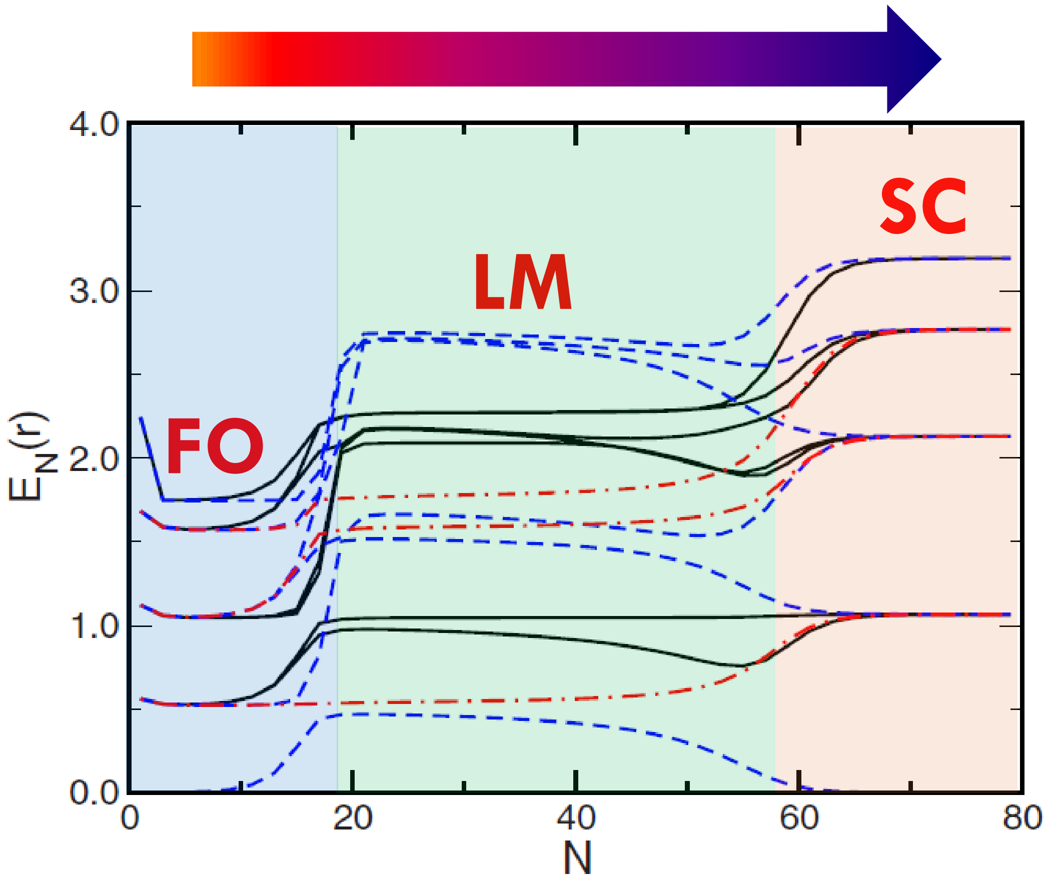
    magnetic susceptibility: $T\chi_{imp} = 0$



RG flow in energy levels

- Each new iteration corresponds to a **lower temperature**
- **RG flow** seen in many-particle energies…

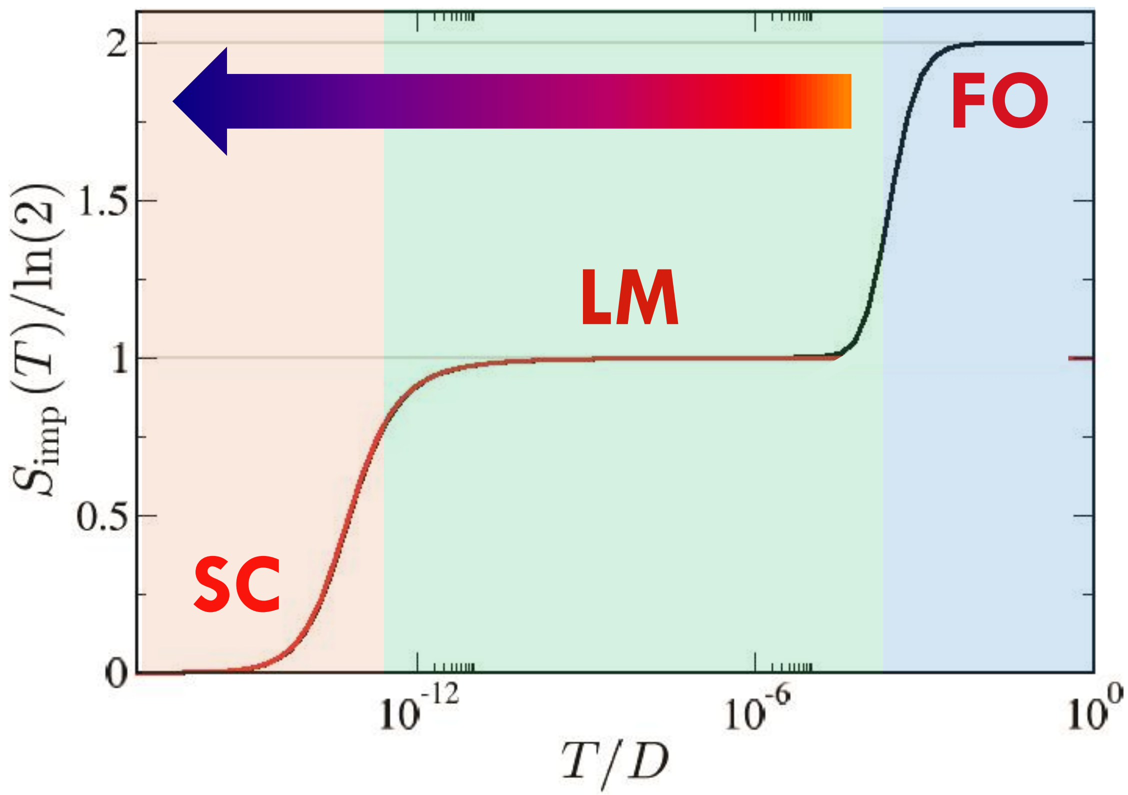
AIM:



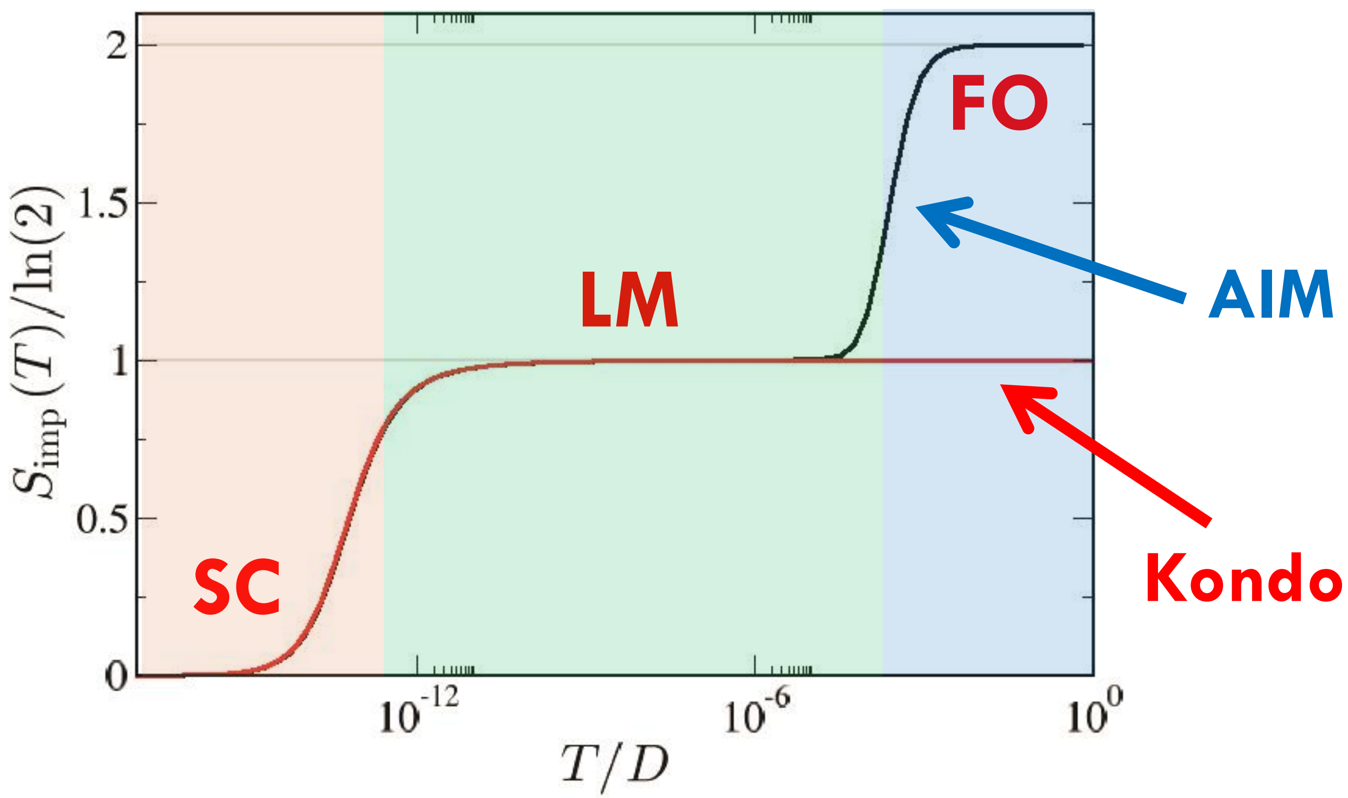
RG flow in thermodynamics

- Each new iteration corresponds to a **lower temperature**
- **RG flow** seen in many-particle energies…
  … also appears in **thermodynamics!**

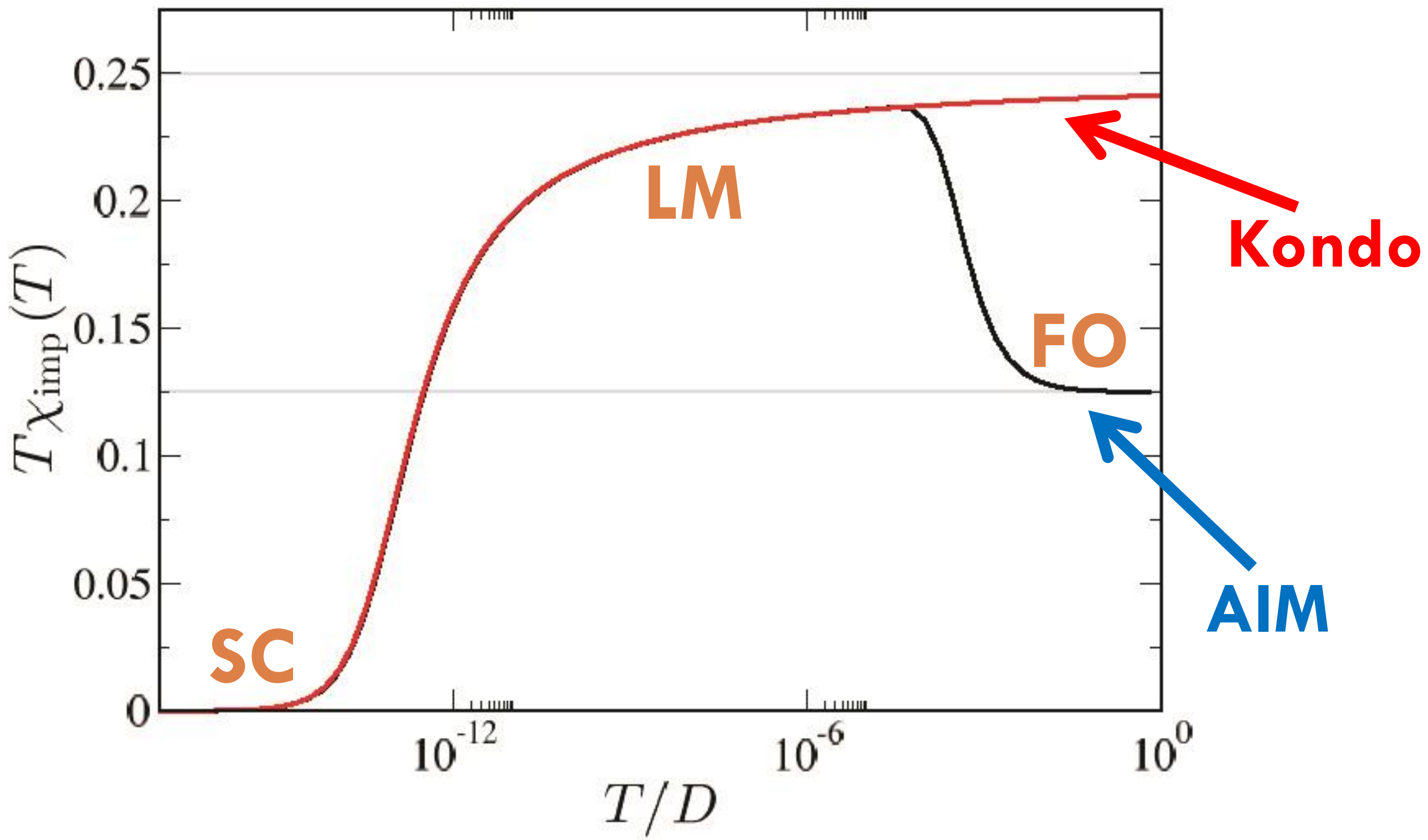
AIM:



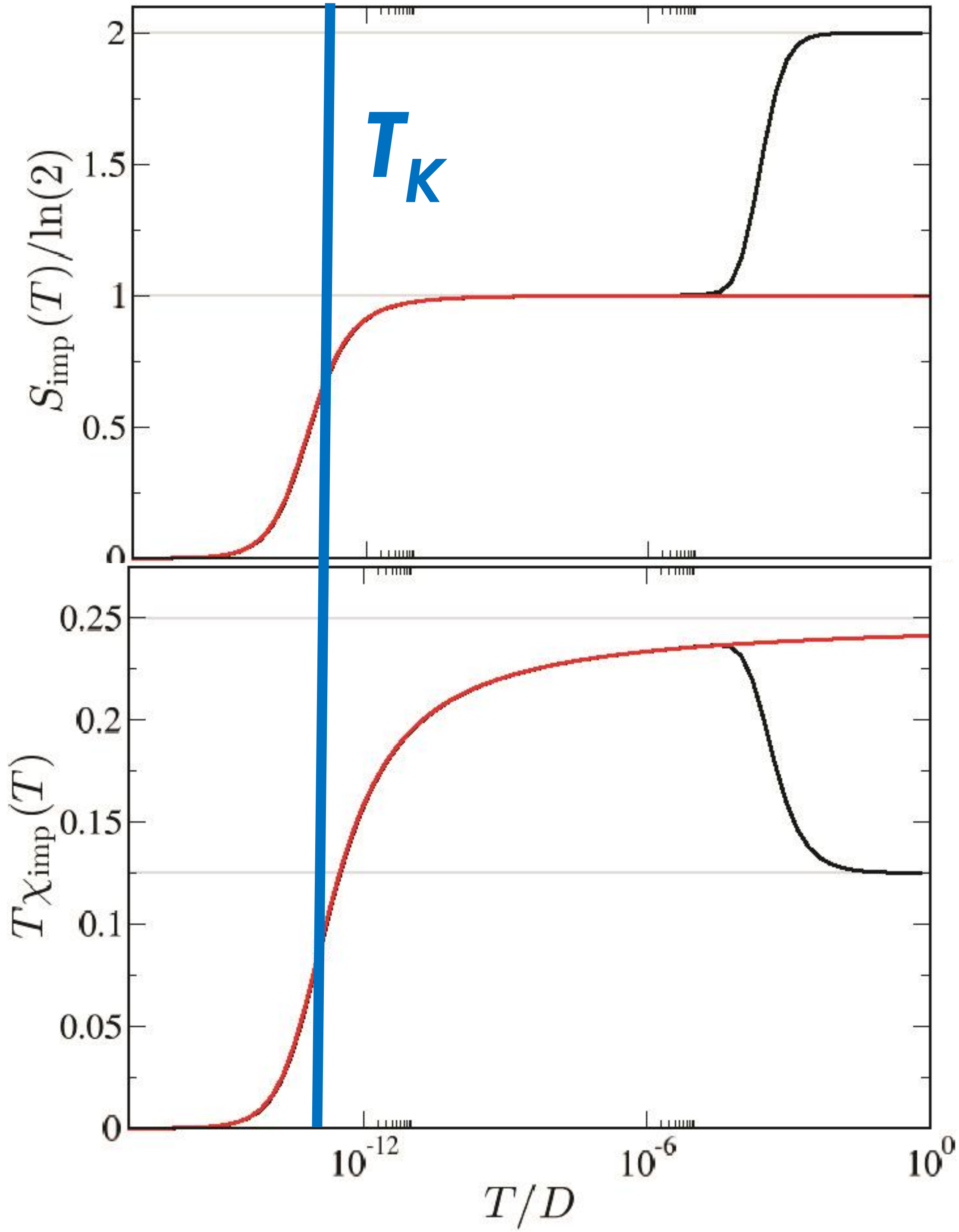
Anderson $\longrightarrow$ Kondo



Magnetic susceptibility



Kondo temperature: **characterizes crossover from LM to SC**

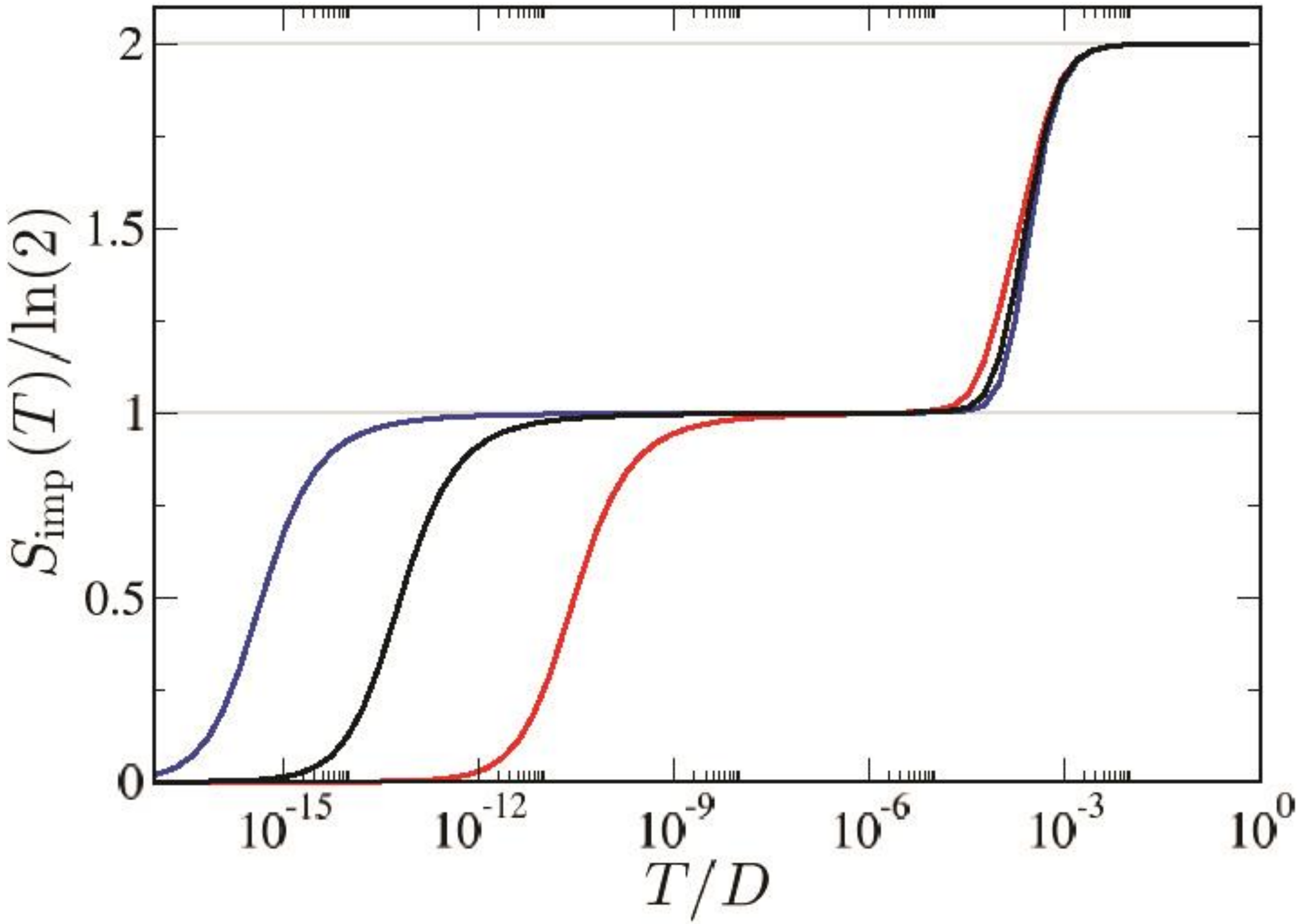


Kondo temperature

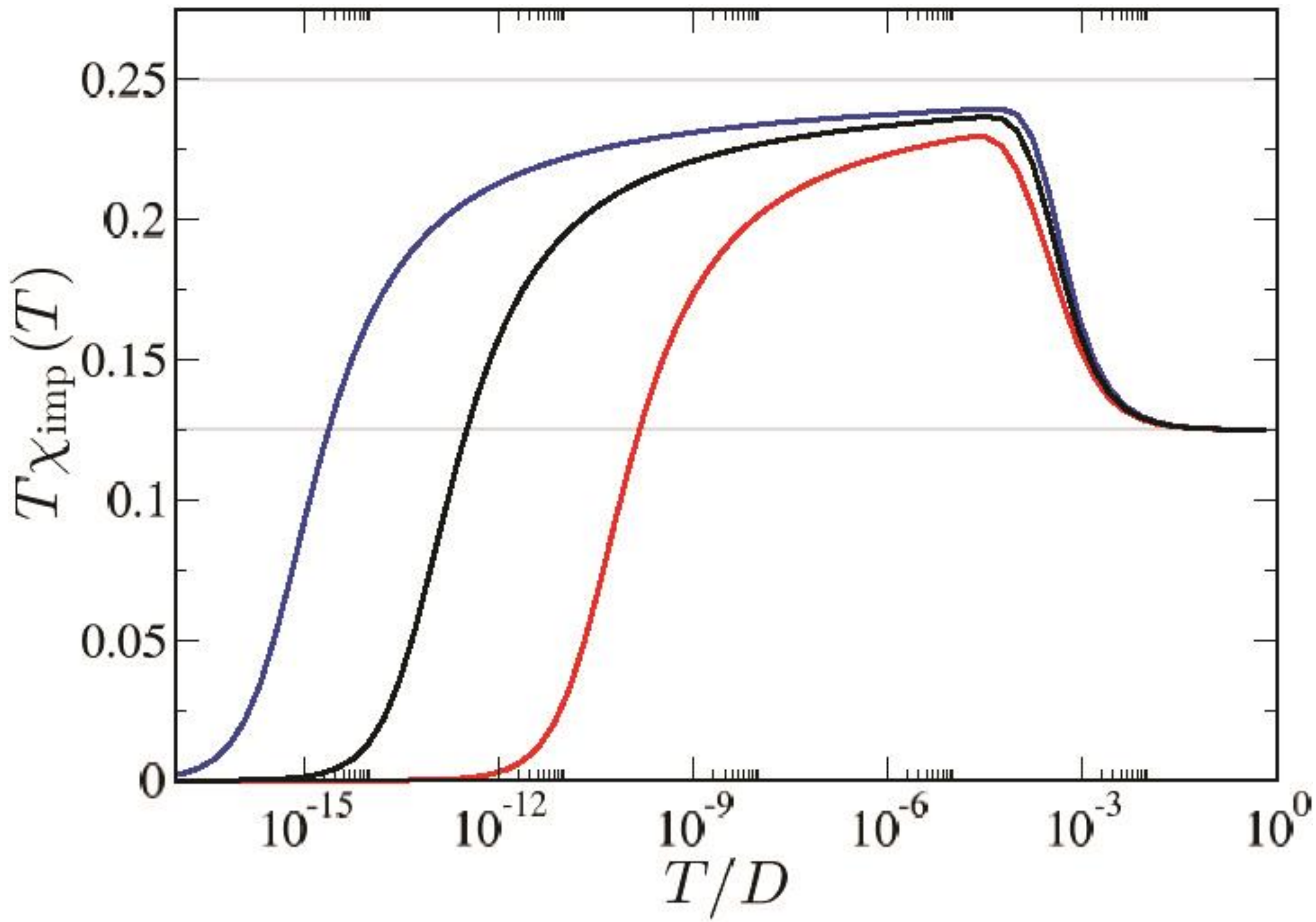
- **Perturbative scaling**
  (2nd order, p-h symmetric, wide flat band)
  - **Kondo Model:** $T_K \sim D \exp\left[-1/\left(\rho J\right)\right]$
  - **Anderson Model (via SWT):** $T_K \sim D \exp\left[-8\Gamma/\left(\pi U\right)\right]$

- **Confirmed asymptotically by NRG (for small *J* or large *U*).**

Scaling and universality

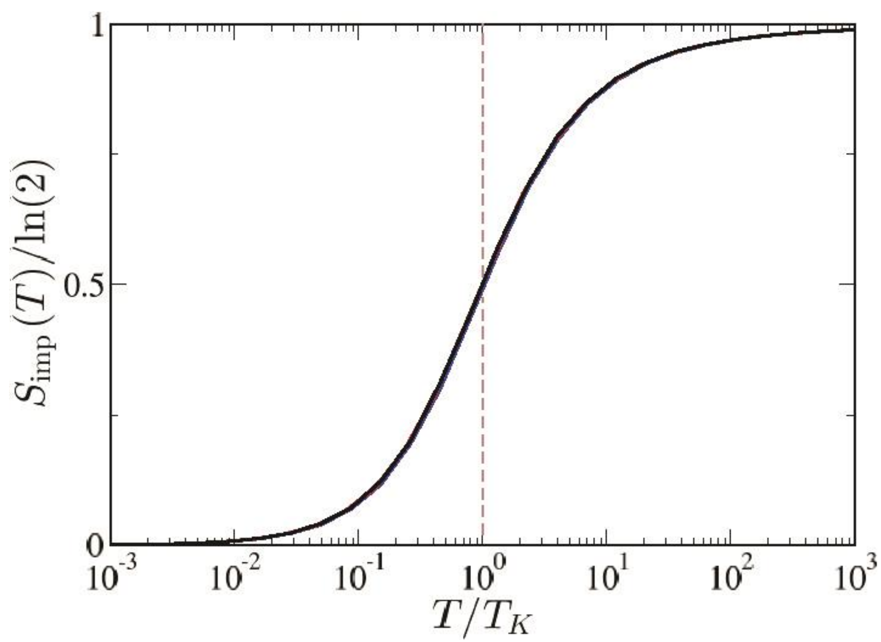


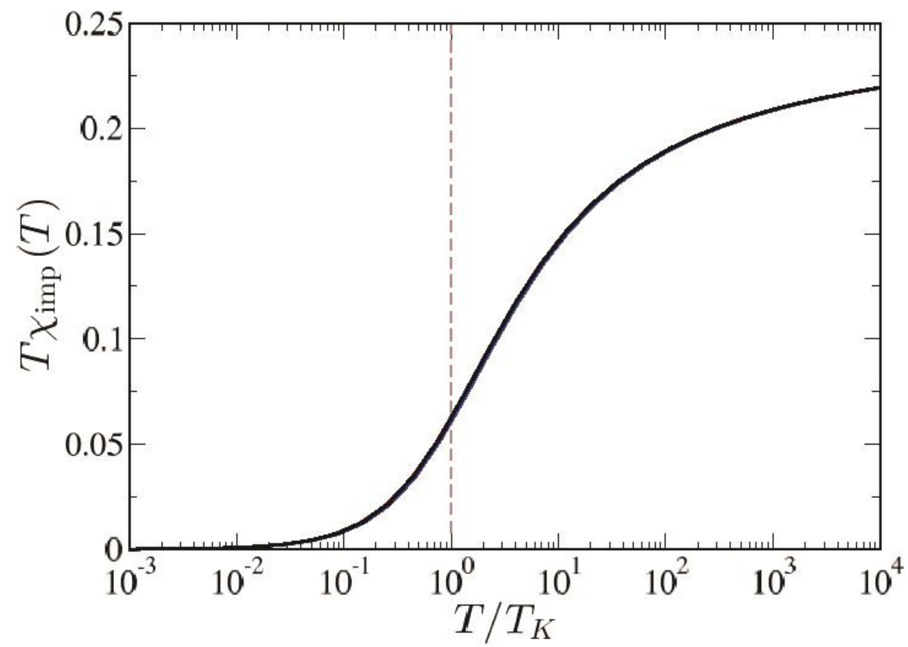
Scaling and universality



Scaling and universality

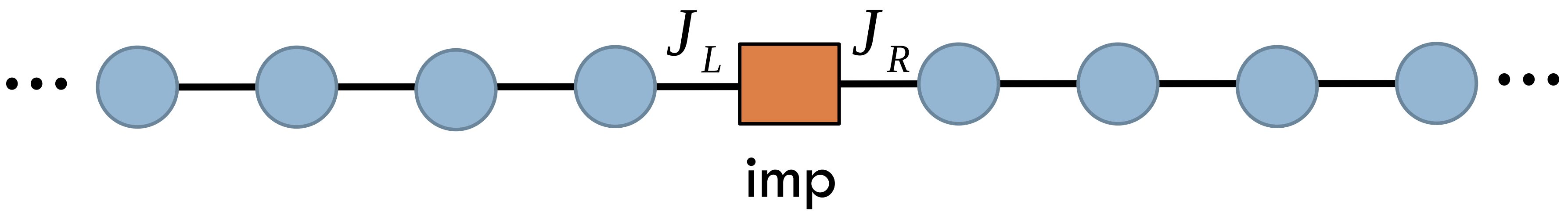
- RG flow between LM and SC fixed points is **UNIVERSAL!**
- Details of model are unimportant (AIM or Kondo)
  - **Except for determining crossover Kondo scale, T_K**
- **Scaling collapse** of data in terms of T/T_K





Other applications of NRG

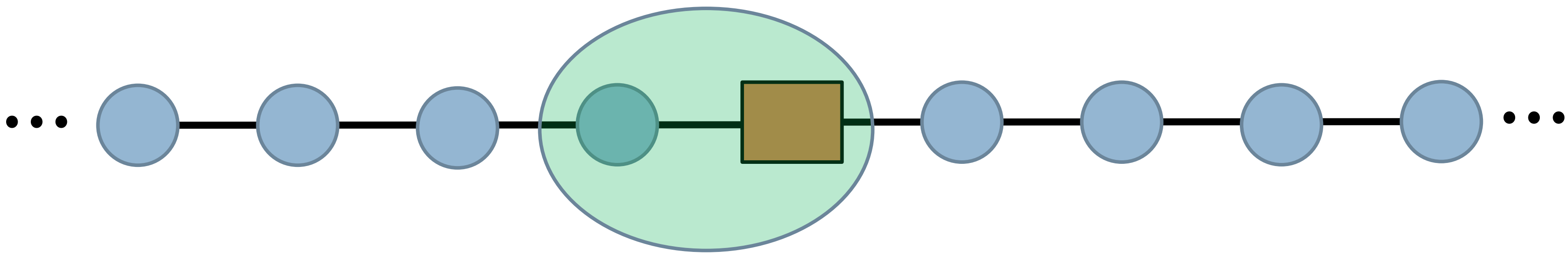
- Example: two-channel Kondo model



$$H_{2CK} = J_L \vec{S}_{imp} \cdot \vec{s}_{0L} + J_R \vec{S}_{imp} \cdot \vec{s}_{0R} + \sum_{\substack{k,\sigma \\ \alpha=L,R}} \varepsilon_k c^\dagger_{k\sigma\alpha} c_{k\sigma\alpha}$$

Other applications of NRG

- Example: two-channel Kondo model

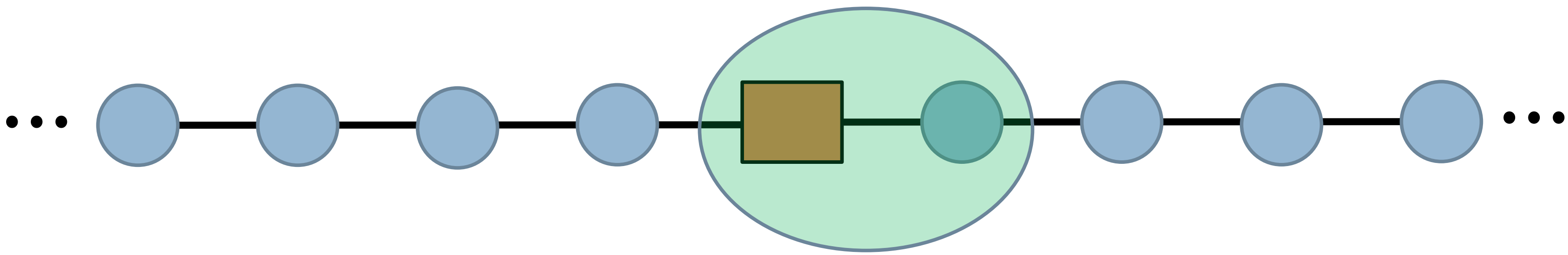


$$H_{2CK} = J_L \vec{S}_{imp} \cdot \vec{s}_{0L} + J_R \vec{S}_{imp} \cdot \vec{s}_{0R} + \sum_{\substack{k,\sigma \\ \alpha=L,R}} \varepsilon_k c^\dagger_{k\sigma\alpha} c_{k\sigma\alpha}$$

$J_L > J_R$: **Kondo effect with left channel**

Other applications of NRG

- Example: two-channel Kondo model

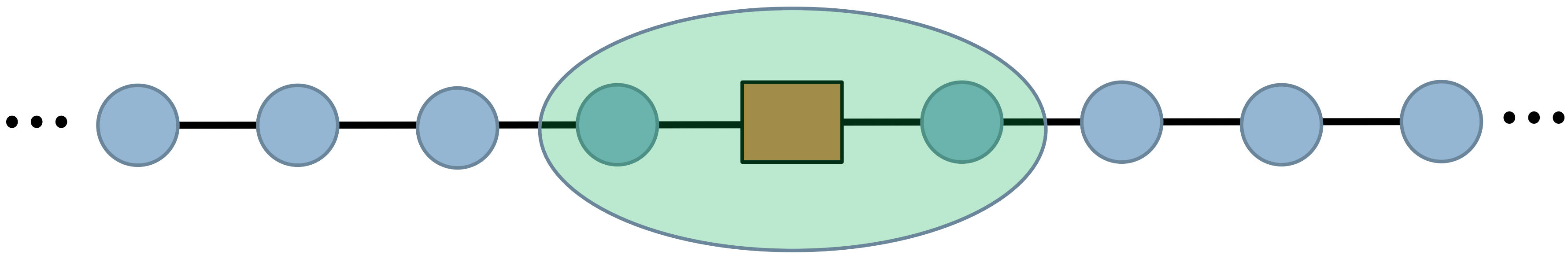


$$H_{2CK} = J_L \vec{S}_{imp} \cdot \vec{s}_{0L} + J_R \vec{S}_{imp} \cdot \vec{s}_{0R} + \sum_{\substack{k,\sigma \\ \alpha = L,R}} \varepsilon_k c^{\dagger}_{k\sigma\alpha} c_{k\sigma\alpha}$$

$J_L < J_R$: **Kondo effect with right channel**

Other applications of NRG

- Example: two-channel Kondo model

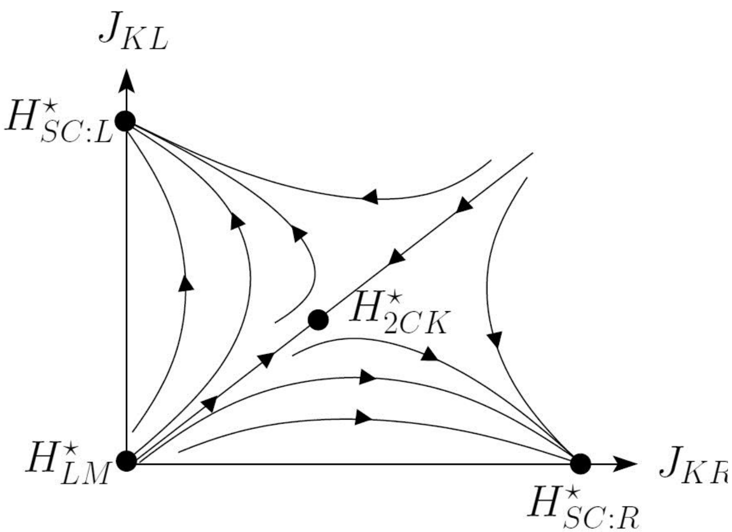


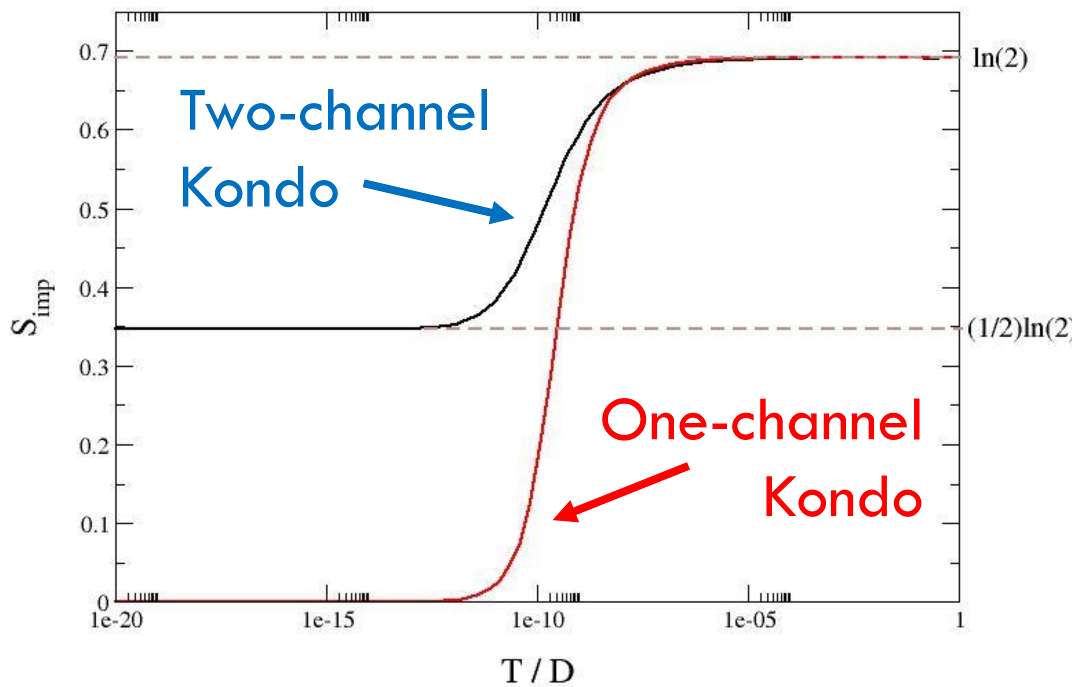
$$H_{2CK} = J_L \vec{S}_{imp} \cdot \vec{s}_{0L} + J_R \vec{S}_{imp} \cdot \vec{s}_{0R} + \sum_{\substack{k,\sigma \\ \alpha=L,R}} \varepsilon_k c^\dagger_{k\sigma\alpha} c_{k\sigma\alpha}$$

  - Strong Coupling FP is **destabilized** when $J_L = J_R$
    - **Different RG flow here!**

Other applications of NRG

- Example: two-channel Kondo model





- Quantum critical physics captured by NRG

Dynamics within NRG

- Dynamical quantities much harder to calculate

- Discretized model produces discretized dynamics: spectral functions consist of **discrete poles**

- Calculate spectral functions using the **Lehmann respresentation…**

Lehmann Representation

- In NRG, we have access to **many-particle** states of the approximate Hamiltonians $\boldsymbol{H_N}$. We want a generalized method for constructing spectral functions…
  - **No single-particle levels for interacting systems!**

Reminder: $$C^{>}(t) = \left\langle \hat{A}(t)\,\hat{B} \right\rangle \quad ; \quad C^{<}(t) = \left\langle \hat{B}\,\hat{A}(t) \right\rangle$$

FT $\Rightarrow$ $$C^{\alpha}(z) = \int_{-\infty}^{\infty} dt\ e^{izt}\, C^{\alpha}(t)$$

Spectrum: $$A(\omega) = -\frac{1}{2\pi}\,\mathrm{Im}\left[C^{>}\left(\omega + i0^{+}\right) + C^{<}\left(\omega + i0^{+}\right) \right]$$

Lehmann Representation

- **Impurity Green functions:**

$$C^{>}(t) = \frac{1}{Z}\sum_i \langle i | e^{-\beta H} e^{iHt} d_\sigma e^{-iHt} d_\sigma^\dagger | i \rangle$$

$$\sum_j | j \rangle\langle j | \qquad \sum_k | k \rangle\langle k |$$

resolution of identity

Lehmann Representation

$$C^{>}(t) = \frac{1}{Z}\sum_{i}\langle i\,|e^{-\beta H} e^{iHt}\, d_\sigma\, e^{-iHt}\, d_\sigma^\dagger\,|i\,\rangle$$

$$= \frac{1}{Z}\sum_{i,j,k}\langle i\,|e^{-\beta H} e^{iHt}|k\,\rangle \times \langle k\,|d_\sigma\, e^{-iHt}|\,j\,\rangle \times \langle j\,|d_\sigma^\dagger|i\,\rangle$$

$$= \frac{1}{Z}\sum_{i,j} e^{-\beta E_i}\, e^{itE_i}\, e^{-itE_j}\,\langle i\,|d_\sigma|\,j\,\rangle \times \langle j\,|d_\sigma^\dagger\,|i\,\rangle$$

$$= \frac{1}{Z}\sum_{i,j} e^{-\beta E_i}\, e^{it(E_i - E_j)}\,\left|\langle i\,|d_\sigma|\,j\,\rangle\right|^2$$

Lehmann Representation

$$C^{>}(\omega) = \frac{1}{Z}\sum_{i,j}\int_{-\infty}^{\infty} d\,t\, e^{i\,\omega\, t}\, e^{-\beta E_i}\, e^{i\,t\left(E_i - E_j\right)} \left|\langle i\,|d_\sigma|\,j\,\rangle\right|^2$$

$$= \frac{1}{Z}\sum_{i,j} e^{-\beta E_i} \left|\langle i\,|d_\sigma|\,j\,\rangle\right|^2 \times 2\pi\,\delta\left(\omega + E_i - E_j\right)$$

Similarly,

$$C^{<}(\omega) = \frac{1}{Z}\sum_{i,j} e^{-\beta E_j} \left|\langle i|d_\sigma|\,j\,\rangle\right|^2 \times 2\pi\,\delta\left(\omega + E_i - E_j\right)$$

Lehmann Representation

Impurity spectral function is given by:

$$A(\omega) = \frac{1}{Z}\sum_{i,j}\left(e^{-\beta E_i} + e^{-\beta E_j}\right)\left|\langle i \,|\, d_\sigma \,|\, j \rangle\right|^2 \times \delta\left(\omega + E_i - E_j\right)$$

in terms of **matrix elements of impurity operators,**
between diagonalized **many-particle eigenstates**

For the generalized quantity $C^{>}_{AB}(t) = \left\langle \hat{A}(t)\ \hat{B}(0) \right\rangle$

$$C^{>}_{AB}(\omega) = \sum_{i,j}\langle j \,|\, \hat{B} \,|\, i \rangle \frac{e^{-\beta E_a}}{Z}\langle i \,|\, \hat{A} \,|\, j \rangle \times \delta\left(\omega - E_j + E_i\right)$$

Dynamics within NRG

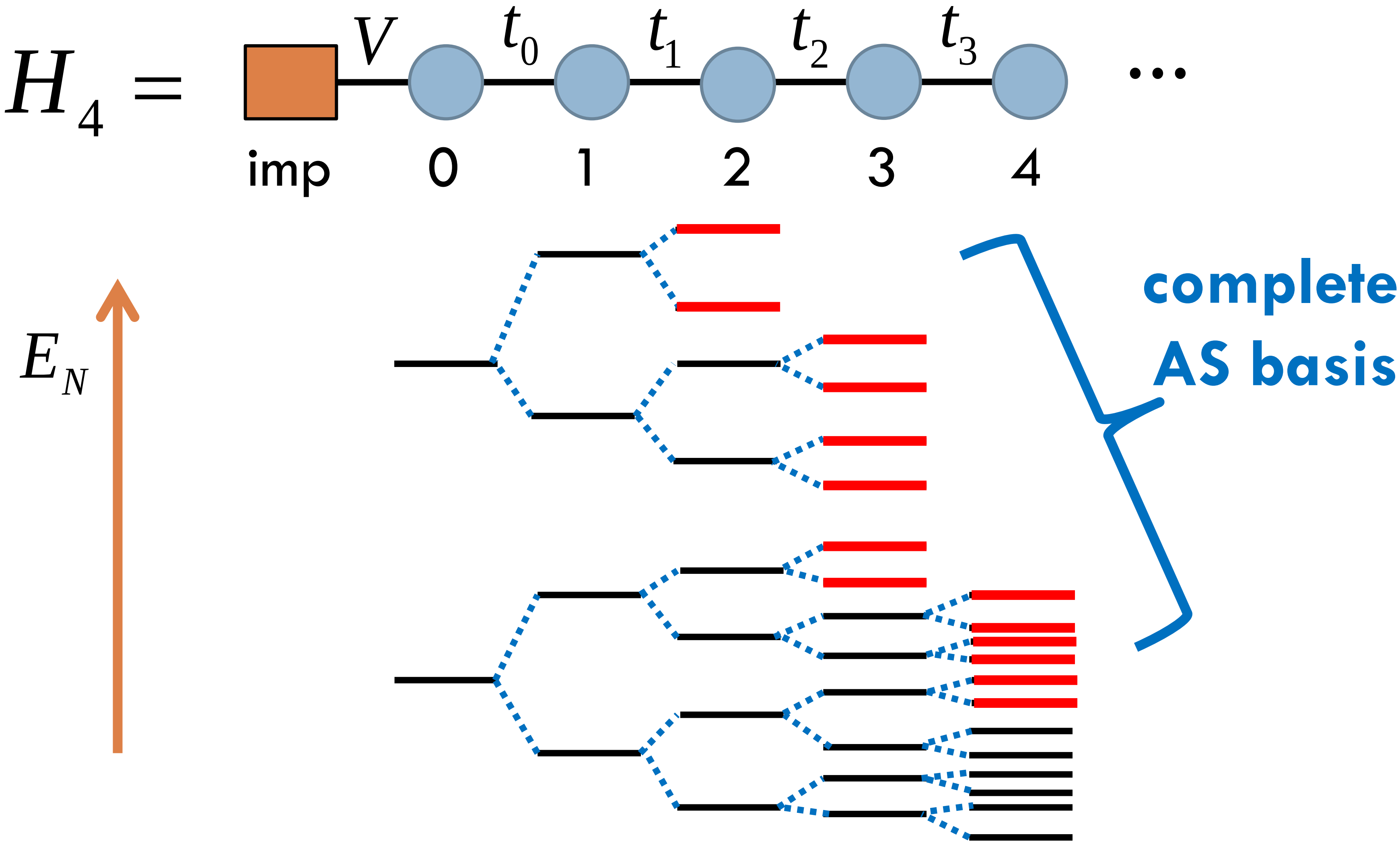
- Simple heuristic approximation at $T=0$
  - Calculate excitations from the ground state at each iteration: need matrix elements $\langle a | \hat{B} | gs \rangle_N$
  - Energy differences at each iteration $\sim \Lambda^{-N/2}$
  - Contributions to entire spectrum at a given energy $\sim \Lambda^{-N/2}$ come from iteration *N*. Combine poles for different *N*.
- Problems:
  - High energies poorly resolved
  - Overcounting
  - Nature of true ground state not known at early iterations

Complete Fock space

- **Discarded states** at each iteration form an approximate but **complete basis**
- Calculate **full density matrix** in this basis, $\hat{\rho} = \dfrac{e^{-\beta \hat{H}}}{Z}$
- Access to **accurate dynamics**
  - Calculated via $\langle ... \rangle = \mathrm{Tr}\left[\hat{\rho} ...\right]$

F. B. Anders, A. Schiller, PRL **95** 196801 (2005)
A. Weichselbaum, J. von Delft, PRL **99** 076402 (2007)
R. Peters, T. Pruschke, F. B. Anders, PRB **74** 245114 (2006)

Dynamics within NRG



Dynamics within NRG

- **Complication:**
  Matrix elements of type $\langle a | \hat{B} | b \rangle_N$ are known in NRG basis (calculated recursively, iteration by iteration)
  - Need unitary rotation of **full density matrix in AS basis** into **NRG basis**
  - Calculate **reduced density matrix** at each iteration
    - From which can also calculate entanglement entropy!

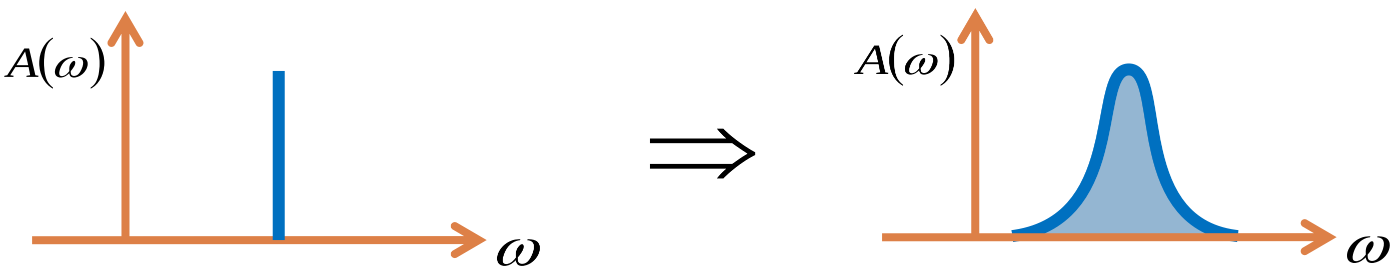
Dynamics within NRG

- **Complication:**
  Discretized model produces discretized dynamics: spectral functions consist of **discrete poles**

  - **Broaden** delta-peaks to recover continuous spectrum
  - Energies distributed on a logarithmic grid
  - Broaden using *logarithmic Gaussians*
  - Low-energy behavior around Fermi level well-sampled

Broadening discrete data

- Replace each delta-peak with a log-Gaussian of the same total weight



  - At each frequency that the spectrum is to be evaluated, sum up the contribution from each broadened pole

Broadening discrete data

$$A(\omega) = \sum_n a_n \, \delta(\omega - \omega_n) \rightarrow \sum_n a_n \, P_b(\omega - \omega_n)$$

$$= \int_{-\infty}^{\infty} d\omega' \sum_n a_n \delta(\omega' - \omega_n) P_b(\omega - \omega')$$

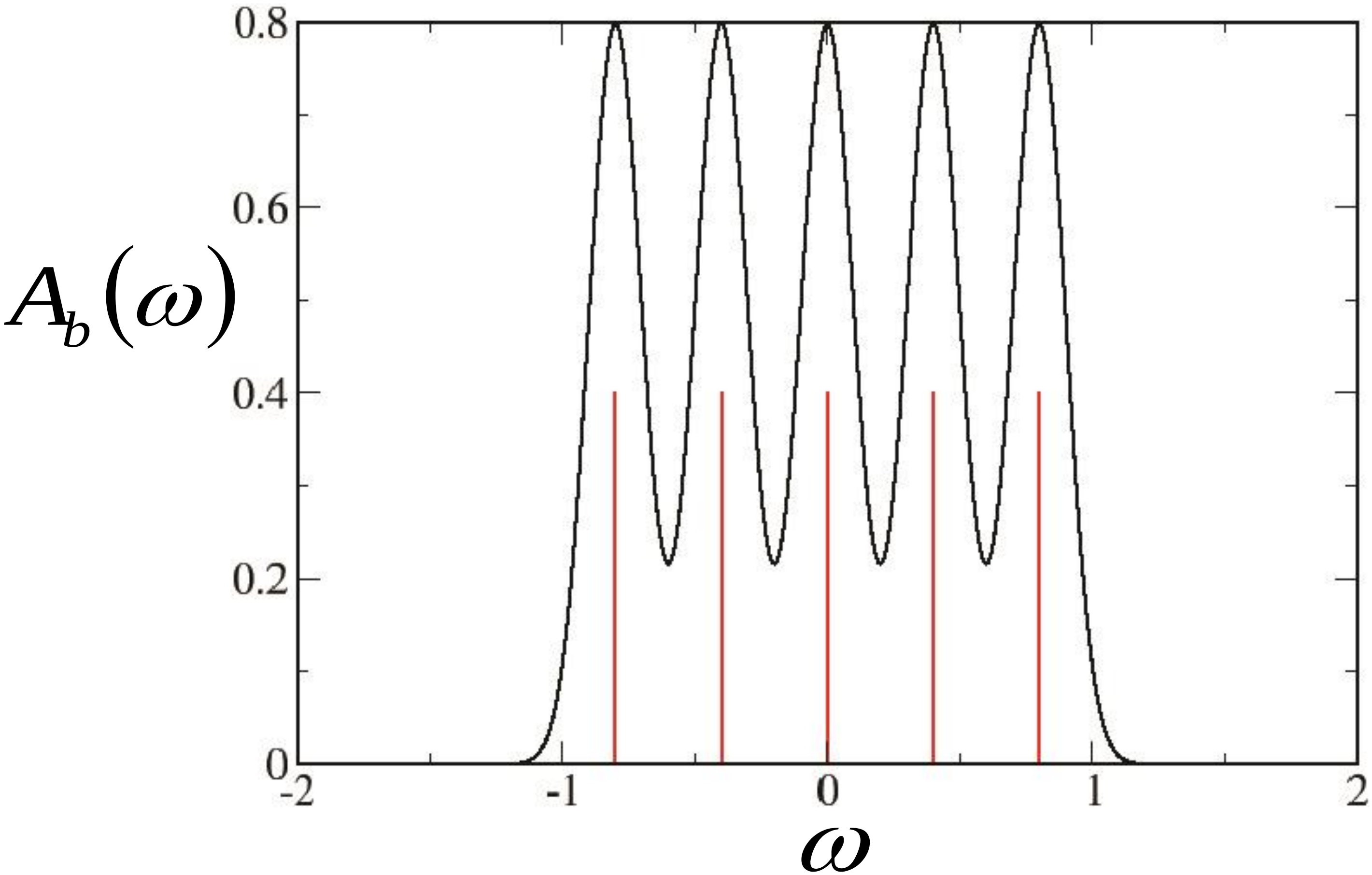
$$= \int_{-\infty}^{\infty} d\omega' \, A(\omega') P_b(\omega - \omega')$$

can exploit convolution theorem and FFT

convolution

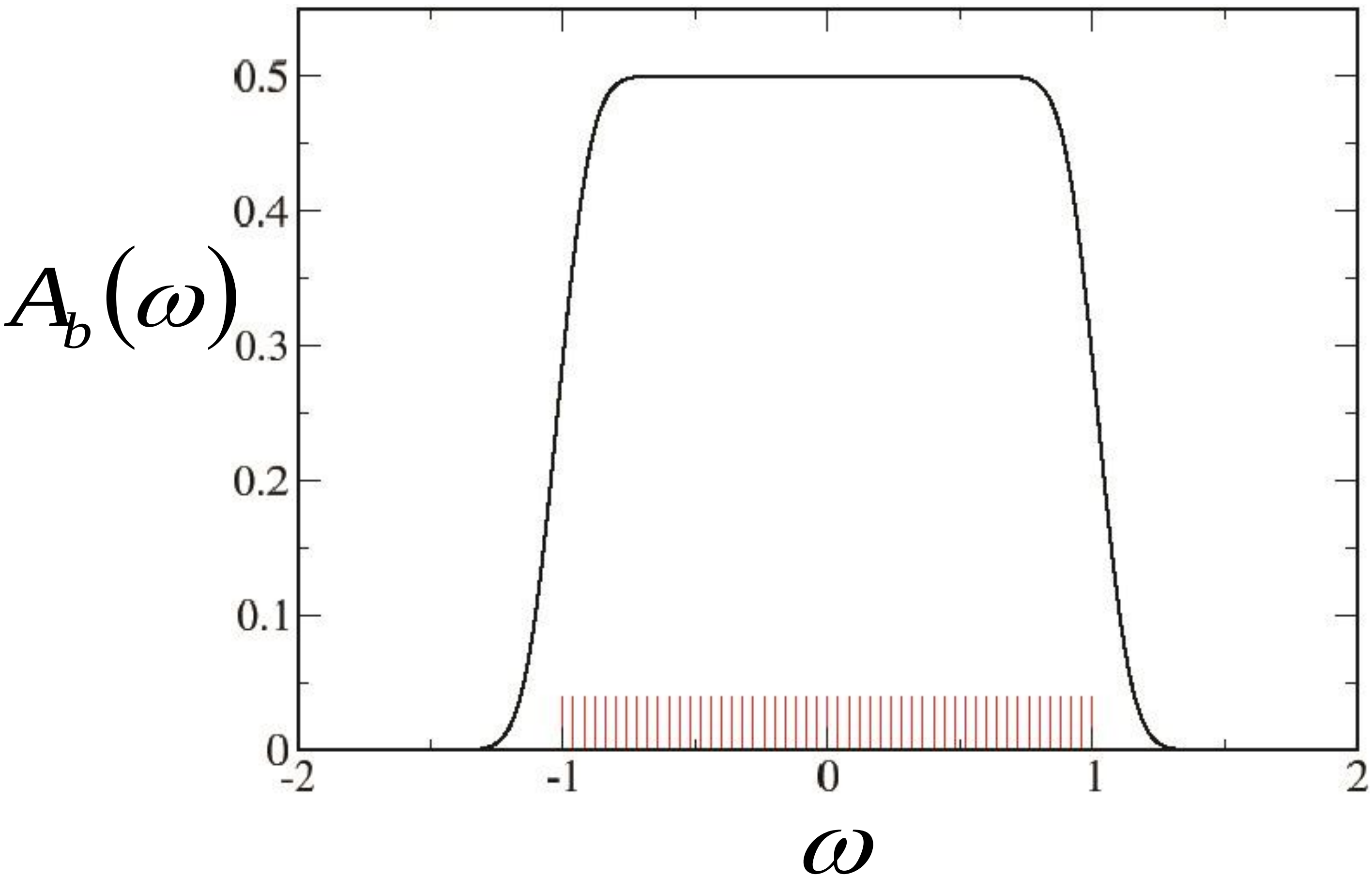
Broadening discrete data

- Example:



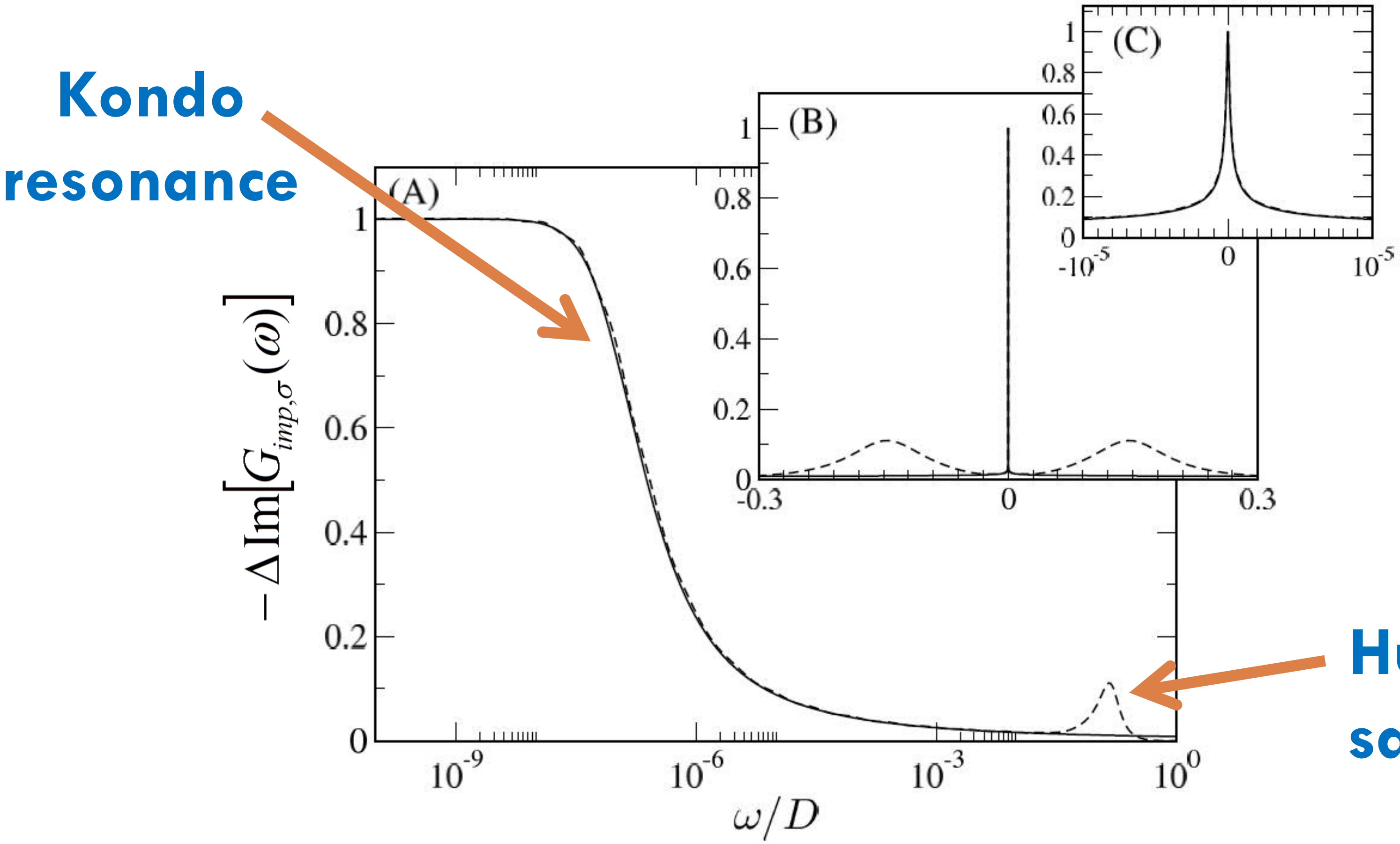
Broadening discrete data

- Example:



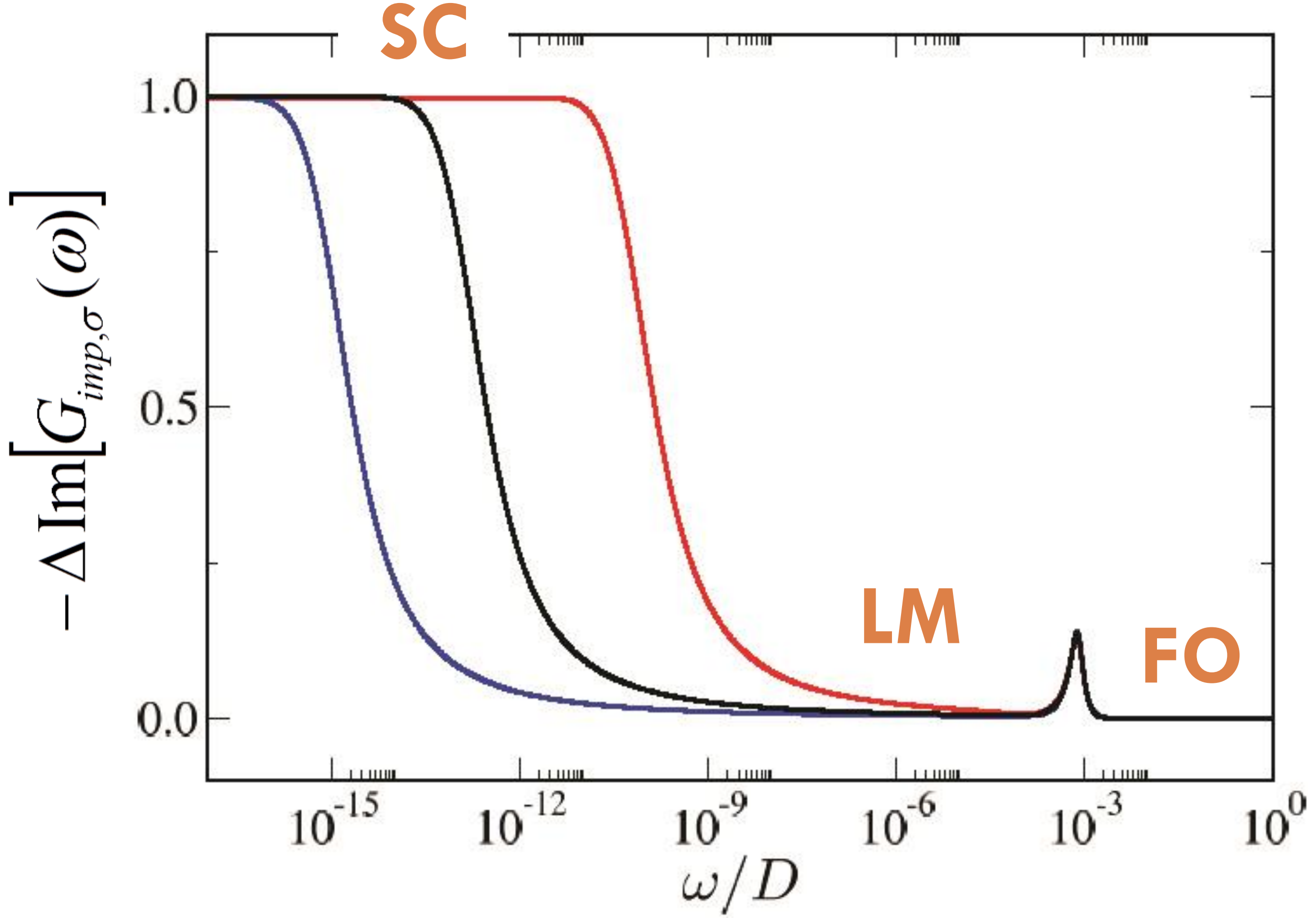
Dynamics within NRG

- Single-particle spectrum of the Anderson model:



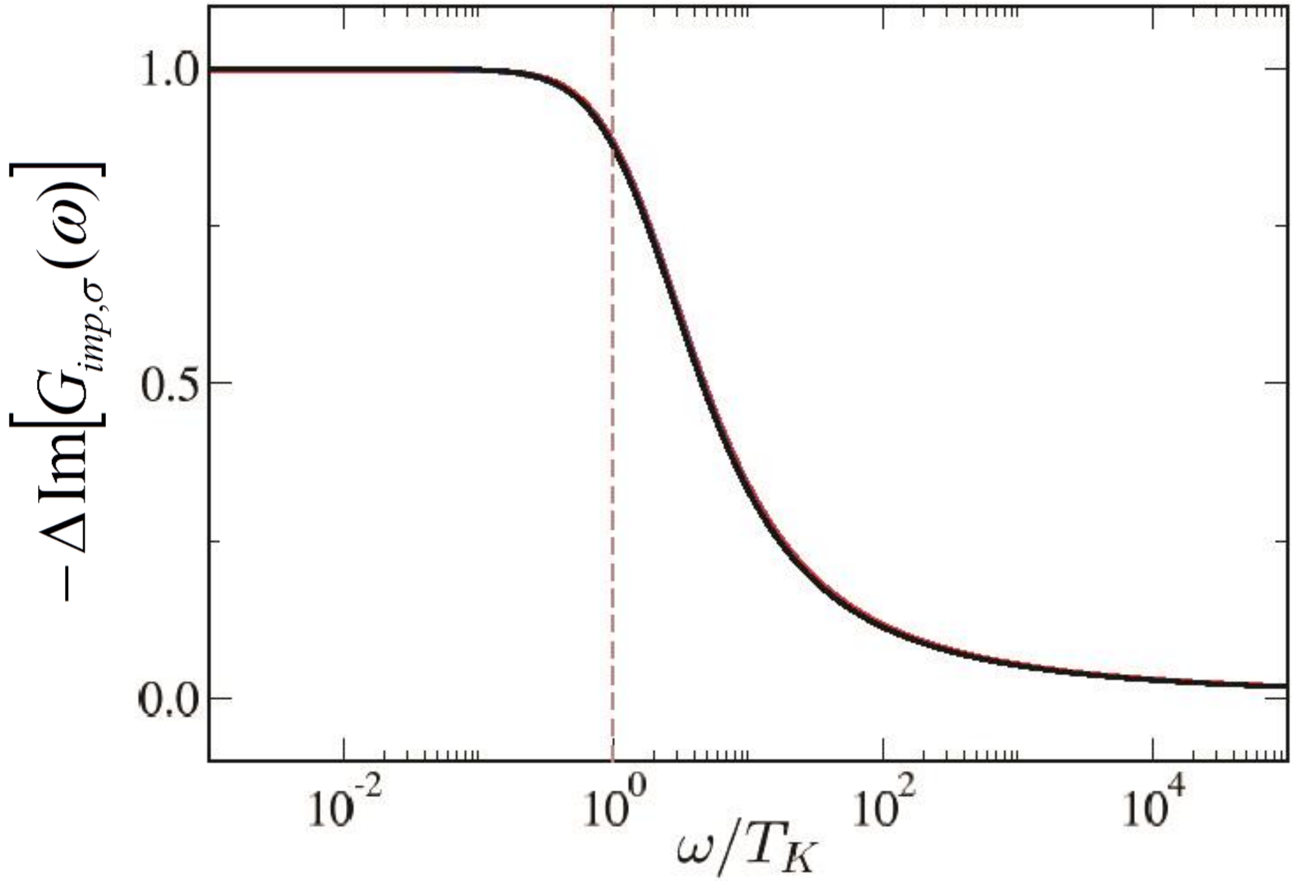
Dynamics within NRG

- Single-particle spectrum of the Anderson model:



Dynamics within NRG

- Universal scaling spectrum of the Anderson model:



Conclusion: NRG for QIP

- Quantum impurity problems appear in various guises:
  - Magnetic impurities in metals
  - Nanostructures
  - Effective models in DMFT
- NRG is a numerically-exact method
  - It exploits the fundamental RG character of QIPs
  - High-energy states are successively discarded, and the physics is examined at progressively lower temperatures
- Exact thermodynamics and dynamics can be calculated
- Versatile: can be applied to generalized problems