Quantum impurity problems (QIP) and numerical renormalization group (NRG): quick introduction

Rok Žitko

Institute Jožef Stefan

Ljubljana, Slovenia

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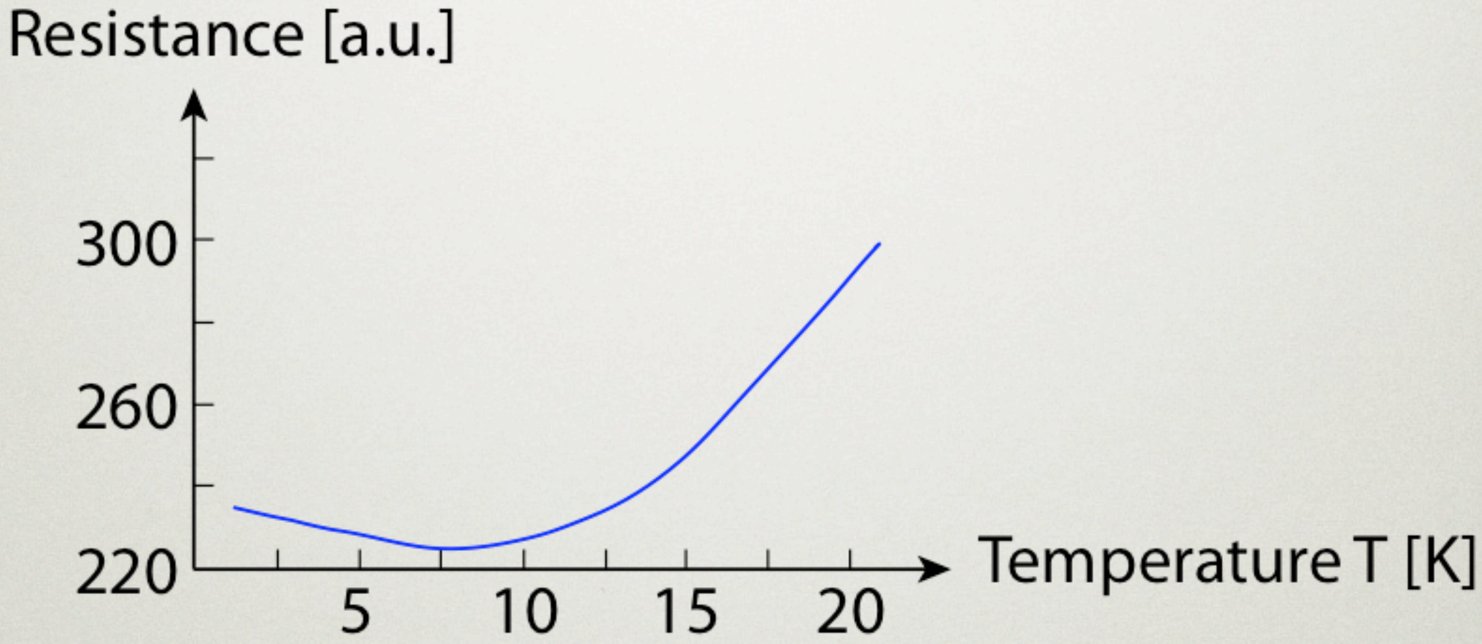
Magnetic Impurities in Metal Hosts

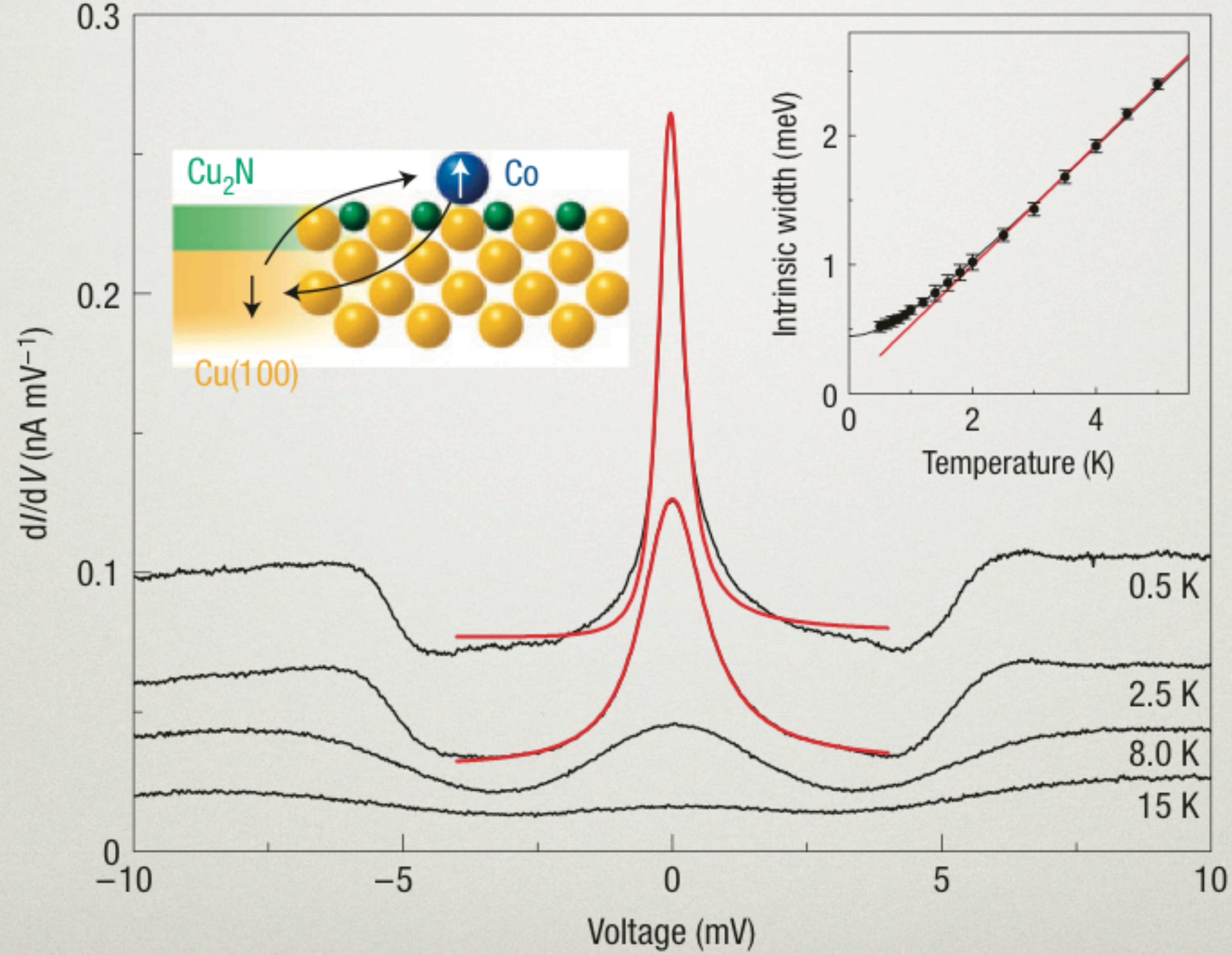
Low-temperature resistance of Au



resistance minimum at <u>finite</u> temperature

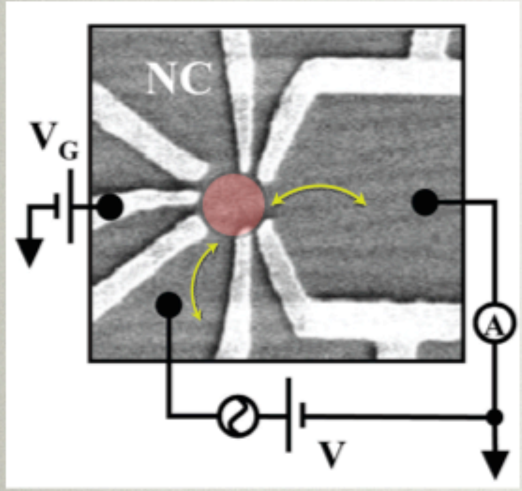
W. J. de Haas and G. J. van den Berg, Physica **3**, 440 (1936)

Magnetic Adatoms on Metal Surfaces

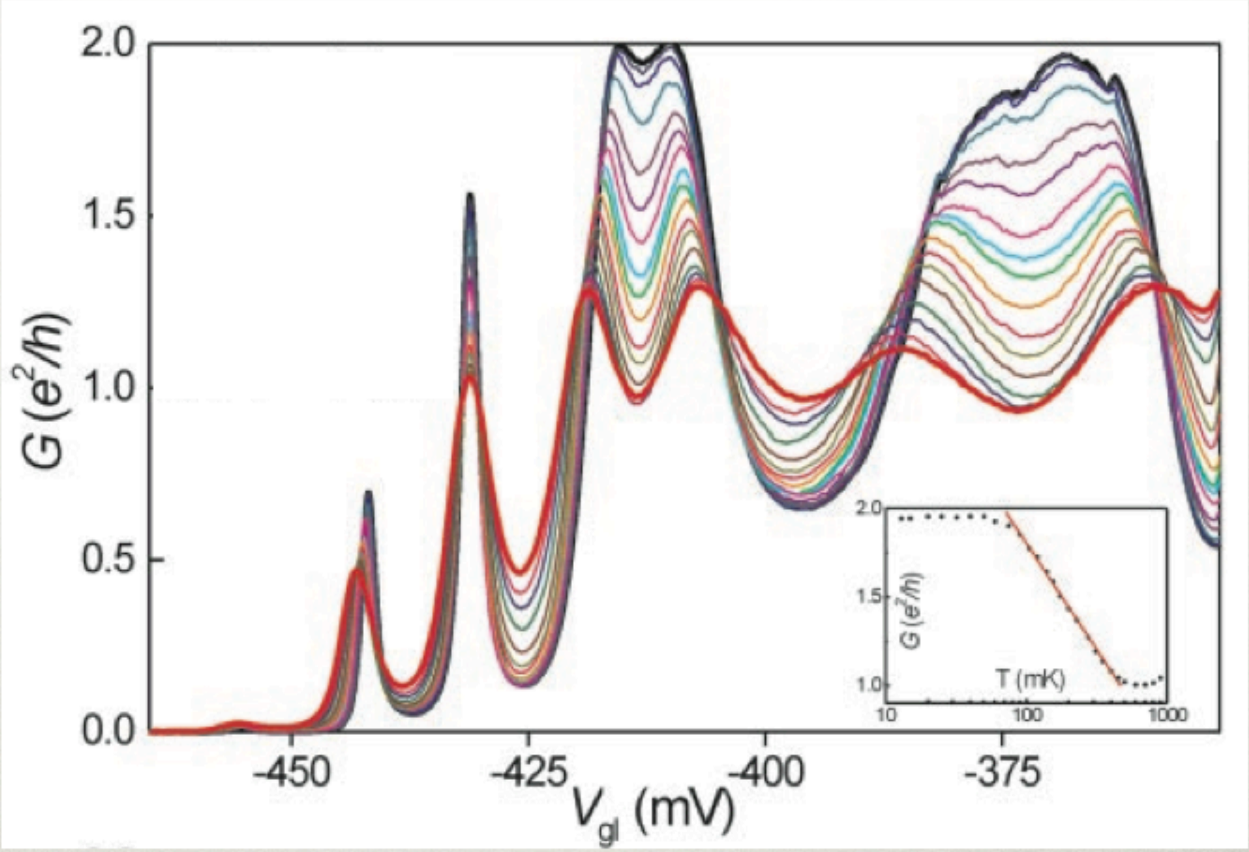


A. Otte et al., Nature Physics **4**, 847 (2008)

Semiconductor Quantum Dots



Grobis et al., PRL 100, 246601 (2008)

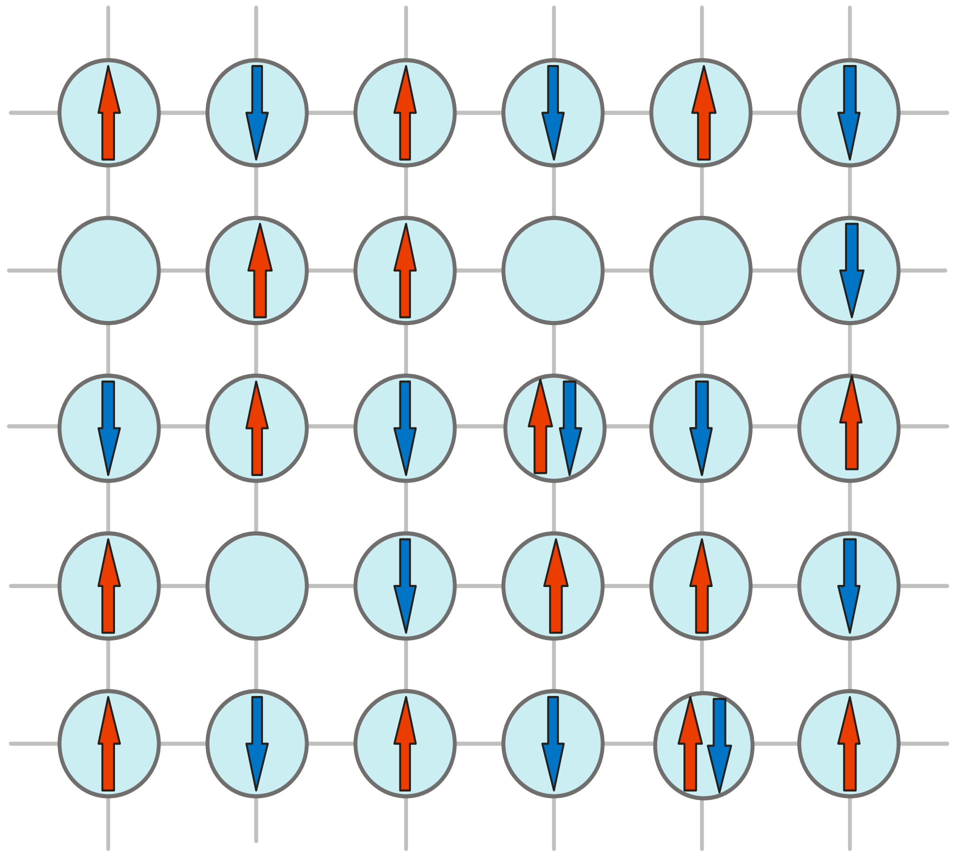


$$G = \left.\frac{\mathrm{d}I}{\mathrm{d}V}\right|_{V=0}$$

unitary conductance: $G=G_0=2e^2/h$

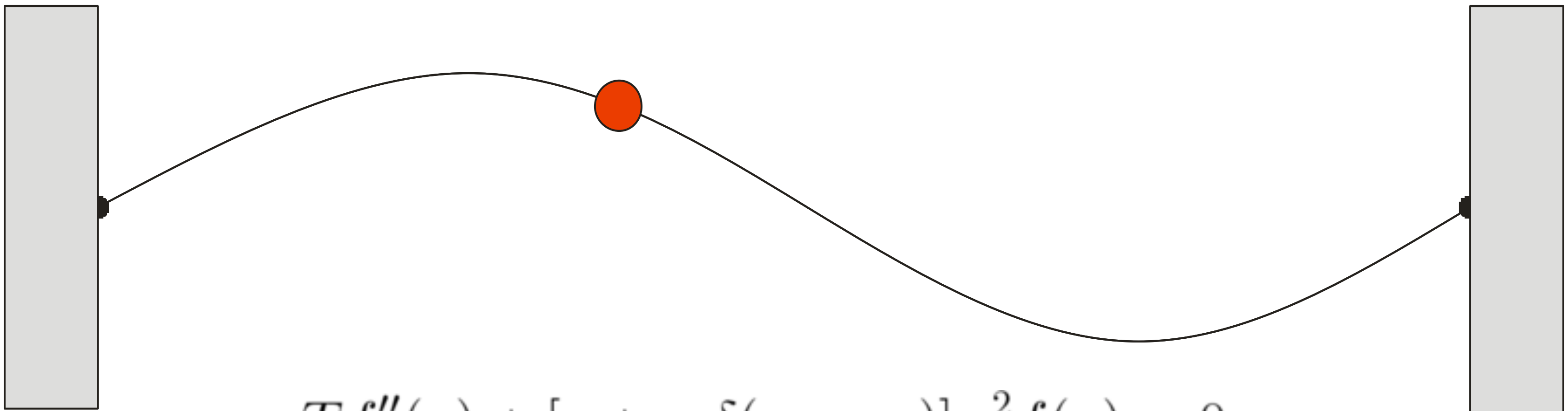
W. G. van der Wiel et al., Science **289**, 2105 (2000)

Dynamical mean-field theory

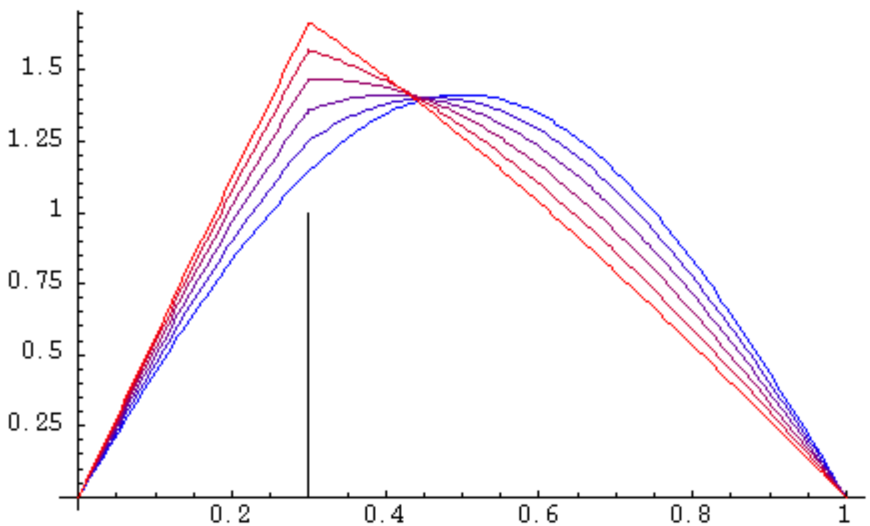


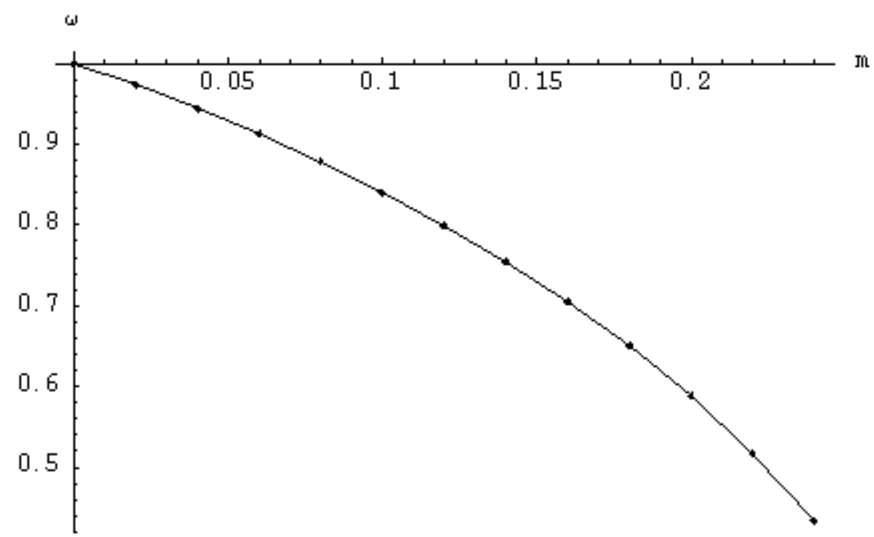
Hubbard model $$H = -t \sum_{\langle i,j \rangle,\sigma} c_{i\sigma}^\dagger c_{i\sigma} - \mu \sum_i n_i + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

"Classical impurity" (potential scattering)

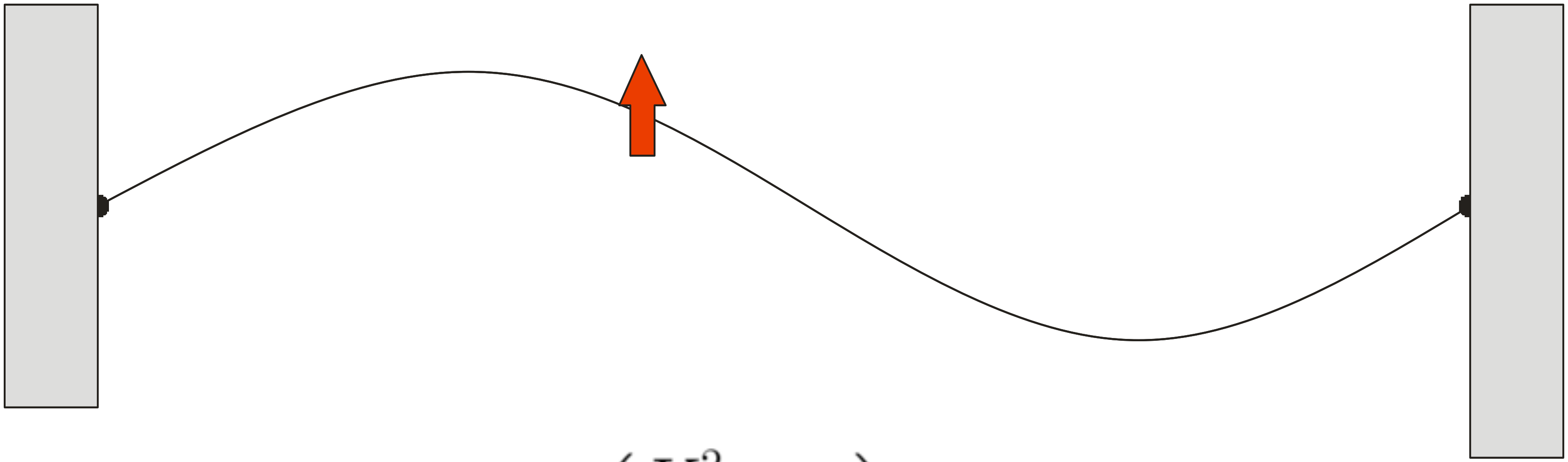


$$T f''(x) + [\rho + m\delta(x - x_0)]\omega^2 f(x) = 0$$





“Quantum impurity” (exchange scattering)



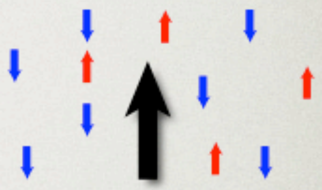
$$H = \sum_i \left(\frac{K_i^2}{2m} - \mu \right) + J\mathbf{S} \cdot \mathbf{s}(x_0)$$

$$\mathbf{s}(x_0) = \sum_i \sum_{\mu\mu'} \psi_{i\mu}^*(x_0) \left(\frac{1}{2} \boldsymbol{\sigma}_{\mu\mu'} \right) \psi_{i\mu'}(x_0)$$

This is the Kondo model!

Kondo Model

$$H = H_{\text{band}} + H_{\text{exch}}$$



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

Fermi sea: gas of non-interacting electrons

$$H_{\text{exch}} = J \, \mathbf{S} \cdot \mathbf{s}$$

exchange coupling

$$\mathbf{S} = \frac{1}{2}\boldsymbol{\sigma}$$ quantum-mechanical spin operator

$$\mathbf{s} = \sum_{\mathbf{k},\alpha,\beta} c^{\dagger}_{\mathbf{k},\alpha} \left(\frac{1}{2} \boldsymbol{\sigma}_{\alpha\beta} \right) c_{\mathbf{k},\beta}$$ spin-density (at $\mathbf{r}$=0)

Nonperturbative behaviour

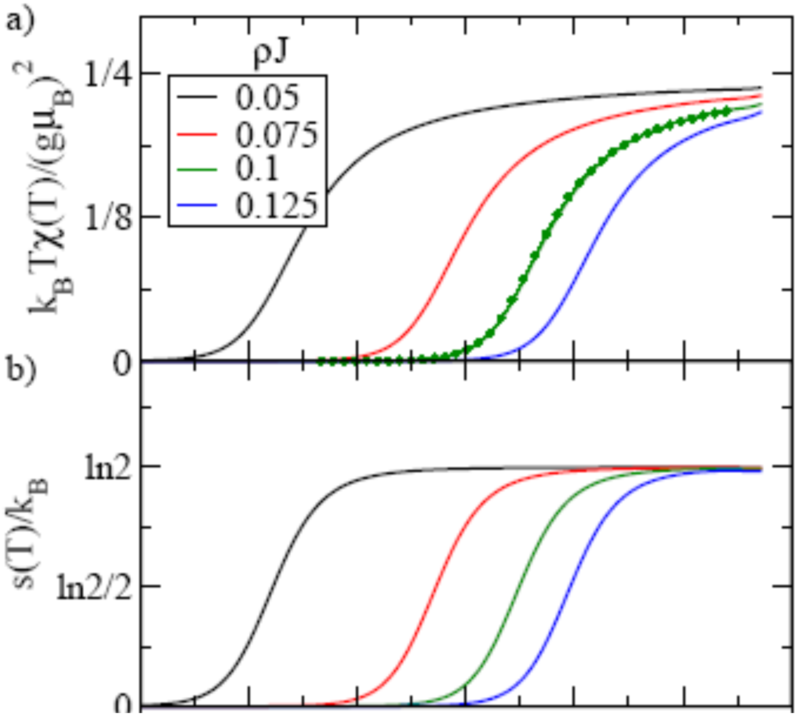
$$M_{\text{imp}}(H) = g\mu_B \left(\langle S_z + S_{z,\text{band}} \rangle - \langle S_{z,\text{band}} \rangle_0 \right)$$

$$\chi_{\text{imp}}(T) = \frac{(g\mu_B)^2}{k_B T} \frac{1}{4}$$

The perturbation theory fails for arbitrarily small J !

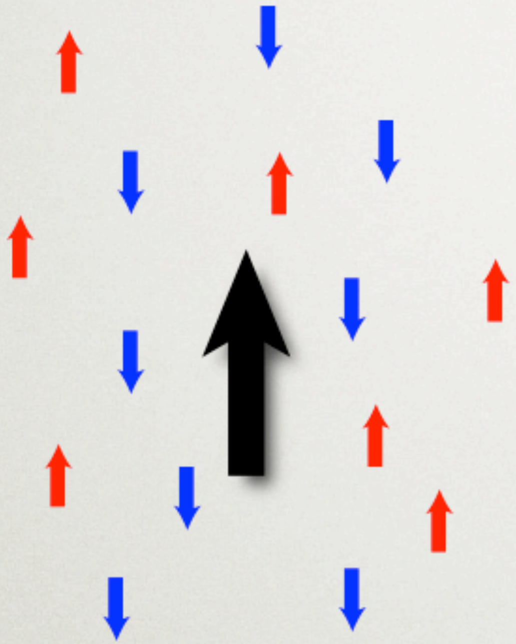
$$k_B T_K \sim D e^{-1/\rho J}$$

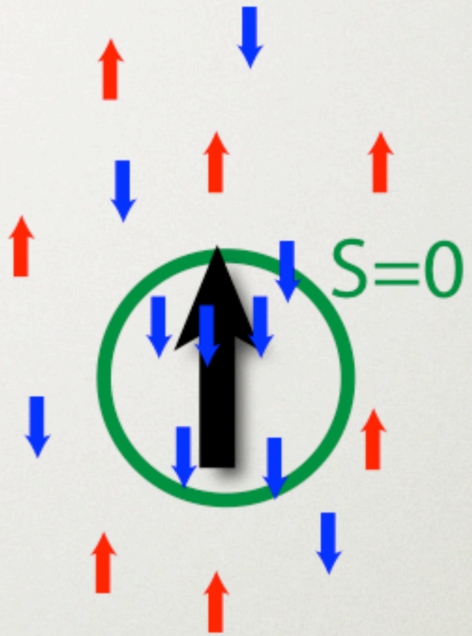
Screening of the magnetic moment



Kondo effect!

Kondo Effect





Kondo singlet

$$T_K = \mathcal{D} \exp\left(-\frac{1}{\rho J}\right)$$

$T \gg T_K$

asymptotic freedom

$T \ll T_K$

infrared slavery

Single-Impurity Anderson Model

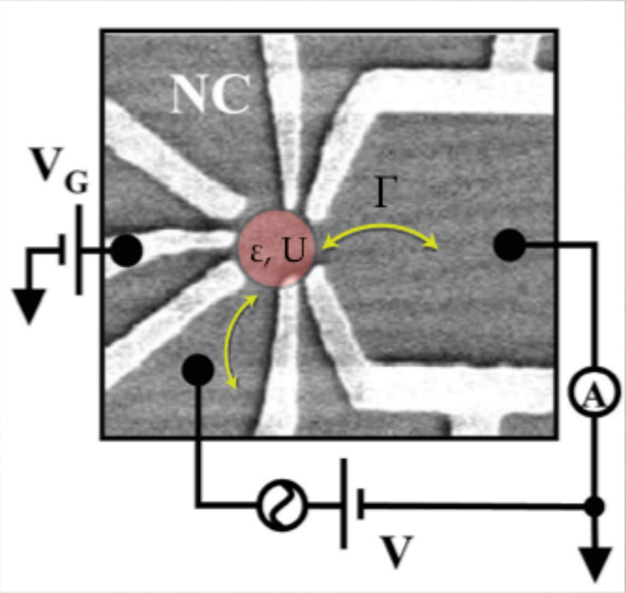
$$H = H_{\text{imp}} + H_{\text{band}} + H_{\text{hyb}}$$

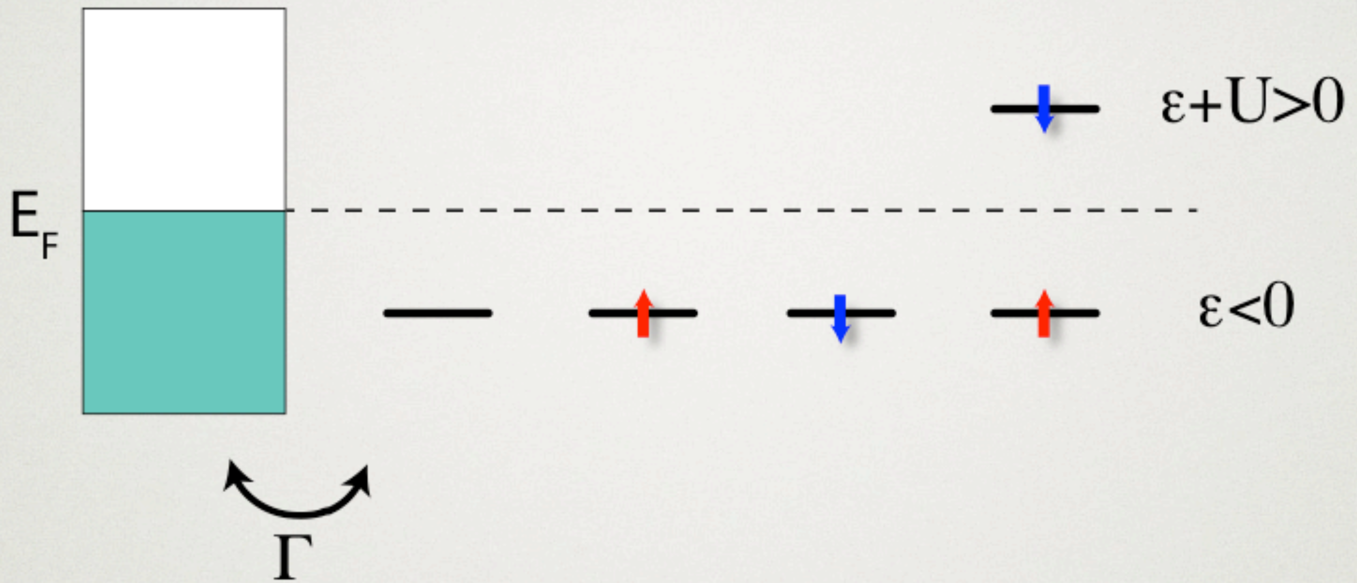
$$H_{\text{imp}} = \sum_{\sigma} \epsilon\, n_\sigma + U\, n_\uparrow n_\downarrow \qquad n_\sigma = d^\dagger_\sigma d_\sigma$$

$$H_{\text{band}} = \sum_{\mathbf{k},\sigma} \epsilon_k\, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$

$$H_{\text{hyb}} = \sum_{k,\sigma} \left(V_k\, c^\dagger_{k,\sigma} d_\sigma + \text{H.c.} \right)$$

$$\Delta(\omega) = \sum_k \frac{|V_k|^2}{\omega - \epsilon_k} \approx i\Gamma$$

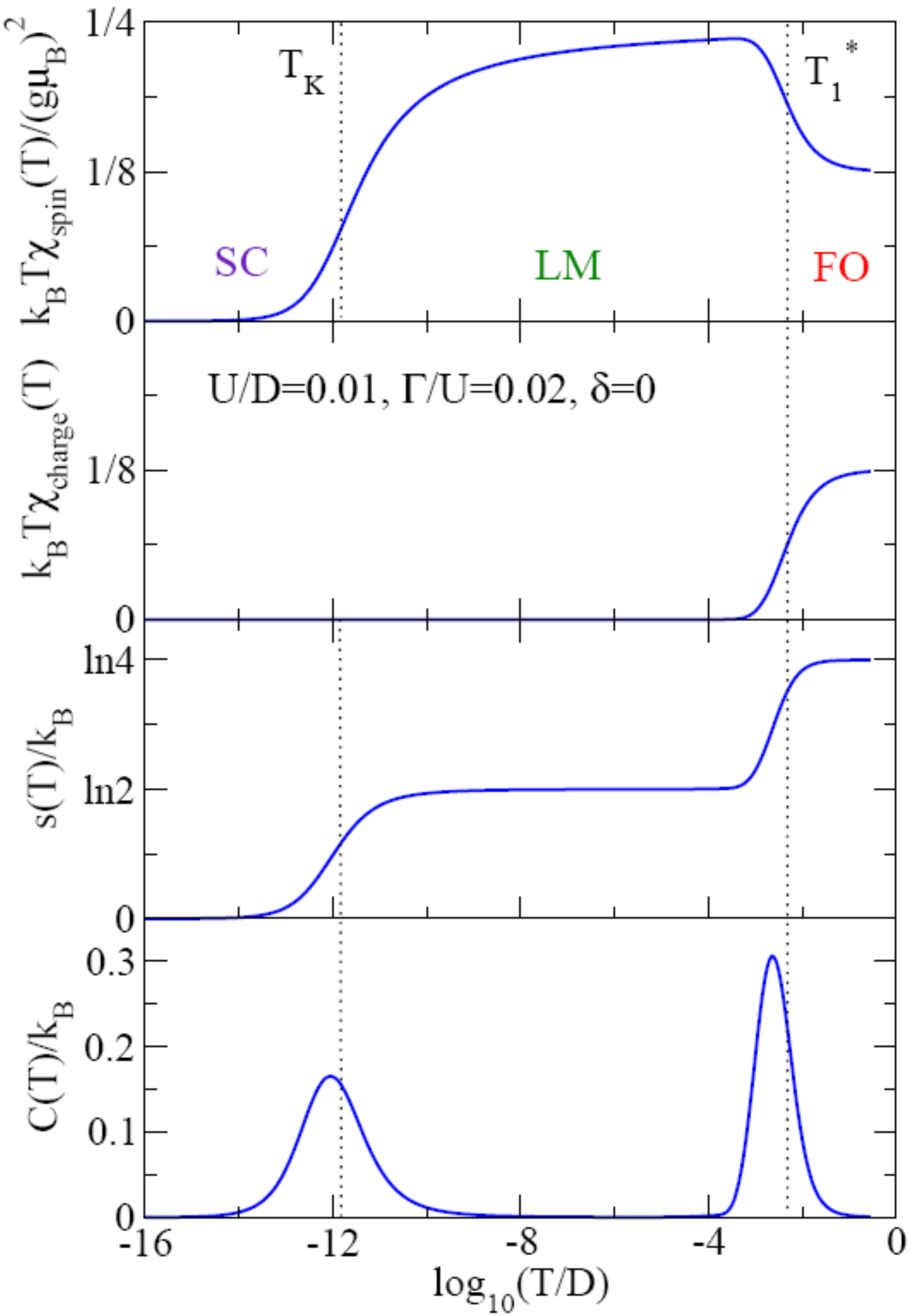




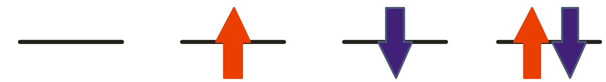
$$\boxed{\delta} = \epsilon + U/2$$

δ=0 is a special "particle-hole symmetric point" with ⟨n⟩=1

$$\rho J = \frac{8U}{\pi\Gamma}$$ Schrieffer-Wolff transformation

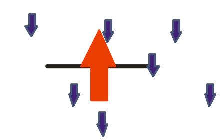


FO: free orbital

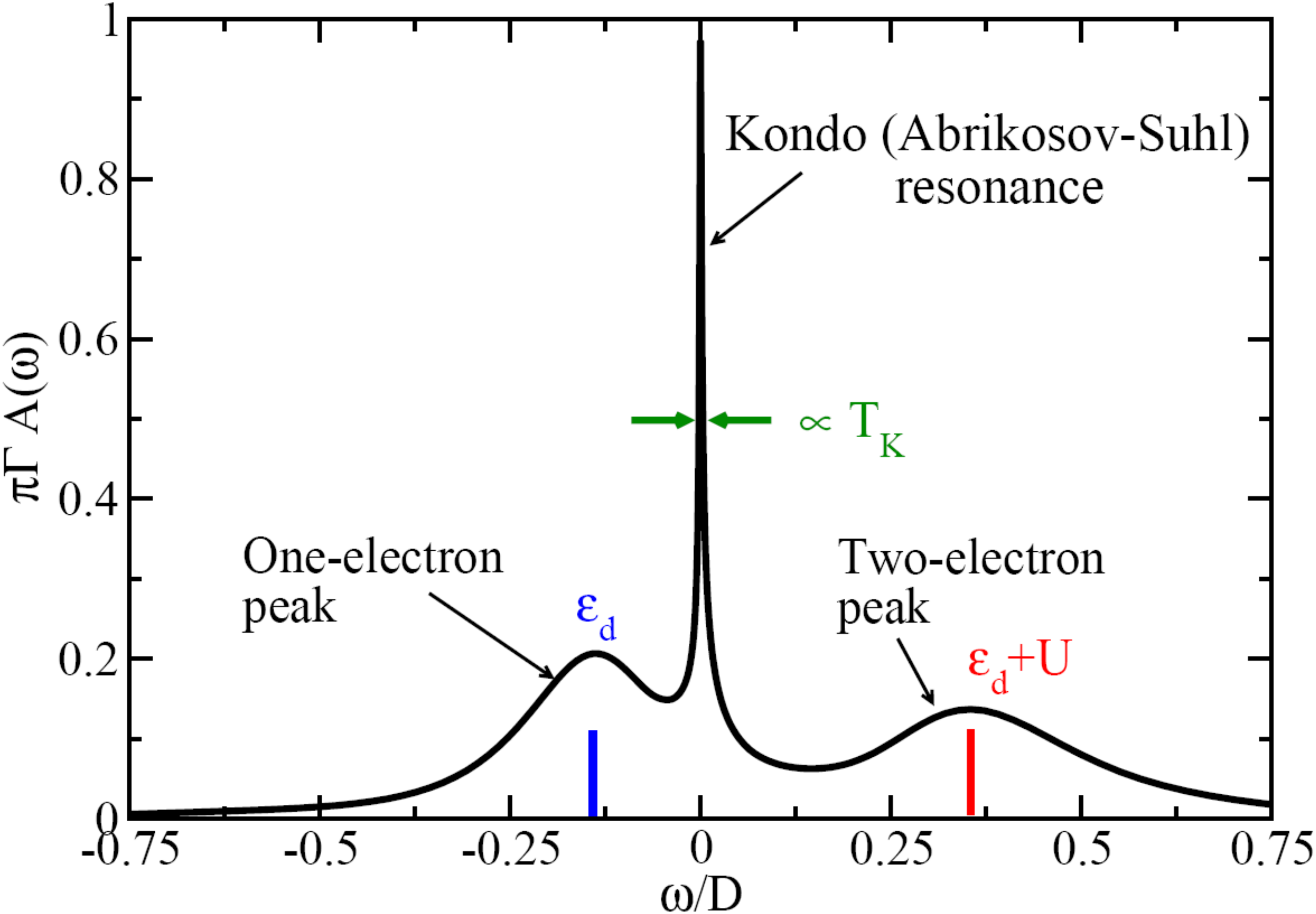


LM: local moment

SC: strong coupling

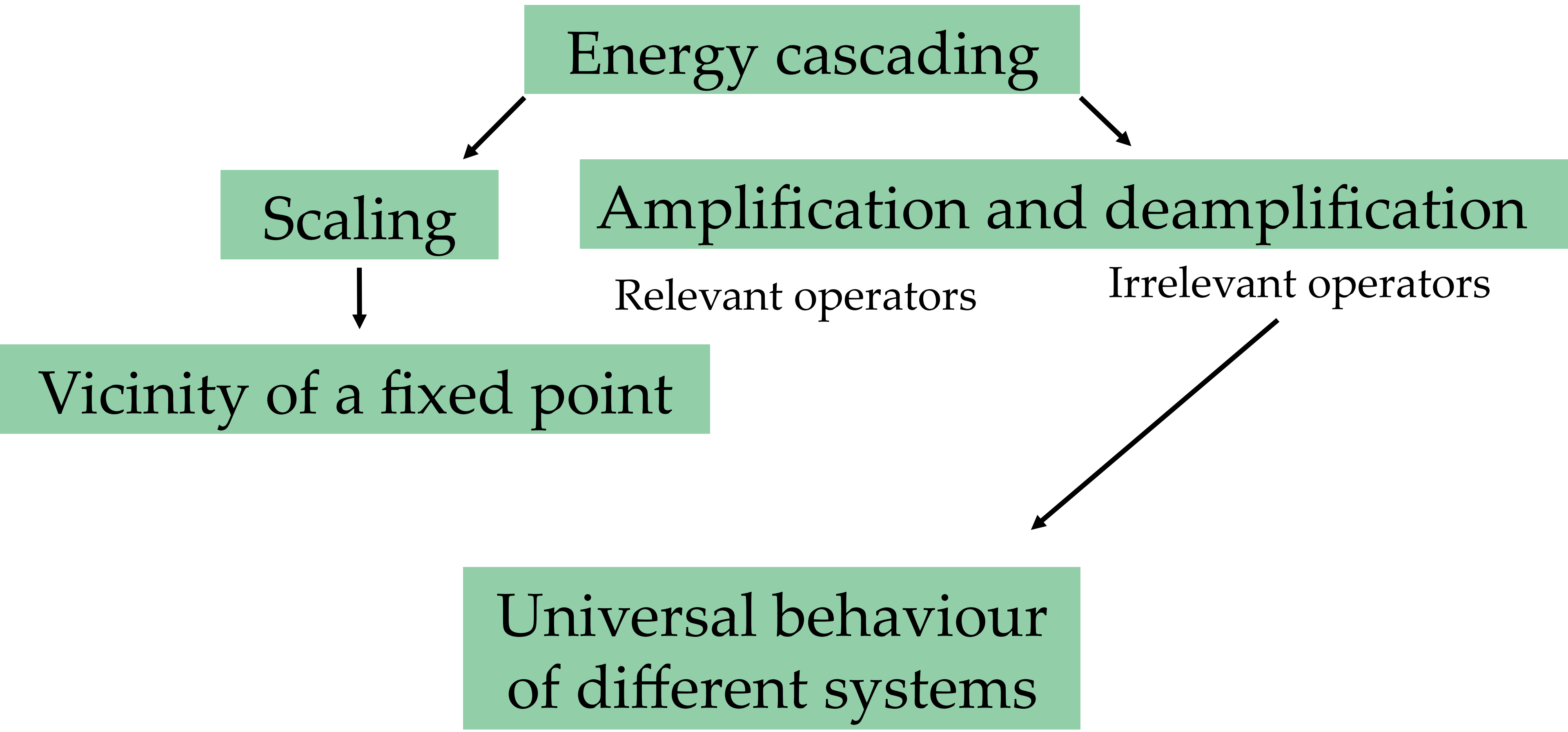


Krishnamurthy, Wilkins, Wilson, PRB **21**, 1003 (1980)



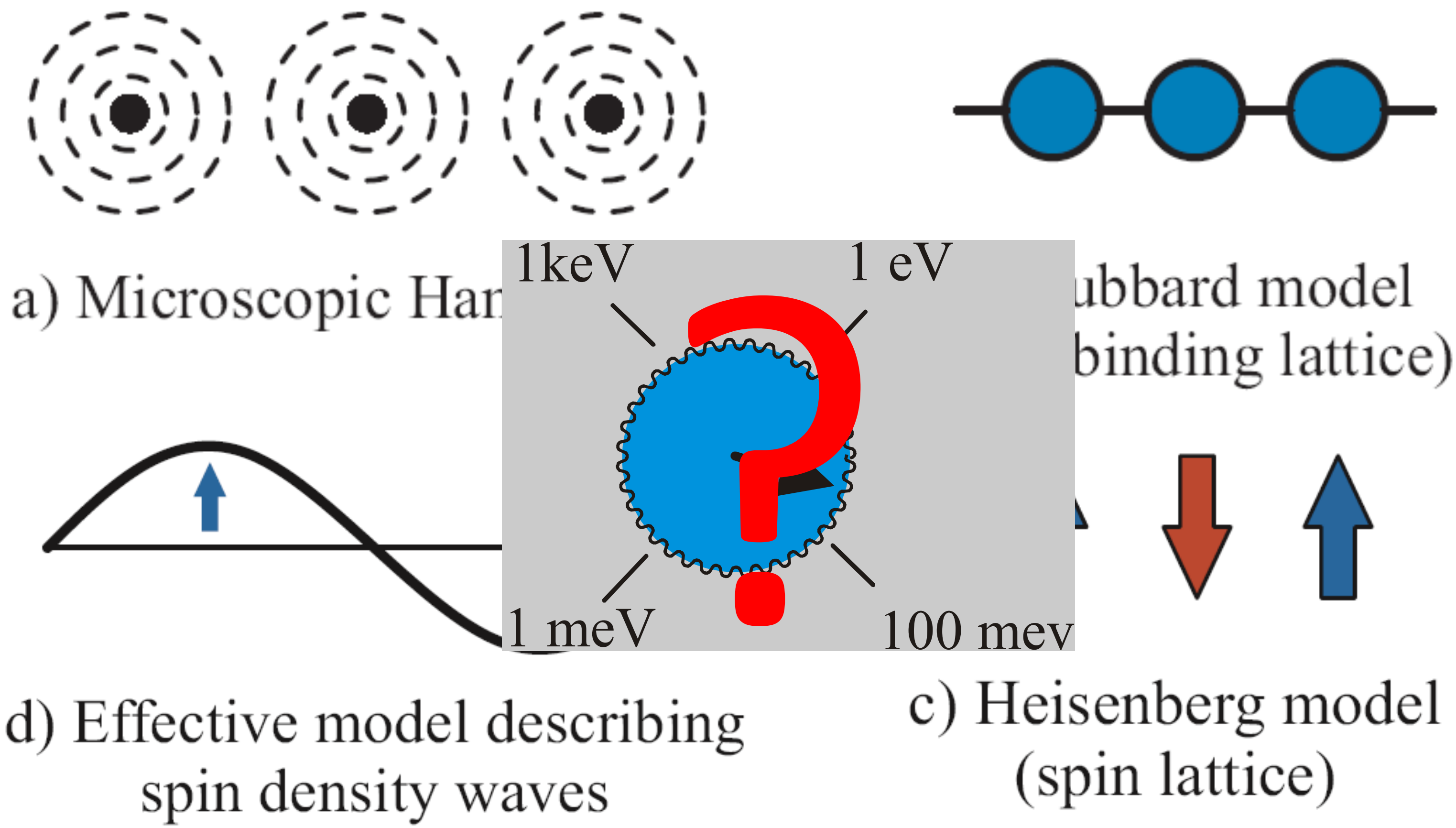
Frota, Oliveira, PRB **33**, 7871 (1986), Costi, Hewson, Zlatić, JPCM **6**, 2519 (1994)

Renormalization group theory

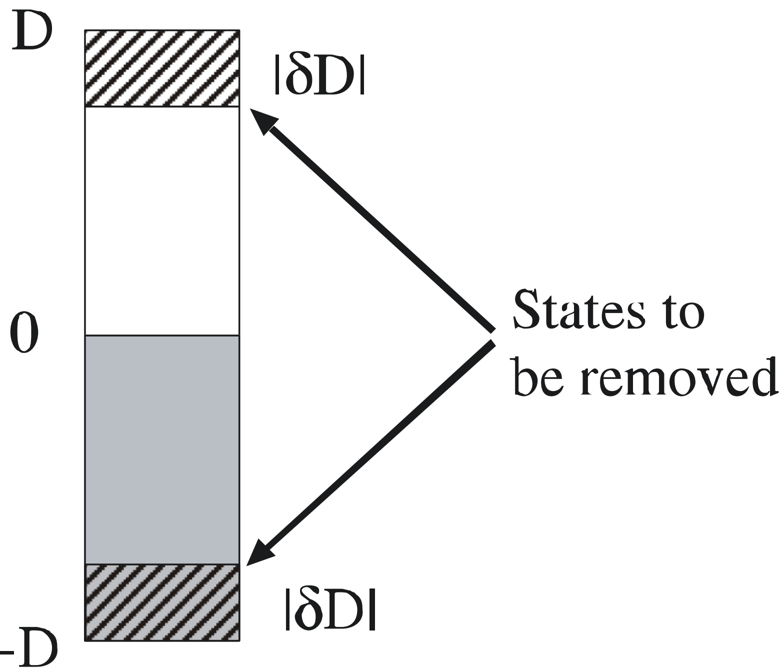


RG explains the universality of critical phenomena in continuous phase transitions. K. G. Wilson, Nobel prize 1982.

Renormalization group



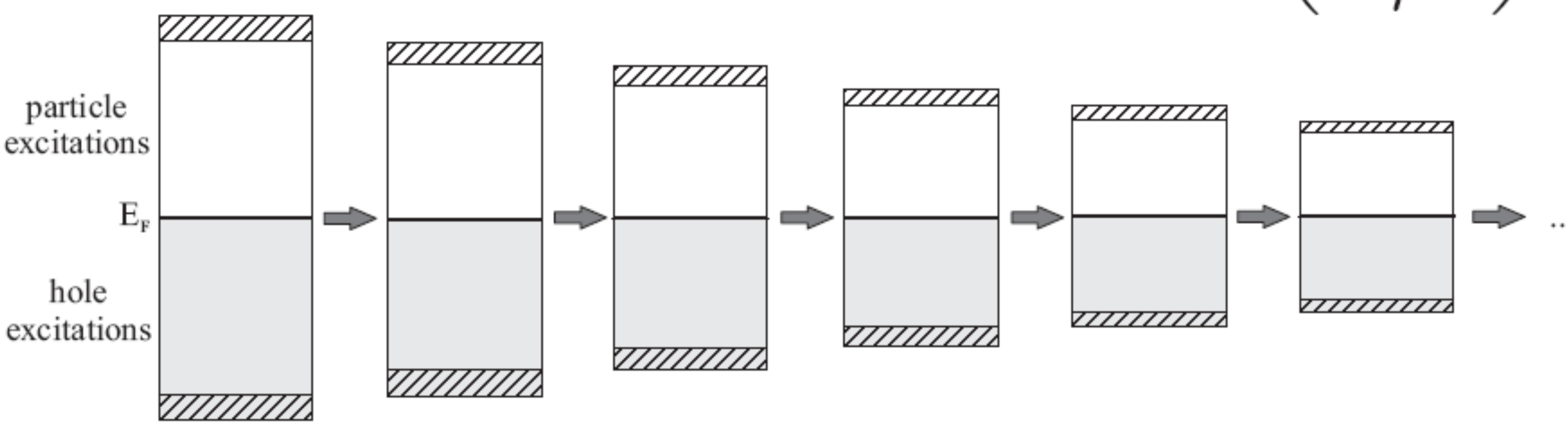
Cutoff renormalization



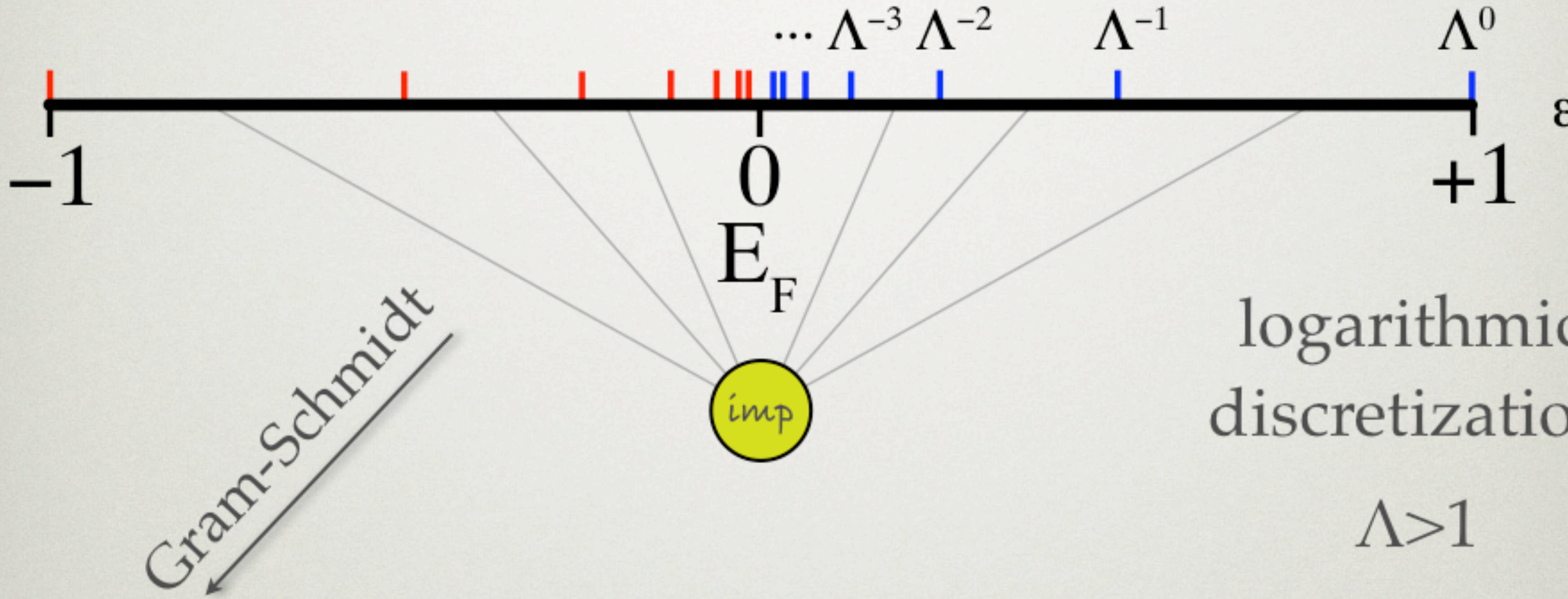
$$\frac{d\mathcal{J}}{d\ln\mathcal{D}} = -\rho\mathcal{J}^2$$

$$\mathcal{J}(\mathcal{D}) = \frac{J}{1 - J\rho\ln(\mathcal{D}/D)}$$

$$T_K \sim D\exp\left(-\frac{1}{\rho J}\right)$$

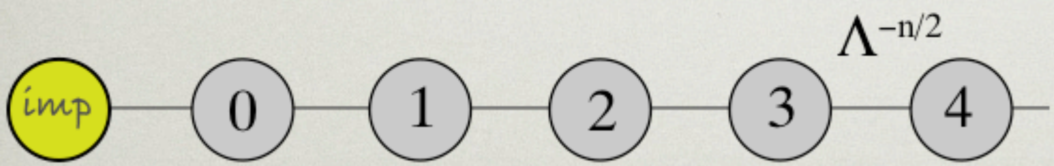


Numerical Renormalization Group



logarithmic discretization

$\Lambda>1$



Wilson's chain

open-source code: http://nrgljubljana.ijs.si/

K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975)

Discretization schemes

$\rho(\varepsilon)$ = density of states in the band

1) Conventional scheme

$$\mathcal{E}_j^z = \frac{\int_{I_j} \rho(\epsilon)\epsilon \, d\epsilon}{\int_{I_j} \rho(\epsilon) d\epsilon}$$

Chen, Jayaprakash, JPCM **7**, L491 (1995); Ingersent, PRB **54**, 11936 (1996); Bulla, Pruschke, Hewson, JPCM **9**, 10463 (1997).

2) Campo-Oliveira scheme

$$\mathcal{E}_j^z = \frac{\int_{I_j} \rho(\epsilon) d\epsilon}{\int_{I_j} \rho(\epsilon)/\epsilon \, d\epsilon}$$

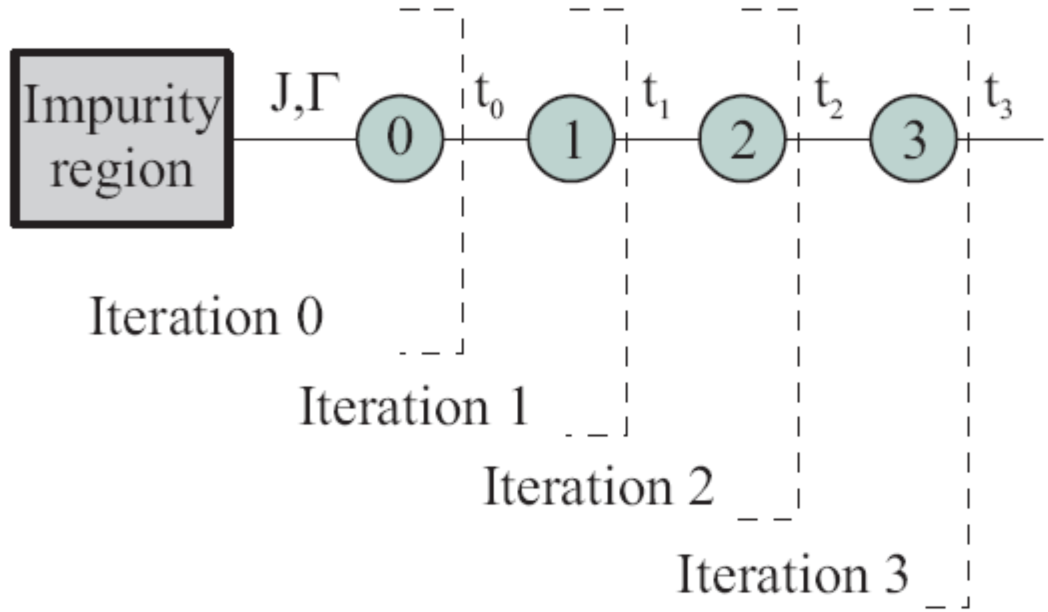
Campo, Oliveira, PRB **72**, 104432 (2005).

3) Scheme without artifacts

$$A_{f_0}(\omega) = \rho(\omega)$$

R. Žitko, Th. Pruschke, PRB **79**, 085106 (2009)
R. Žitko, Comput. Phys. Comm. **180**, 1271 (2009)

Iterative diagonalization

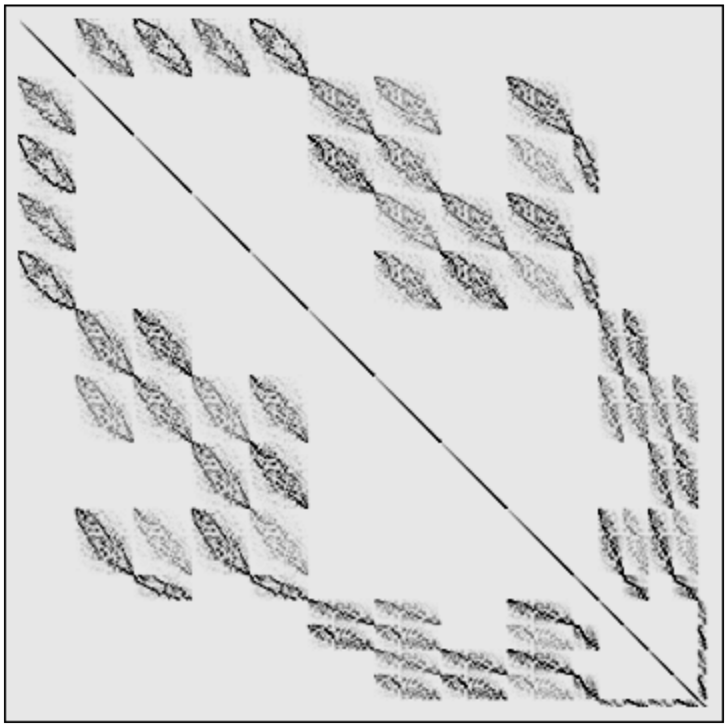


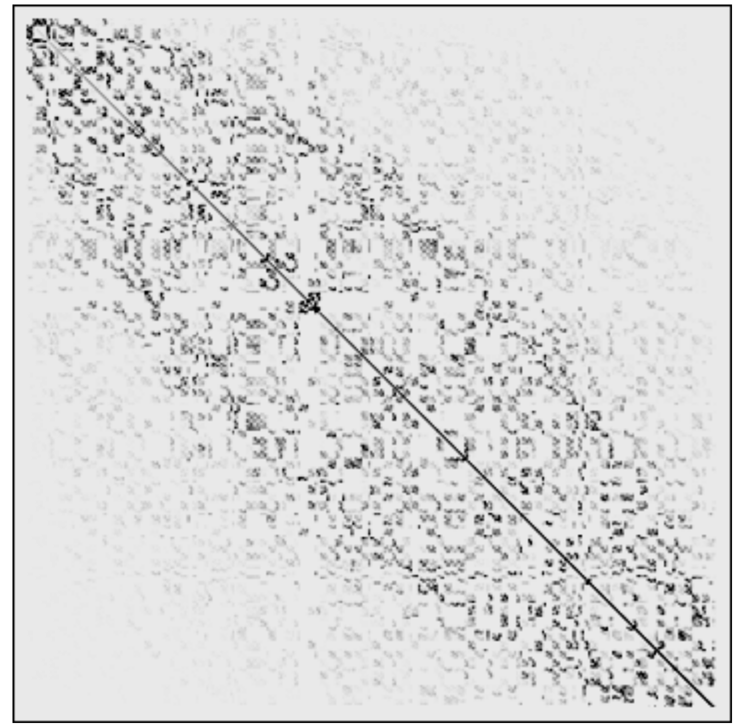
Recursion relation:

$$H_{N+1} = T\left[H_N\right]$$

$$H_{N+1} = \Lambda^{-1/2} H_N + \xi_N \left(f_{N+1,\sigma}^{\dagger} f_{N,\sigma} + f_{N,\sigma}^{\dagger} f_{N+1,\sigma} \right)$$

Energy-scale separation





- Extremely fast (for single-orbital problems)
- Arbitrarily low temperatures
- Real-frequency spectral functions
- Arbitrary local Hamiltonian / hybridization function

Dynamic quantities

We' re interested in correlators such as

$$C(t) = \left\langle T\left[A(t)B(0) \right] \right\rangle$$

or their Fourier transforms

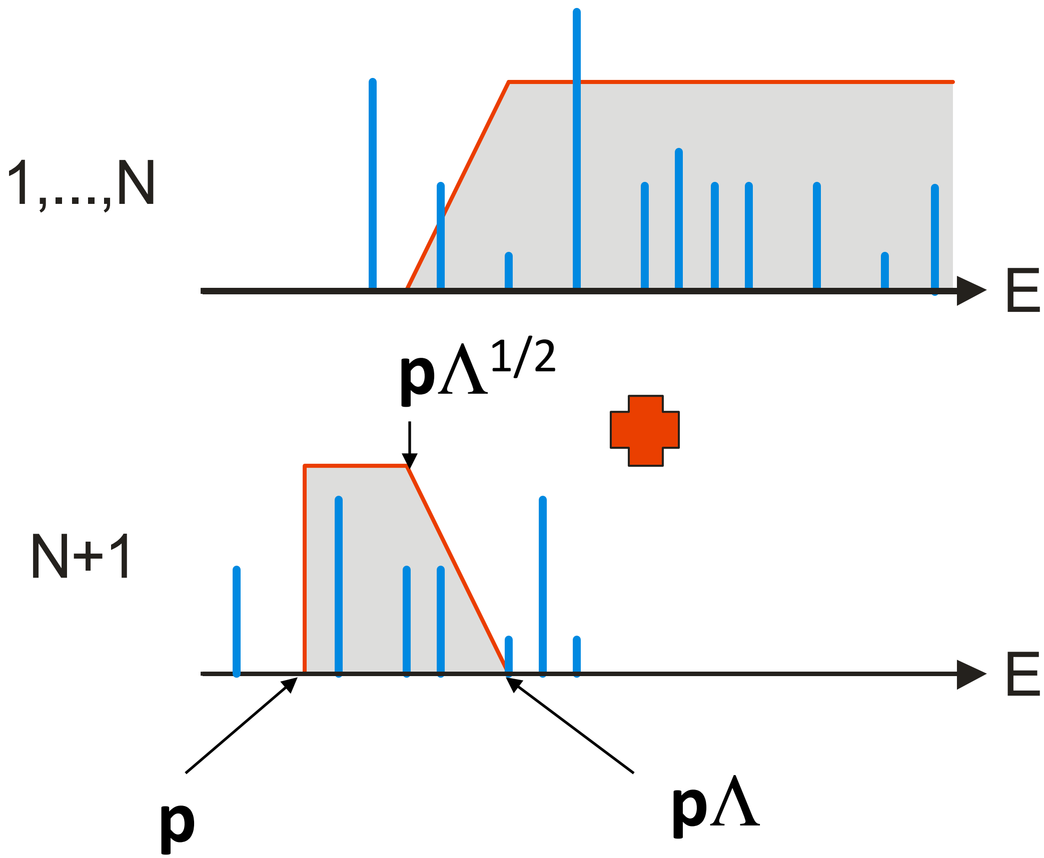
$$C(\omega) = \int_{-\infty}^{+\infty} e^{i\omega t} \left\langle T\left[A(t)B(0) \right] \right\rangle dt$$

Spectral decomposition (Lehmann representation):

$$C^R(\omega) = \frac{1}{\sum_n e^{-\beta E_n}} \sum_{n,m} \left\langle m \middle| A \middle| n \right\rangle^* \left\langle m \middle| B \middle| n \right\rangle \frac{e^{-\beta E_n} + e^{-\beta E_m}}{\omega + E_n - E_m + i\delta}$$

Frota, Oliveira, PRB **33**, 7871 (1986); Sakai, Shimizu, Kasuya, JPSJ **58**, 3666 (1989); Costi, Hewson, Zlatić, JPCM **6**, 2519 (1994); Hofstetter, PRL **85**, 1508 (2000).

Patching



p: patching parameter (in units of the energy scale at N+1-th iteration)

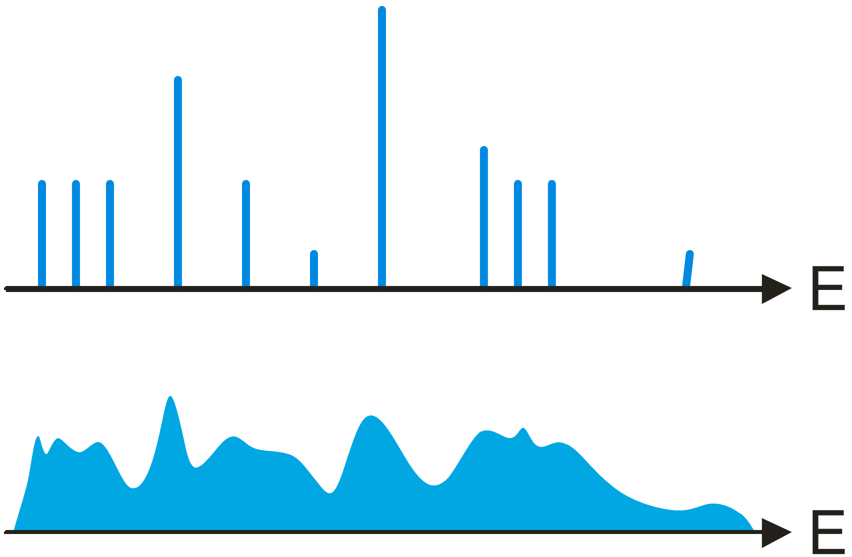
Bulla, Costi, Vollhardt, PRB **64**, 045103 (2001).

Alternatively: **complete Fock space** approach.

Peters, Pruschke, Anders, PRB **74**, 245114 (2006)

Weichselbaum, von Delft, PRL **99**, 076402 (2007).

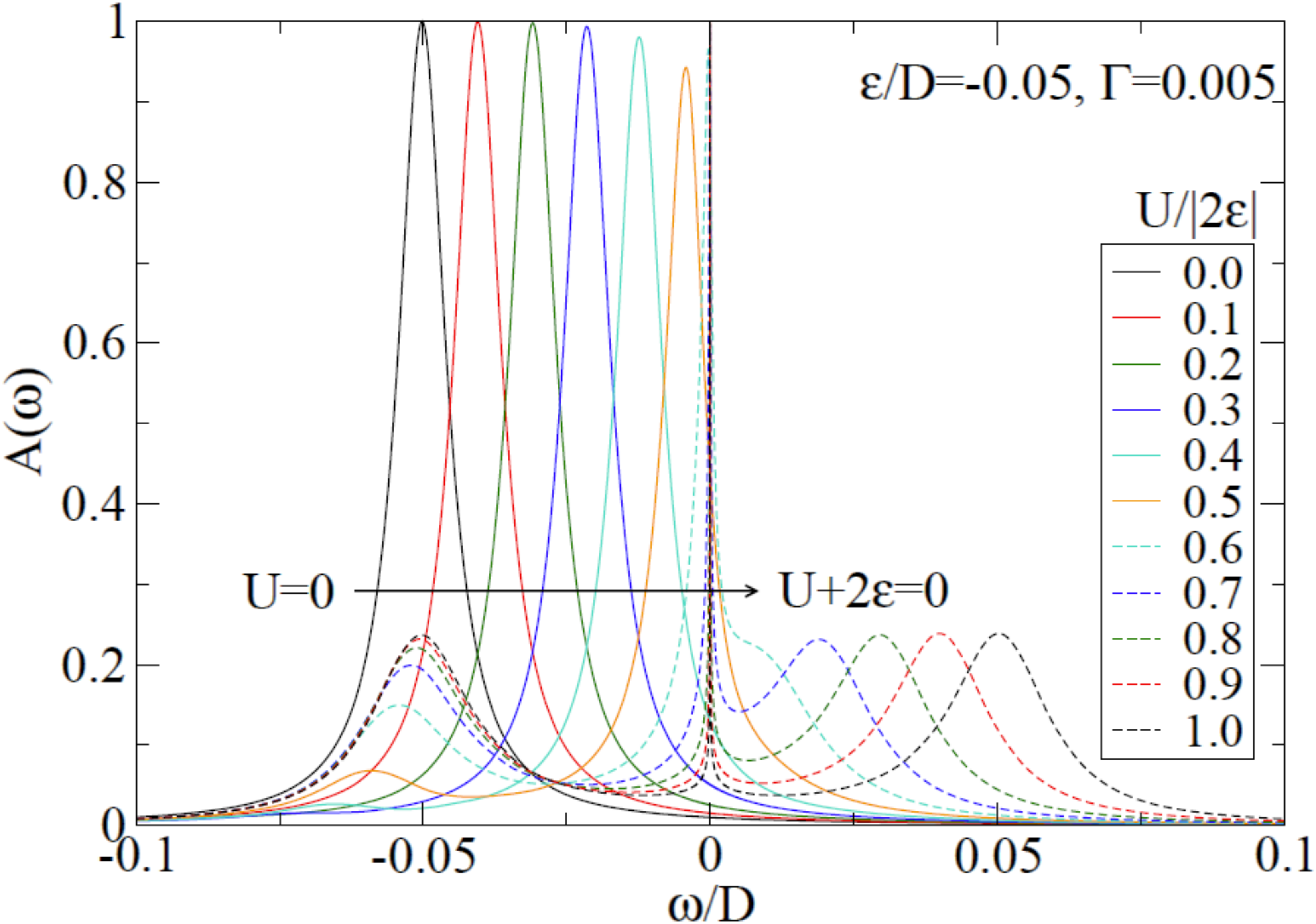
Broadening



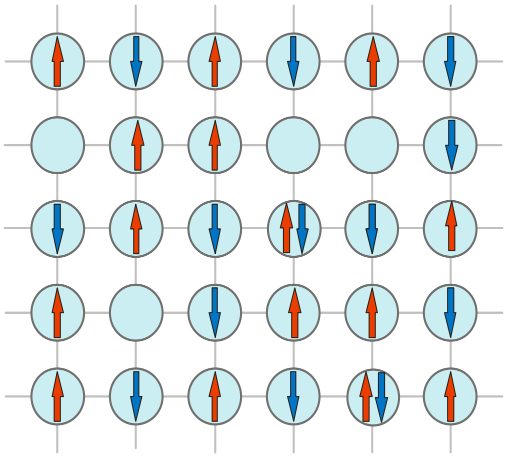
$$P(\omega, E) = \frac{1}{\sqrt{2\pi}\eta_E} e^{-\frac{(\omega - E)^2}{2\eta_E^2}}$$

$$\eta_E = \eta \ |E|$$

High-resolution spectral functions



Dynamical mean-field theory



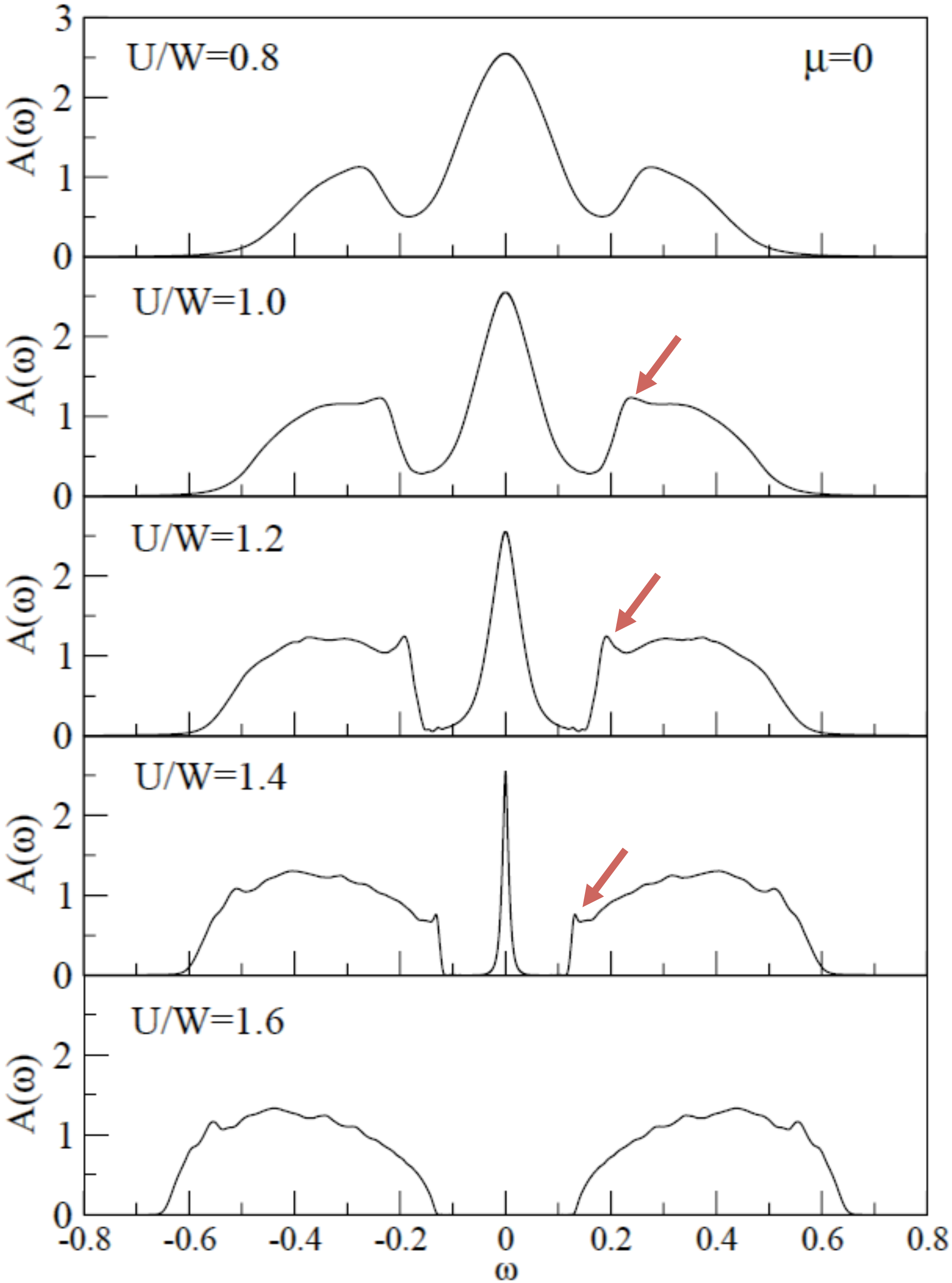
Hubbard model

$$H = -t \sum_{\langle i,j \rangle,\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} - \mu \sum_i n_i + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$G_{\mathrm{latt}}(\boldsymbol{k}, \omega) = \frac{1}{\omega + \mu - \epsilon_{\boldsymbol{k}} - \Sigma_{\mathrm{latt}}(\boldsymbol{k}, \omega)}$$

$$\Sigma_{\mathrm{latt}} = \Sigma(\omega)$$

$$\mathcal{G} = \frac{1}{G^{-1} + \Sigma} = \frac{1}{z - \Delta(z)}$$



Hubbard model on the Bethe lattice, PM phase

inner band-edge features

See also DMRG study, Karski, Raas, Uhrig, PRB **72**, 113110 (2005).

Tools: SNEG and NRG Ljubljana

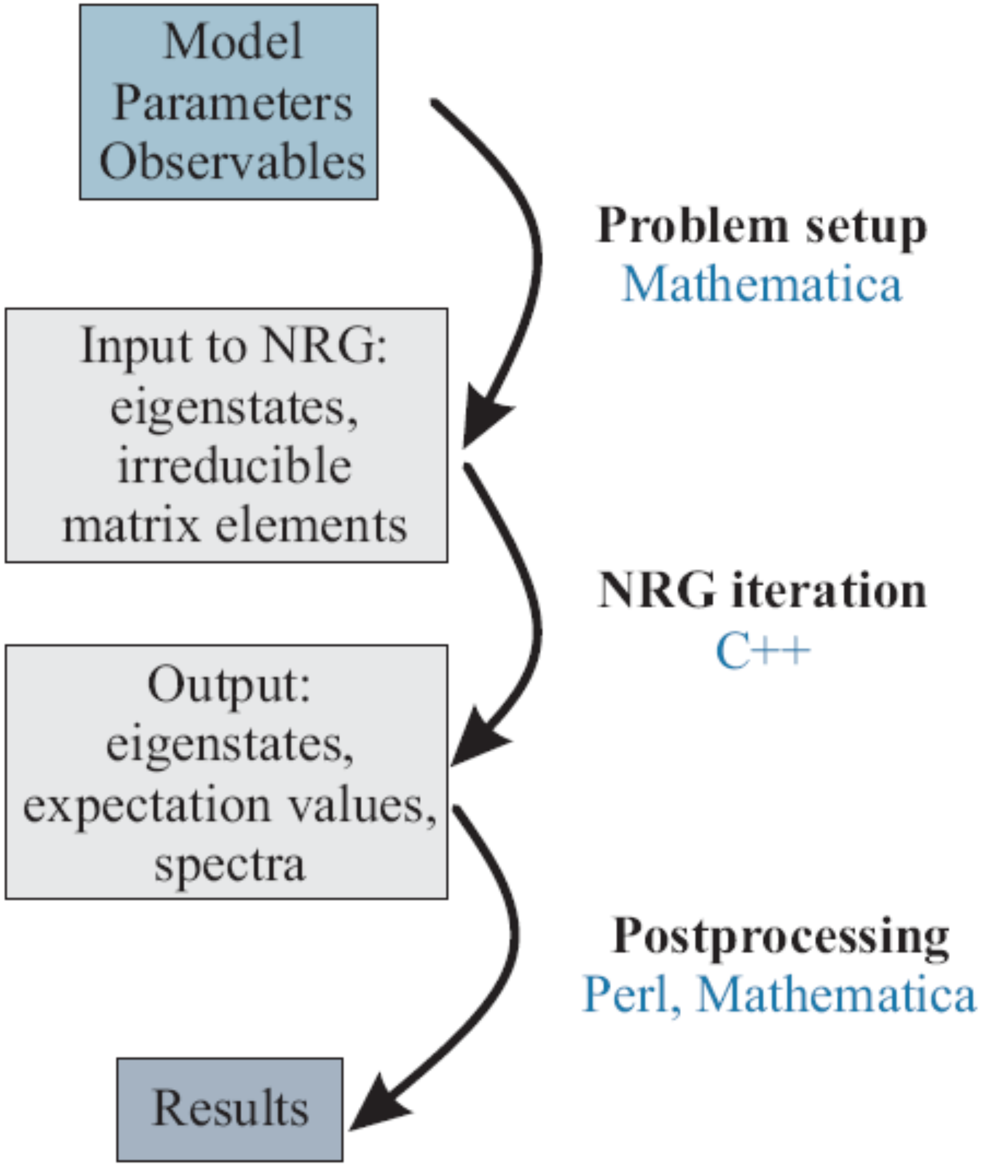
Add-on package for the computer algebra system Mathematica for performing calculations involving non-commuting operators

Efficient general purpose numerical renormalization group code

- flexible and adaptable
- highly optimized (partially parallelized)
- easy to use

Both are **freely available** under the GPL licence:

http://nrgljubljana.ijs.si/



nrginit

nrgrun

various
scripts

Lectures plan

- 1a. Introduction to QIP and NRG
- 1b. Discretization, z-averaging, thermodynamics, flow diagrams

- 2a. Implementing NRG, handling second quantization expressions, parallelization issues
- 2b. **Tutorial**: getting the code to run, basic calculations

- 3a. Spectral function calculations, self-energy trick, DMNRG, patching, complex Fock space basis approaches
- 3b. **Tutorial**: themodynamics and flow diagrams for Kondo model and SIAM

- 4a. More on spectral functions: systematic errors, broadening issues
- 4b. **Tutorial**: spectral function for SIAM, T matrix for Kondo model

- 5a. Transport properties
- 5b. **Tutorial**: Kondo peak splitting in magnetic field, transport properties, conductance and thermopower in SIAM

- 6a. NRG as impurity solver in dynamical mean-field theory, self-consistency, Broyden mixing
- 6b. **Tutorial**: Hubbard model, MIT at half-filling, bad metal behavior

- 7a. Underscreening, overscreening, (singular,regular,non)-Fermi liquids
- 7b. **Tutorial**: S=1 Kondo model, two-channel Kondo model

- Optional: phonons, impurities in superconductors, multi-impurity models

Reference works

- Wilson, RMP 1975
- Krishnamurthy, Wilkins, Wilson, 2xPRB 1980
- Hofstetter, PRL 2000
- Anders, Schiller, Peters, Pruschke, Weichselbaum, von Delft, several papers, 2005-2008
- Bulla, Costi, Pruschke, RMP 2008