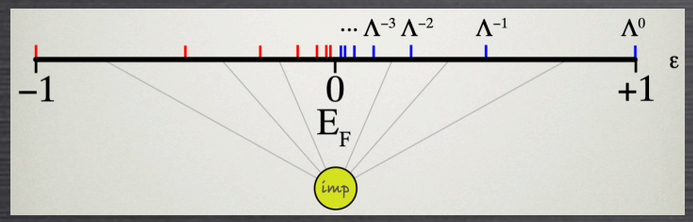
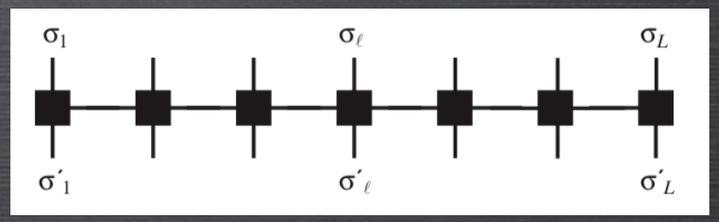
Solvers for quantum impurity problems (with superconducting baths)

Lecture 2: numerical renormalization group





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Part 1: General considerations

Effective hamiltonian

= description valid on a certain energy/length scale

Parameters can be extracted from the experiment.

What terms to retain:

- symmetry considerations
- energy considerations
- relevance of operators (renormalization group)

Example: from Hubbard model to Heisenberg model

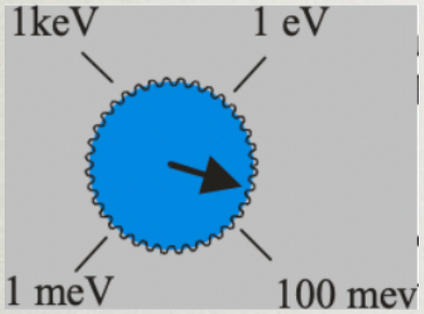
$$H = -t \sum_{ij,\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

large U, <n>=1

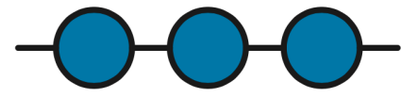
i.e., for Mott insulators

$$H = J \sum_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \qquad J = \frac{4t^2}{U}$$

$$[S^x, S^y] = iS^z \quad \mathbf{S}^2 = S(S+1)$$

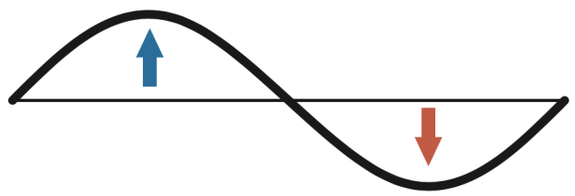


a) Microscopic Hamiltonian



b) Hubbard model
(tight-binding lattice)

c) Heisenberg model
(spin lattice)



d) Effective model describing
spin density waves

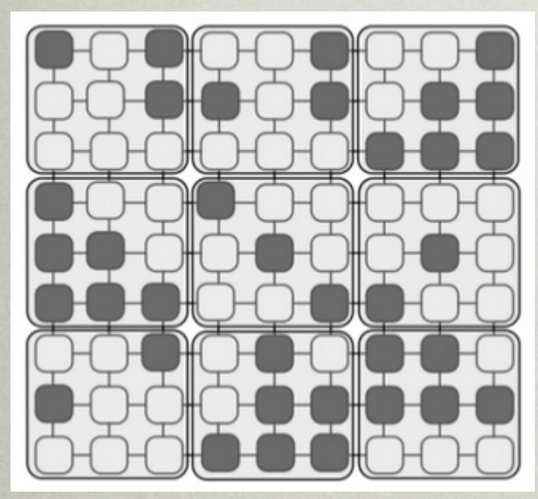
P.W. Anderson: Basic notions of condensed matter physics (1984)

Renormalization group

1) procedure for finding relations between the effective descriptions of the same physical system on different energy scales

Approaches:

- by integrating out high-energy degrees of freedom by coarse graining
- unitary transformations and truncation



coarse graining

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

RG transformation

2) framework for discussing relations between physical theories

Energy cascading

Scaling

Amplification and deamplification

Relevant operators

Irrelevant operators

Vicinity of a fixed point

Universal behaviour
of different systems

Fixed points, (ir)relevant operators

$$H^* = T[H^*]$$

$$H_N = H^* + \delta H_N$$

$$H_{N+1} = T[H^* + \delta H] = H^* + L[H^*] \cdot \delta H + \mathcal{O}[\delta H_N^2]$$

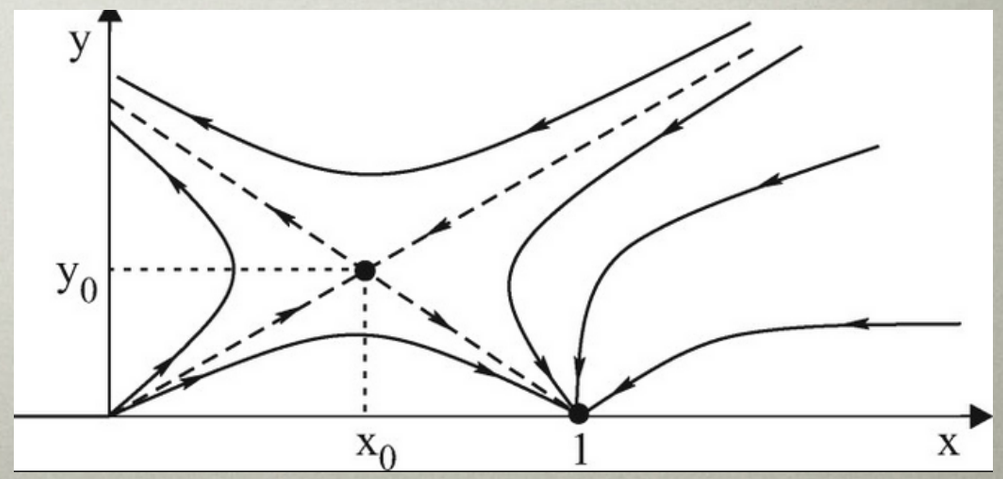
$$L[H^*] \cdot O = \lambda O$$

$$\delta H_N = \sum_m c_m \lambda_m^N O_m$$

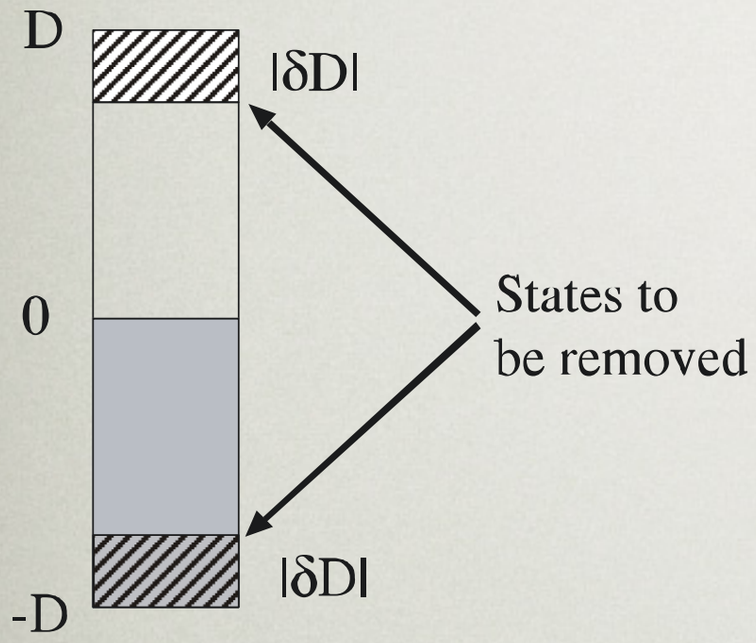
$\lambda > 1$ relevant operator

$\lambda < 1$ irrelevant operator (universality!)

$\lambda = 1$ marginal operator



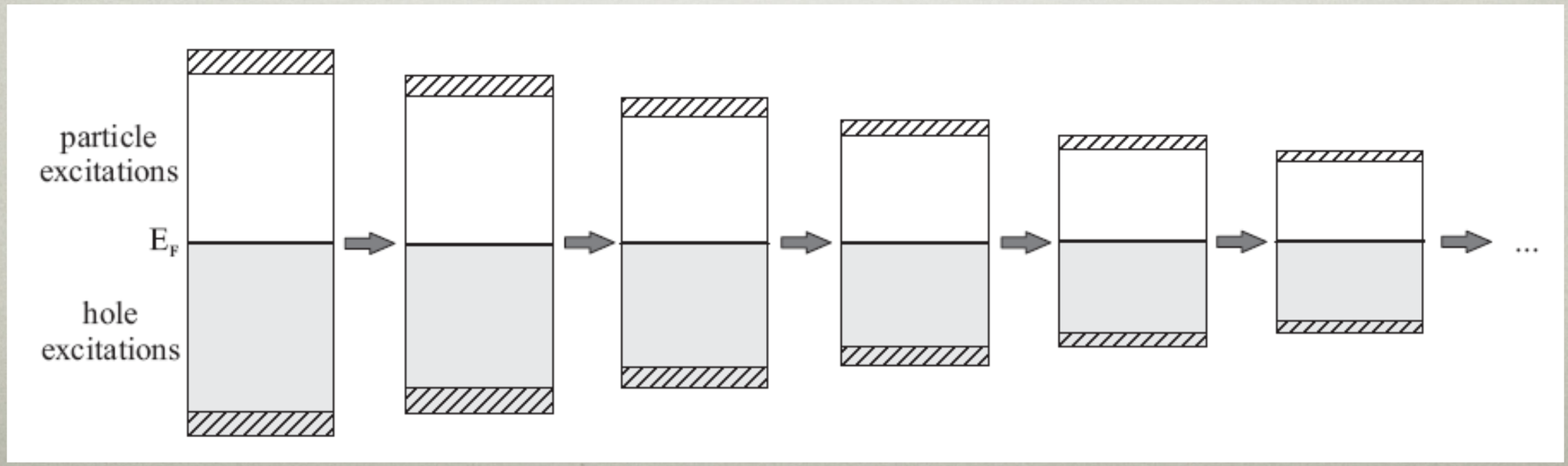
Cutoff renormalization

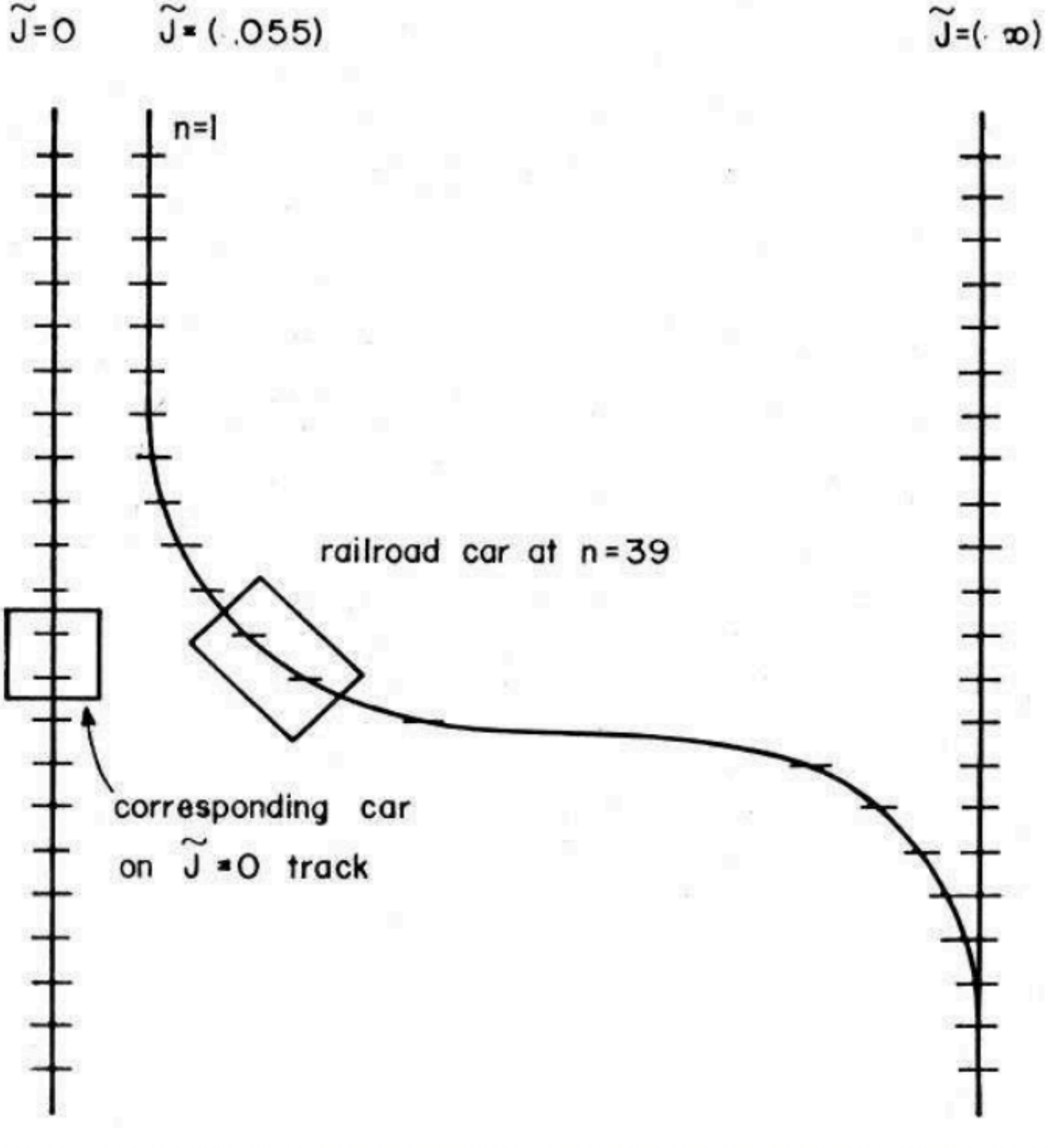


$$\frac{d\mathcal{J}}{d\ln\mathcal{D}} = -\rho\mathcal{J}^2$$

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

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




$\tilde{J}=0$
$\tilde{J}=(.055)$
$\tilde{J}=(\infty)$
n=1
railroad car at n=39
corresponding car
on $\tilde{J}=0$ track

Universality

Kadanoff (1960s)

Stable fixed points define universality classes.

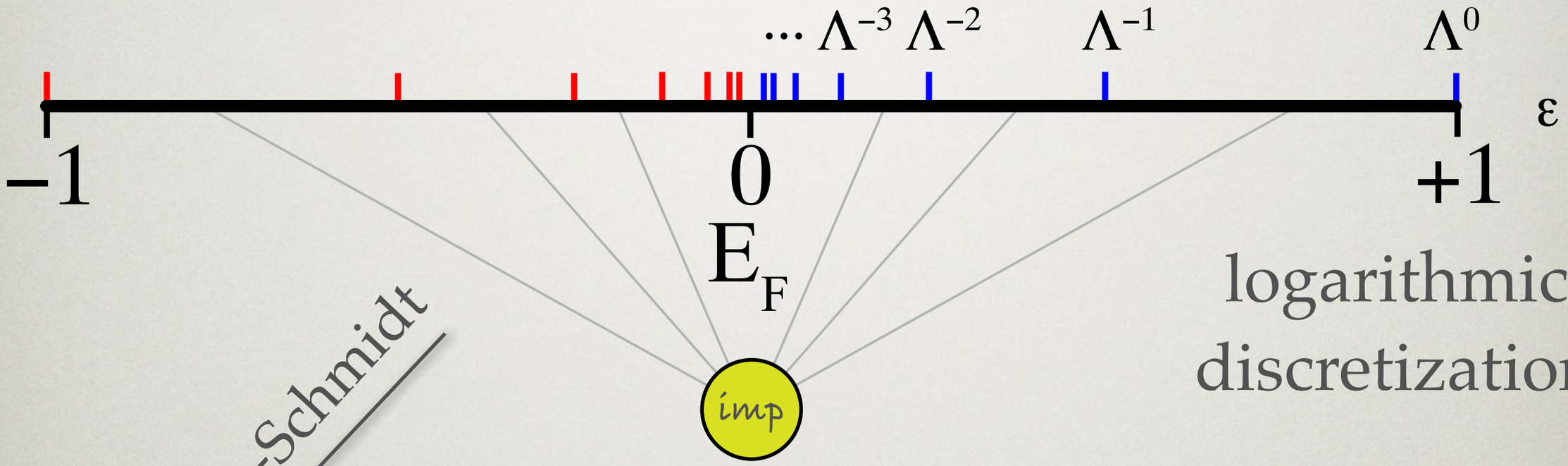
Dictated by dimensionality, degrees of freedom, symmetry.

Usually discrete sets of fixed points for a given family of Hamiltonians, or low-dimensional sets (lines, sheets, etc.) parametrized by coefficients corresponding to "marginal operators".

Part 2: The algorithm

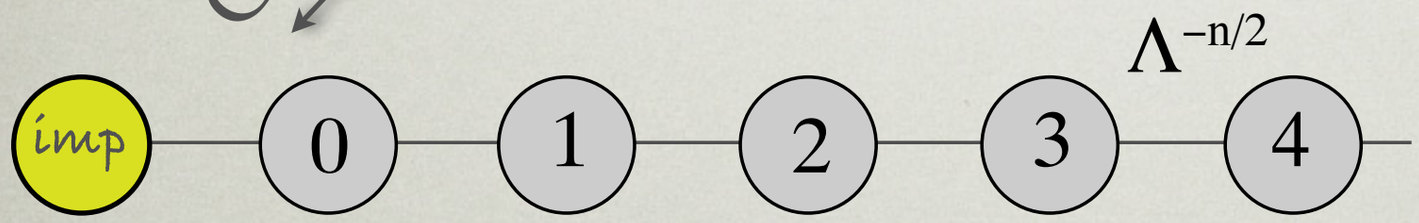
Numerical Renormalization Group

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



logarithmic discretization

$\Lambda > 1$



Wilson's chain

http://nrgljubljana.ijs.si/

NRG

Nondiagrammatic RG transformation which are solved numerically.

- Reduction to a 1D problem
- Logarithmic discretization
- Mapping to a "hopping Hamiltonian"
- Iterative diagonalization of hopping Hamiltonian

Reduction to a 1D model

Because the impurity is point-like, the Hamiltonian maps to a 1D model.

k-space basis:

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + \sum_{\mathbf{k}} \left(V_{\mathbf{k}} c^\dagger_{\mathbf{k}} d + \text{H.c.} \right) + H_{\text{imp}}$$

Lanczos algorithm

chain basis:

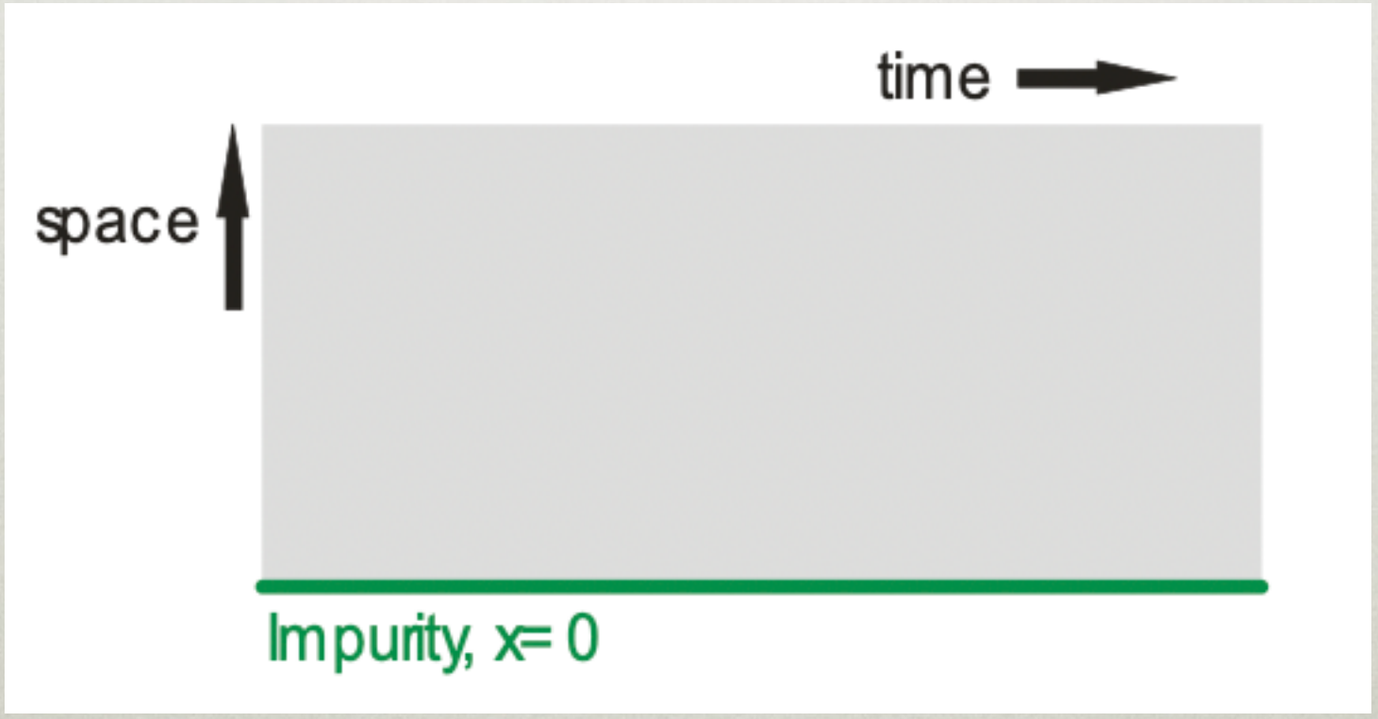
$$H = V(f_0^\dagger d + \text{H.c.}) + \sum_{n \geq 0} \left[\epsilon_n f_n^\dagger f_n + t_n \left(f_n^\dagger f_{n+1} + \text{H.c.} \right) \right] + H_{\text{imp}}$$

noninteracting 1D chain with interacting impurity attached to the edge

starting point for conformal field theory (CFT) approach

BOUNDARY CONFORMAL FIELD THEORY

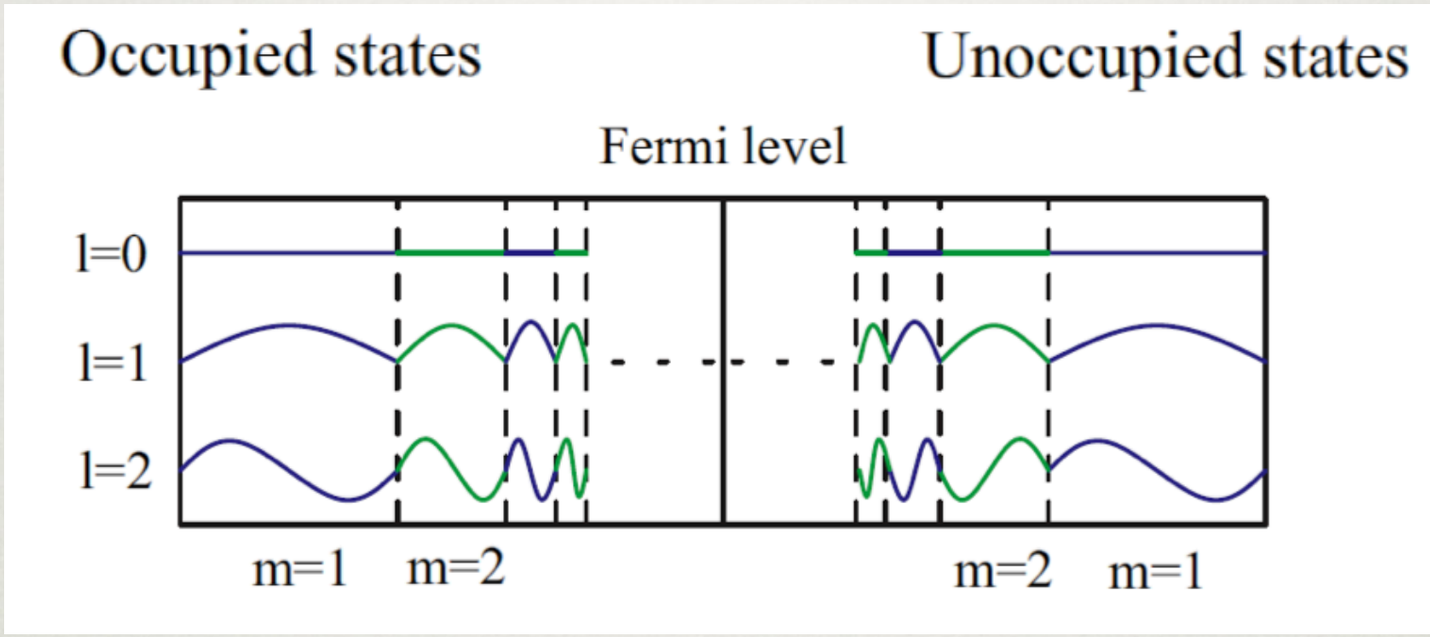
Kondo model = 1D relativistic quantum field theory with massless particles
→ conformal symmetry
Interpretation of the Kondo effect as fusion of impurity degrees of freedom by the continuum

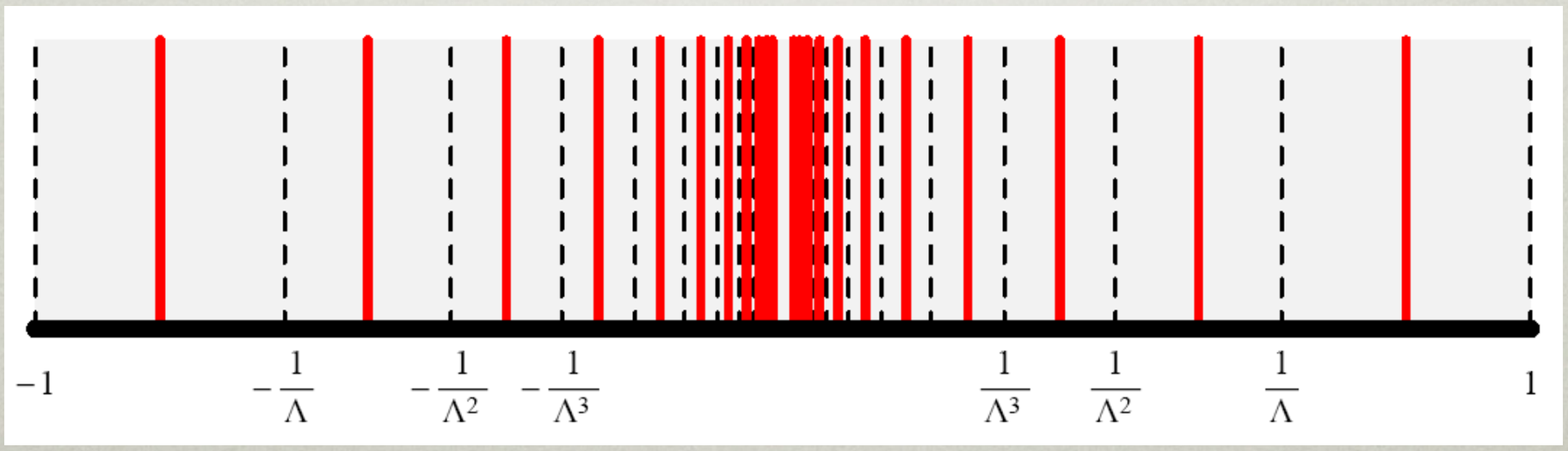


I. Affleck, Nucl. Phys. B (1990)

METHOD

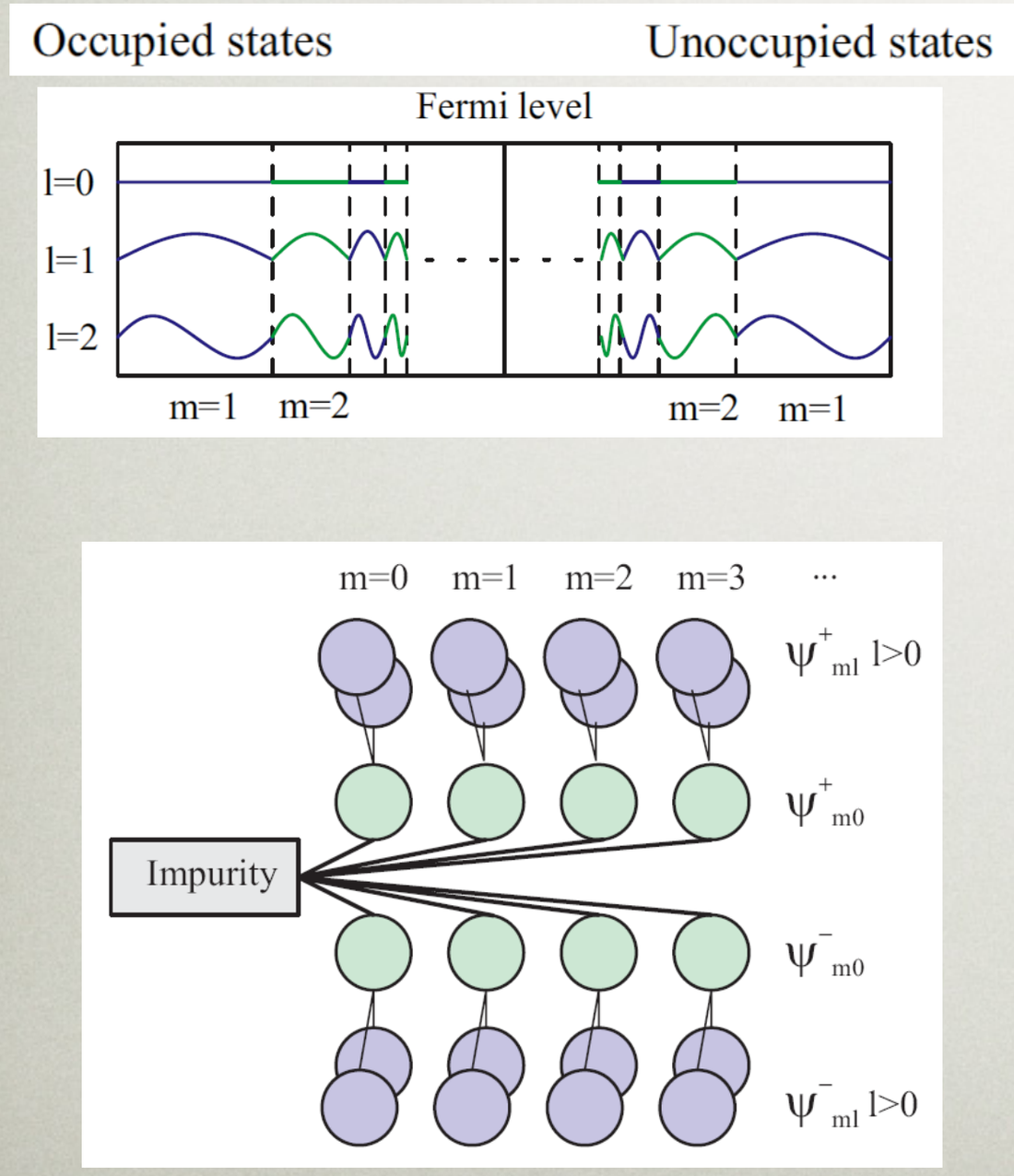
Logarithmic discretization





good sampling of the states near the Fermi energy

REPRESENTATIVE STATES

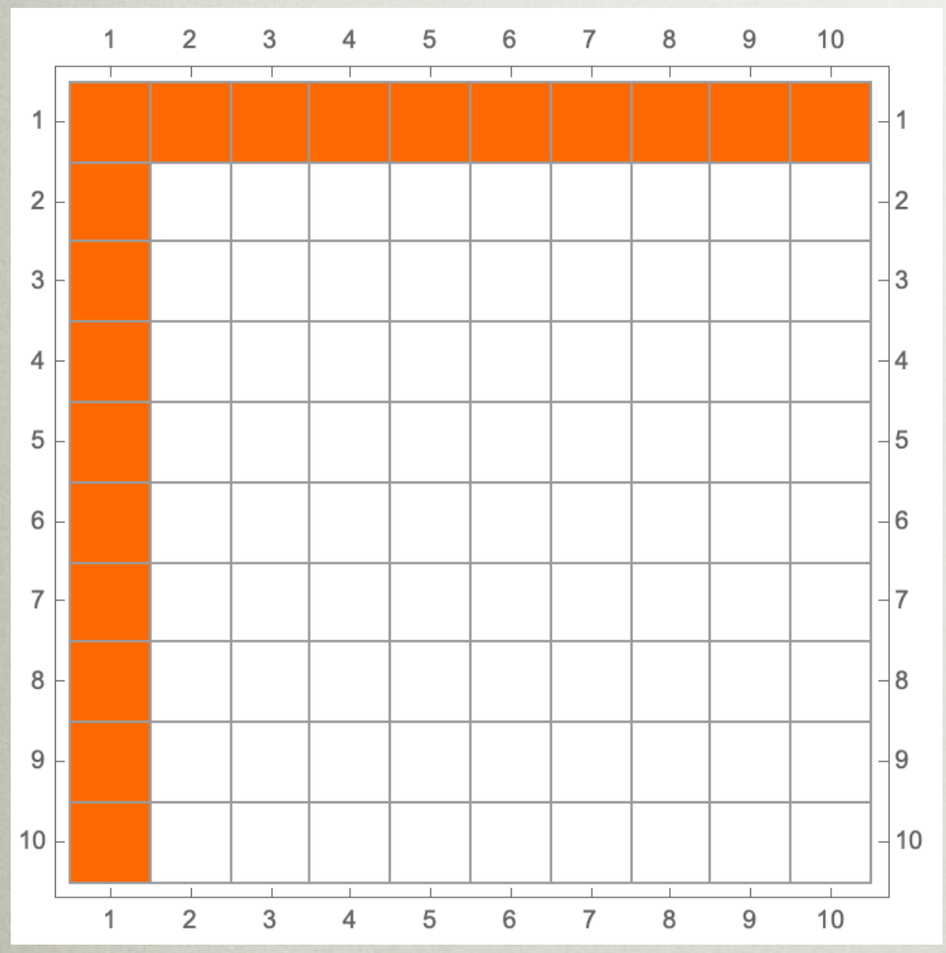


We keep only l=0.

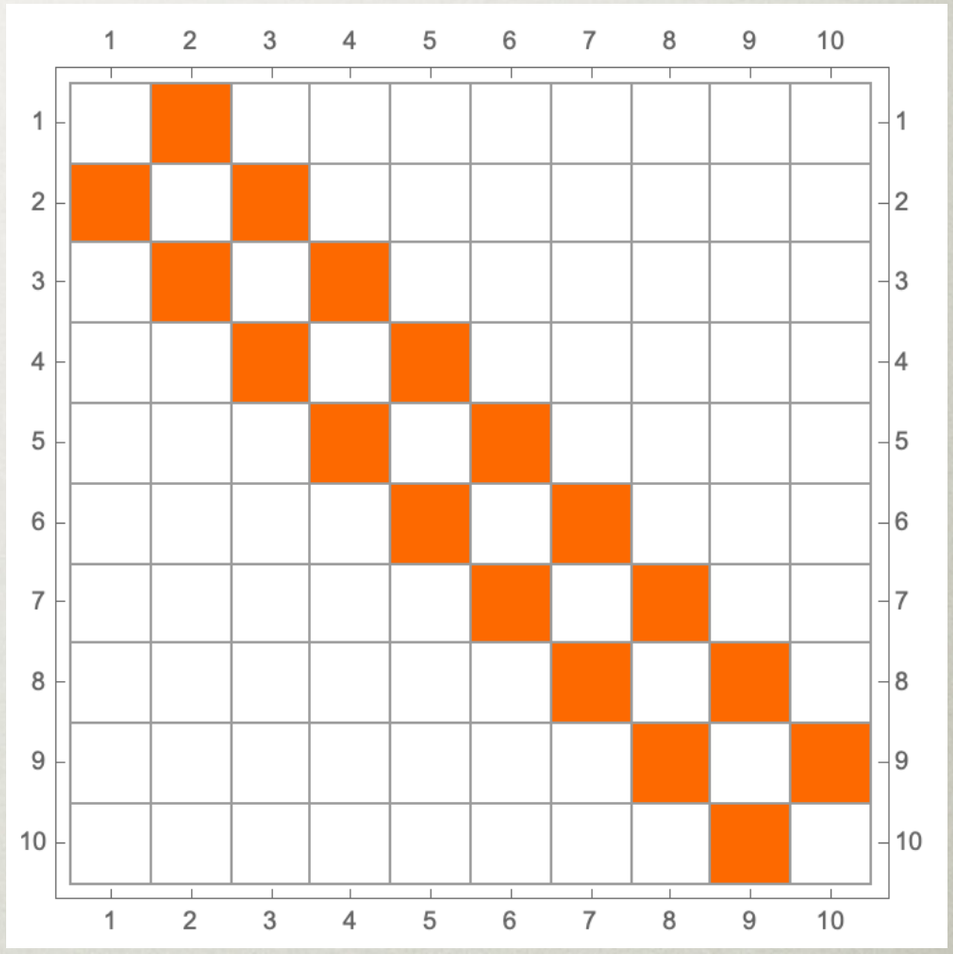
These are the “representative states”

TRIDIAGONALISATION

Another application of the Lanczos (Gram-Schmidt) procedure.



star
representation

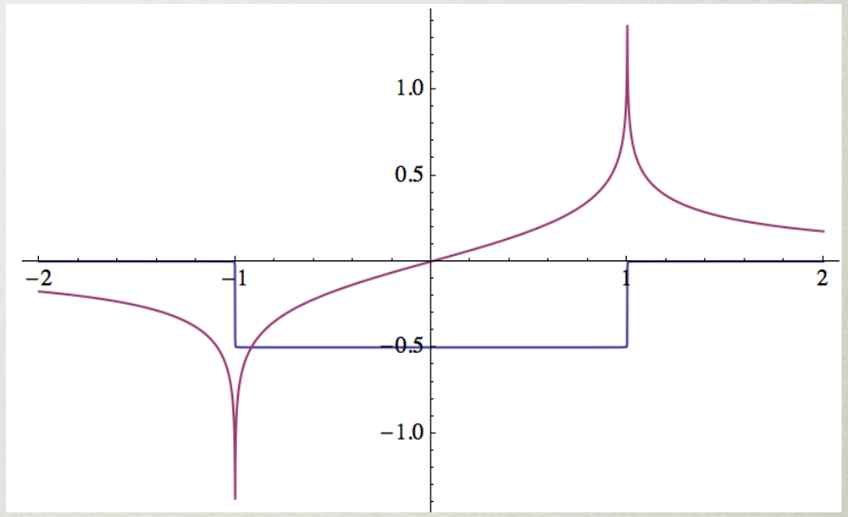


chain
representation

Exact results for flat band

$$\rho(\epsilon) = \frac{1}{2D} \quad \text{for} \quad -D < \epsilon < D$$

$$\Delta(z) = \frac{\Gamma}{2\pi} \ln \frac{z+1}{z-1}$$



$$\Gamma(\epsilon) = \pi\rho(\epsilon)V^2 = \mathrm{Im}\Delta(\epsilon + i0^+)$$

$$t_i = D\frac{(1+\Lambda^{-1})(1-\Lambda^{-i-1})}{2\sqrt{1-\Lambda^{-2i-1}}\sqrt{1-\Lambda^{-2i-3}}}\Lambda^{-i/2}$$

$$A_\Lambda = \frac{\ln\Lambda}{2}\frac{1+\Lambda^{-1}}{1-\Lambda^{-1}}$$

Good exercise in Legendre polynomials and Bonnet recursion formula!

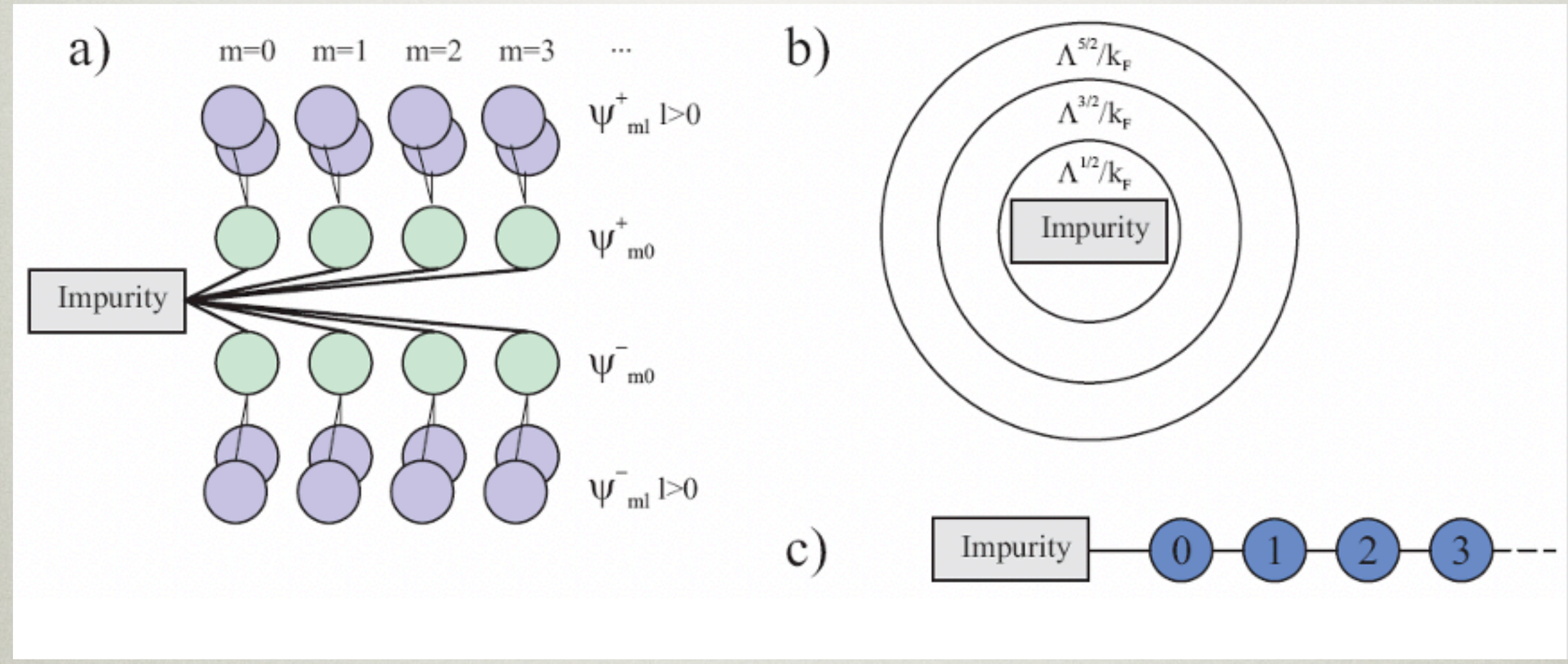
Zero-th site of the Wilson chain

$$f^\dagger_{0\mu} = \frac{1}{\sqrt{N_c}} \sum_k c^\dagger_{k\mu}$$

This is the conduction-band orbital at the position of the impurity.

More generally:

$$V f^\dagger_{0\mu} = \frac{1}{\sqrt{N_c}} \sum_k V_k c^\dagger_{k\mu} \qquad |V|^2 = \frac{1}{N_c} \sum_k |V_k|^2$$

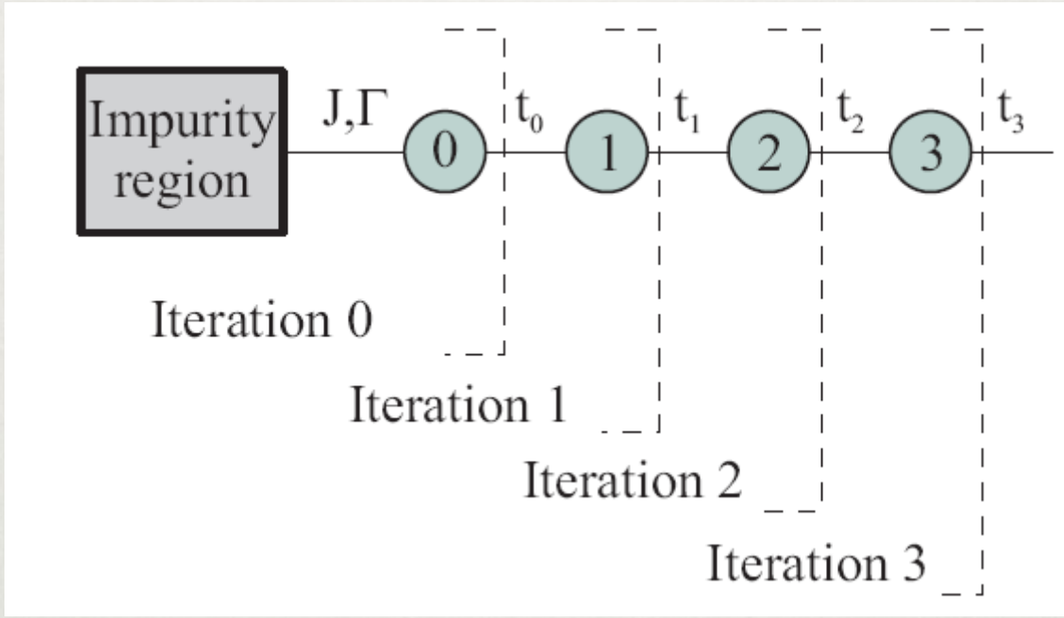

a)
m=0
m=1
m=2
m=3
...
ψ^{+}_{ml} l>0
ψ^{+}_{m0}
Impurity
ψ^{-}_{m0}
ψ^{-}_{ml} l>0
b)
$\Lambda^{5/2}/k_F$
$\Lambda^{3/2}/k_F$
$\Lambda^{1/2}/k_F$
Impurity
c)
Impurity
0
1
2
3

Initial Hamiltonian

$$H_0 = H_{\text{imp}} + \sum_\sigma \epsilon_0 f_{0\sigma}^\dagger f_{0\sigma} + \sqrt{\frac{\xi_0}{\pi}} \sum_\sigma \left(d_\sigma^\dagger f_{0\sigma} + f_{0\sigma}^\dagger d_\sigma \right)$$

$$H_0 |r\rangle_0 = E_0(r) |r\rangle_0$$

Iterative diagonalization



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

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

Basis construction

$$|Q,S_z,r;1\rangle_{N+1} = |Q+1,S_z,r\rangle_N,$$

$$|Q,S_z,r;2\rangle_{N+1} = c^\dagger_{N+1\uparrow}\left|Q,S_z-\frac{1}{2},r\right\rangle_N,$$

$$|Q,S_z,r;3\rangle_{N+1} = c^\dagger_{N+1\downarrow}\left|Q,S_z+\frac{1}{2},r\right\rangle_N,$$

$$|Q,S_z,r;4\rangle_{N+1} = c^\dagger_{N+1\uparrow}c^\dagger_{N+1\downarrow}|Q-1,S_z,r\rangle_N.$$

Symmetries

$\mathrm{SU}(2)_{\mathrm{spin}}$

$$\mathbf{S} = \sum_{\mu\mu'} d^\dagger_\mu \left(\frac{1}{2} \boldsymbol{\sigma}_{\mu\mu'} \right) d_{\mu'}$$

$$\boldsymbol{\sigma} = \{\sigma^x, \sigma^y, \sigma^z\}$$

$$S^z = \frac{1}{2}\left(d^\dagger_\uparrow d_\uparrow - d^\dagger_\downarrow d_\downarrow \right)$$

$$S^+ = S^x + iS^y = d^\dagger_\uparrow d_\downarrow$$

$$S^- = S^x - iS^y = d^\dagger_\downarrow d_\uparrow$$

Total spin: $\mathbf{S}_{\mathrm{total}} = \sum_i \mathbf{S}_i$

Basis construction

$$|r;s\rangle_{N+1} = |r\rangle_N \otimes |s(N+1)\rangle$$

$(\mathbf{q},\mathbf{s})$	States $(\mathbf{k})$
$(-1,0)$	1
$(0,\frac{1}{2})$	$a^\dagger_\uparrow$
$(1,0)$	$a^\dagger_\downarrow a^\dagger_\uparrow$

(a) One channel

$(\mathbf{q},\mathbf{s})$	States $(\mathbf{k})$
$(-2,0)$	1
$(-1,\frac{1}{2})$	$b^\dagger_\uparrow,\ a^\dagger_\uparrow$
$(0,0)$	$b^\dagger_\downarrow b^\dagger_\uparrow,\ \frac{1}{\sqrt{2}}\left(a^\dagger_\downarrow b^\dagger_\uparrow - a^\dagger_\uparrow b^\dagger_\downarrow\right),\ a^\dagger_\downarrow a^\dagger_\uparrow$
$(0,1)$	$b^\dagger_\uparrow a^\dagger_\uparrow$
$(1,\frac{1}{2})$	$a^\dagger_\uparrow b^\dagger_\downarrow b^\dagger_\uparrow,\ b^\dagger_\uparrow a^\dagger_\downarrow a^\dagger_\uparrow$
$(2,0)$	$a^\dagger_\uparrow a^\dagger_\downarrow b^\dagger_\uparrow b^\dagger_\downarrow$

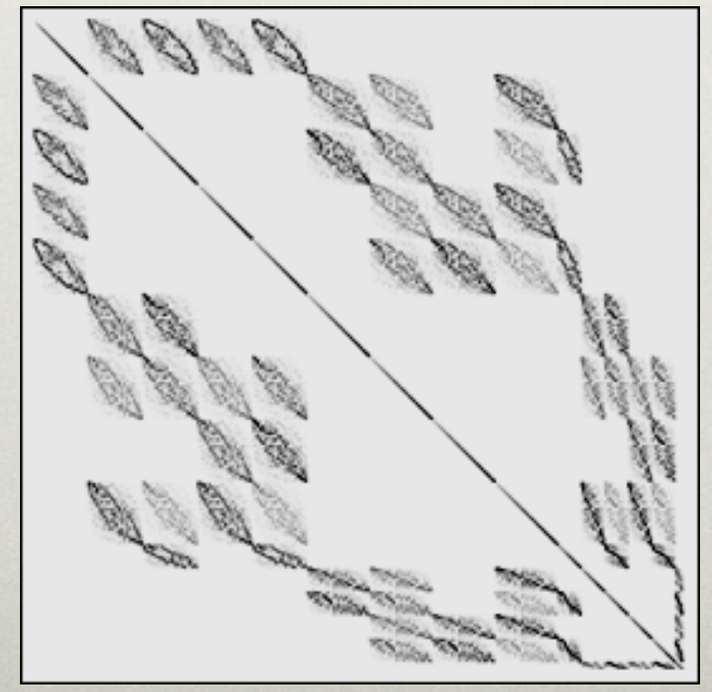
(b) Two channels

$$|QSS_z ri\rangle_{N+1} = \sum_{\mu=-S(i)}^{S(i)} \left\langle g_i^\mu(SS_z);S(i),\mu|SS_z\right\rangle \ |F_i(QS)f_i^\mu(S_z)r\rangle_N \otimes |i,\mu\rangle$$

Hamiltonian matrix generation

$$H_{N+1}(rs, r's') = {}_{N+1}\langle r; s|H_{N+1}|r'; s'\rangle_{N+1}$$

$$H_{N+1} = \sqrt{\Lambda} H_N + X_{N,N+1} + Y_{N+1}$$



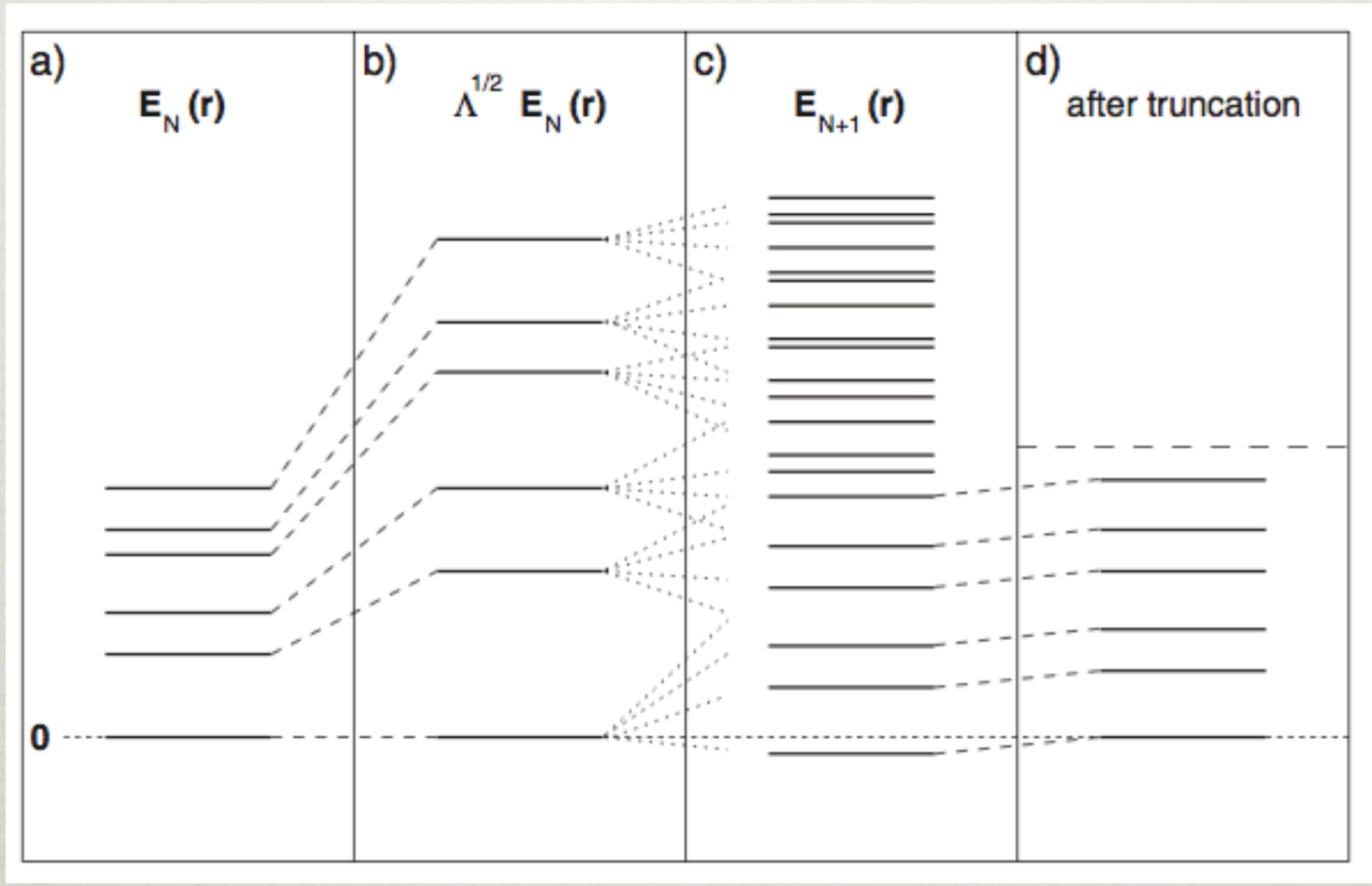
Matrix diagonalisation

- Full diagonalisation with `dsyev/zheev`
- Partial diagonalisations with `dsyevr/zheevr`

Largest amount of the processor time spent here!

$$|QS\omega\rangle = \sum_{ri} U_{QS}(\omega, ri)|QSri\rangle$$

Truncation

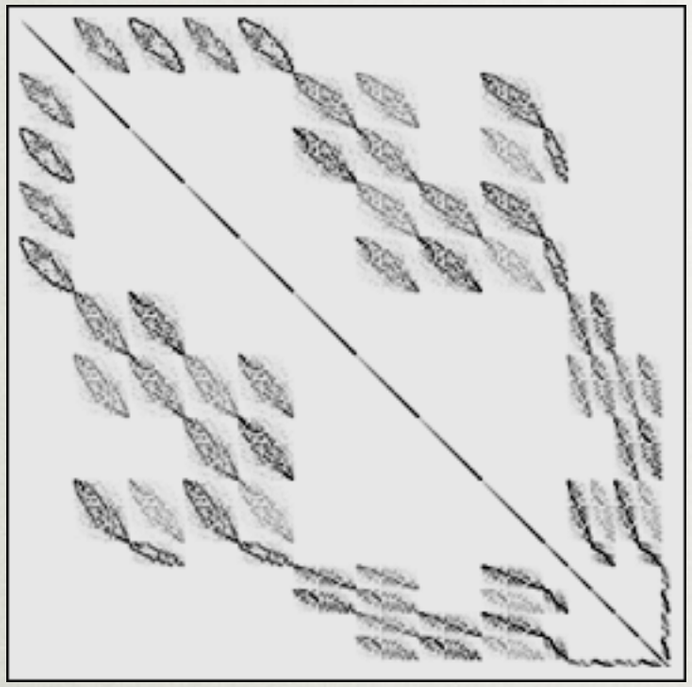


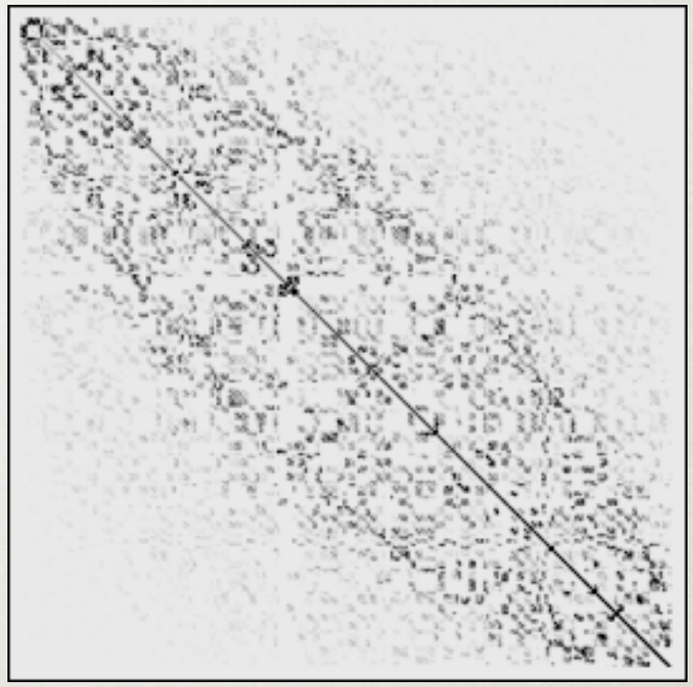
rescaling

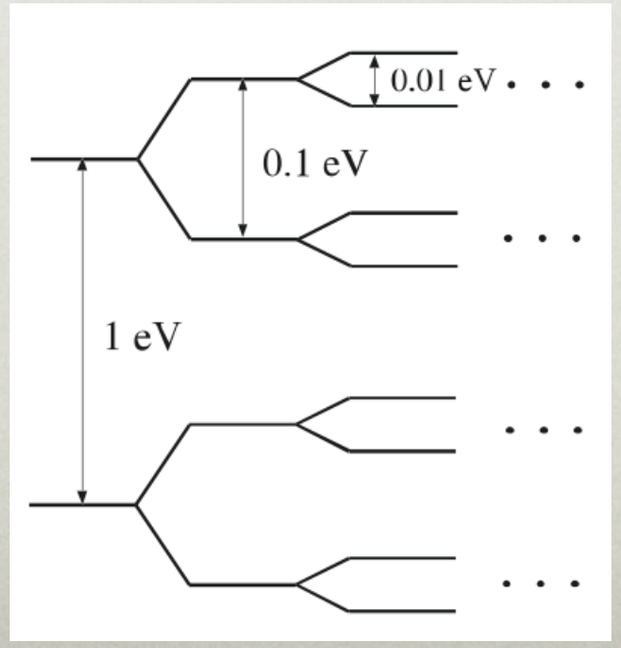
Characteristic energy scale

$$T_N \propto \frac{D}{k_B} \Lambda^{-N/2} / \bar{\beta} \qquad \bar{\beta} \sim 1$$

Energy-scale separation

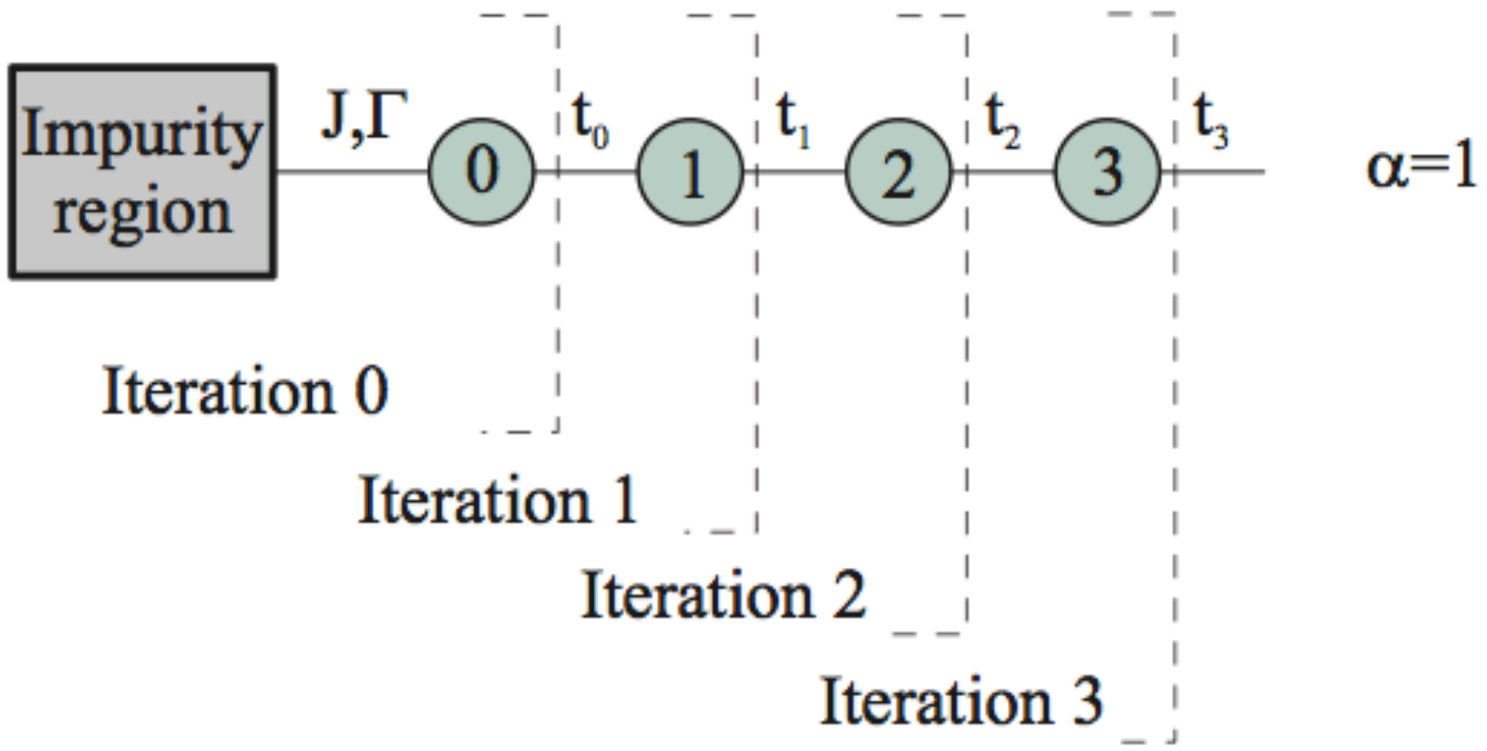




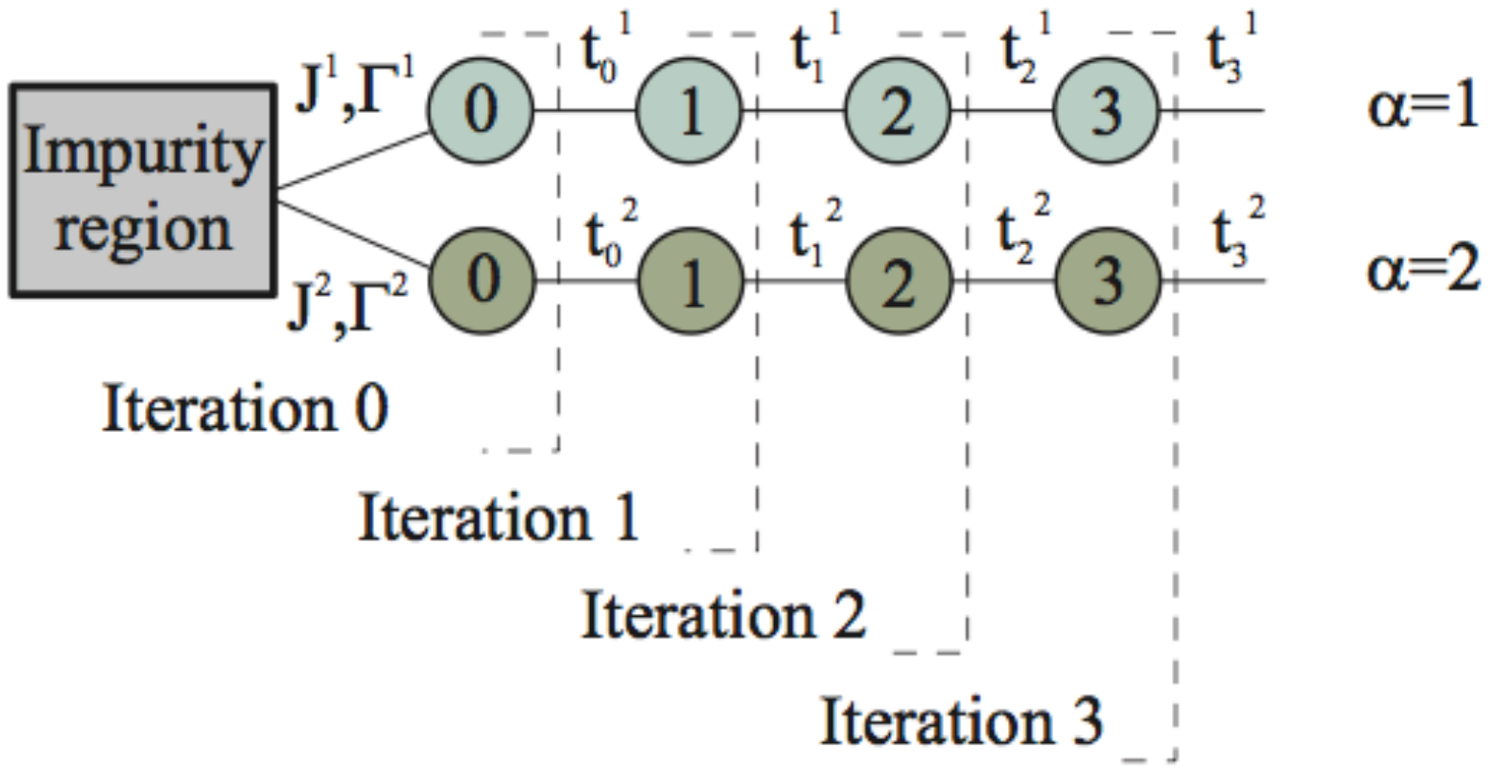


Energy scales are **locally** coupled

a) One-channel case



b) Two-channel case



•Number of states:

– 4^N (single-channel – impurity couples to a single continuum of conduction band states)

–16^N (two-channel – two different continuums)

•We only keep states up to some cut-off energy, or some finite number of states (few 1000): good approximation!

Recalculation of operators

$$|w\rangle_{N+1} = \sum_{rs} U(w, rs)|r; s\rangle_{N+1}$$

$$\langle w|O|w'\rangle_{N+1} = \sum_{rs,r's'} U^*(w, rs)U(w', rs')\langle rs|O|r's'\rangle_{N+1}$$

$$= \sum_{s} \sum_{rr'} U^*(w, rs)O^{(N)}_{rr'}U(w', r's)$$

Wigner-Eckart theorem

O is a **spherical tensor operator** of rank M if:

$$\begin{aligned}\left[J_z, O_\mu^M\right] &= \mu O_\mu^M \\ \left[J_+, O_\mu^M\right] &= A(M,\mu) O_{\mu+1}^M \\ \left[J_-, O_\mu^M\right] &= A(M,-\mu) O_{\mu-1}^M\end{aligned}$$

$$A(M,\mu) = \sqrt{(M-\mu)(M+\mu+1)}$$

$$\langle \alpha, j, j_z | O_\mu^M | \alpha', j', j_z' \rangle = \left\langle j' j_z'; M\mu | j j_z \right\rangle \langle \alpha, j \| O^M \| \alpha', j' \rangle$$

For a more general treatment of non-Abelian symmetries in NRG, see
A. I. Toth, C. P. Moca, O. Legeza, G. Zarand, PRB 78, 245109 (2008),
A. Weichselbaum, Annals of Physics 327, 2972-3047 (2012).

Recalculation of operators

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$$= \sum_{s} \sum_{rr'} U^*(w, rs)O^{(N)}_{rr'}U(w', r's)$$

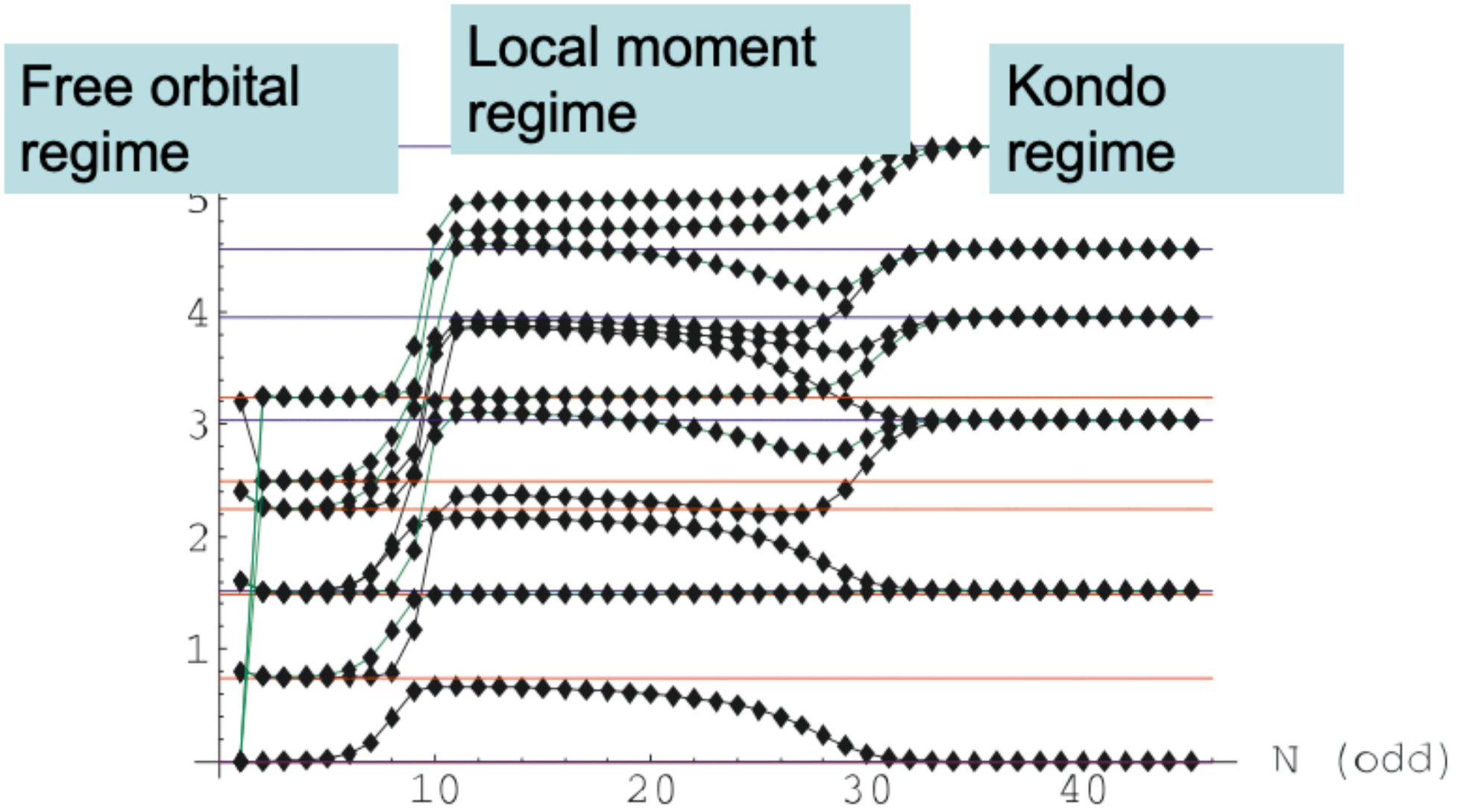
With symmetries:

$$\langle QS\omega\|\hat{O}\|Q'S'\omega'\rangle_{N+1} = \frac{\langle QSS_z\omega|\hat{O}_\mu|Q'S'S'_z\omega'\rangle_{N+1}}{\langle S'S'_z; M\mu|SS_z\rangle}$$

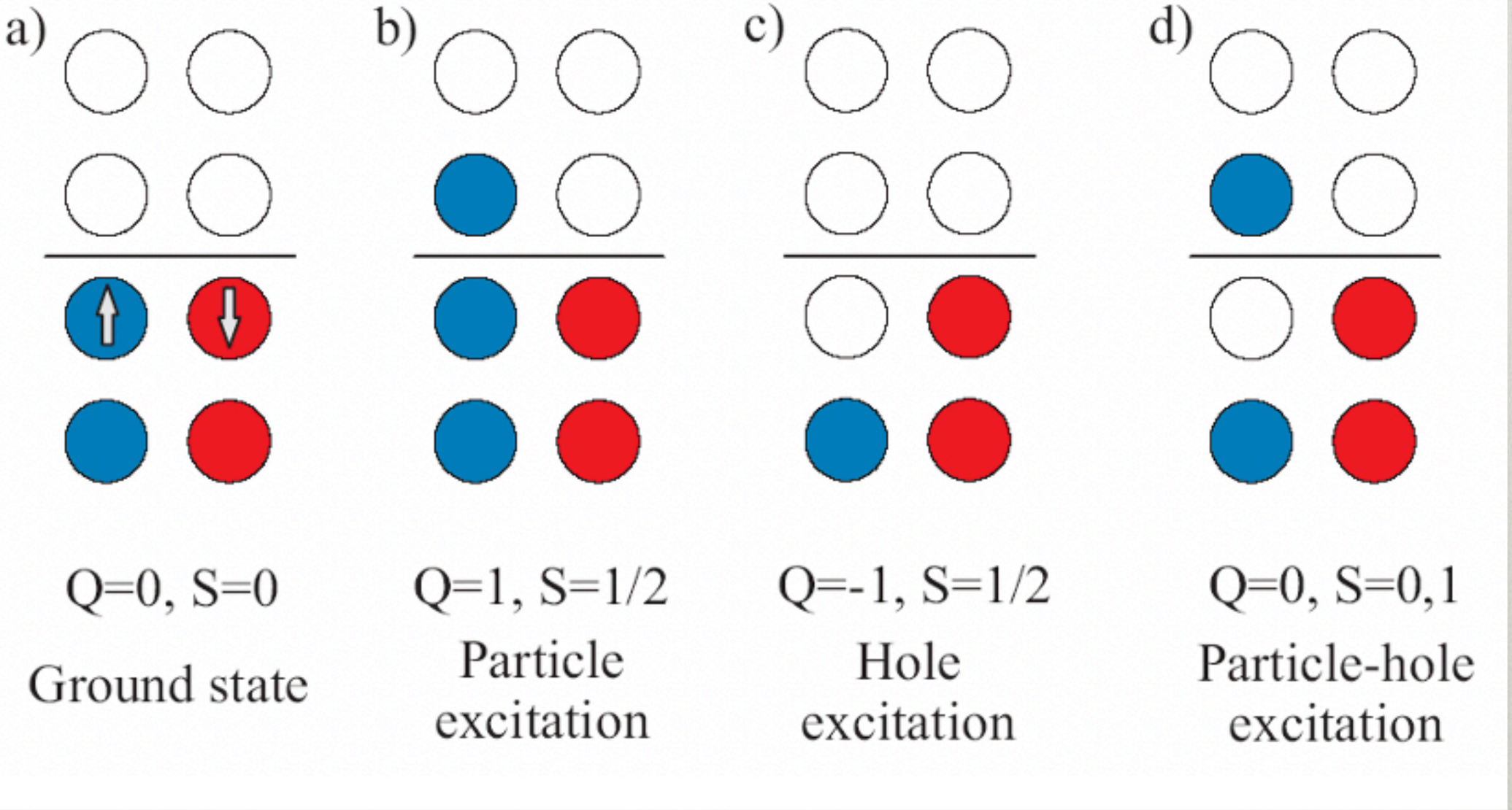
$$\langle QS\omega\|\hat{O}\|Q'S'\omega'\rangle_{N+1} = \sum_{ii'} C(QS, Q'S', ii') \sum_{rr'} U_{QS}(\omega, ri)U_{Q'S'}(\omega', r'i')\langle F_i(QS)r\|\hat{O}\|F_{i'}(Q'S')r'\rangle_N$$

Part 3: analysis of results

Example: RG flow for the Anderson model



Renormalization flow of excitation energies.


a)
b)
c)
d)
Q=0, S=0
Ground state
Q=1, S=1/2
Particle excitation
Q=-1, S=1/2
Hole excitation
Q=0, S=0,1
Particle-hole excitation

Ground state and excited states

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

thermodynamics:

$$Z = \mathrm{Tr}\left[e^{-\beta H}\right] = \sum_n e^{-\beta E_n} \qquad \beta = \frac{1}{k_B T}$$

dynamics:

$$x(t) = \int_{-\infty}^{t} \chi(t-t')\, h(t')\, \mathrm{d}t$$

$$\chi(t-t') = -i\langle [A(t), B(t')] \rangle$$

Kubo formalism, linear response

Green's functions - review

$$G_{AB}(t) = \langle\langle A; B\rangle\rangle_t := -i\theta(t)\langle[A(t), B(0)]_\pm\rangle$$

+ if A and B are fermionic operators
- if A and B are bosonic operators

canonical:

$$\langle\hat{O}\rangle = \mathrm{Tr}\left[\rho\hat{O}\right] \qquad \rho = \frac{e^{-\beta H}}{Z}$$

$$Z = \mathrm{Tr}[e^{-\beta H}]$$

grand canonical:

$$\rho = \frac{e^{-\beta K}}{\mathcal{Z}}$$

$$\mathcal{Z} = \mathrm{Tr}[e^{-\beta K}]$$

$$K = H - \mu N$$

Heisenberg representation: $A(t) = e^{iHt}Ae^{-iHt}$ $\qquad A(t) = e^{iKt}Ae^{-iKt}$

Green's function in frequency domain

Laplace transformation:

$$G_{AB}(z) = \langle\langle A; B\rangle\rangle_z = \int_0^\infty \mathrm{d}t e^{izt} \langle\langle A; B\rangle\rangle_t, \quad \Im z > 0$$

Inverse Laplace transformation:

$$G_{AB}(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}\omega e^{-i(\omega+i\delta)t} G_{AB}(\omega + i\delta)$$

Impurity Green's function (for SIAM):

$$G(z) = \langle\langle d; d^\dagger \rangle\rangle_z$$

Spectral decomposition

Correlation functions: $C^{>}_{AB} = \langle A(t)B \rangle \qquad C^{<}_{AB} = \langle BA(t) \rangle$

$$C^{>,<}_{AB}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} C^{>,<}_{AB}(t)$$

$$G_{AB}(t) = -i\theta(t)(C^{>}_{AB}(t) + \epsilon C^{<}_{AB}(t))$$

ε=+1 if A and B are fermionic, otherwise ε=-1.

Spectral representation: $G_{AB}(z) = \int_{-\infty}^{\infty} \mathrm{d}\omega \frac{\rho_{AB}(\omega)}{z - \omega}$

Spectral function: $\rho_{AB}(\omega) = \frac{1}{2\pi} \left(C^{>}_{AB}(\omega) + \varepsilon C^{<}_{AB}(\omega) \right)$

Lehmann representation

$$p_n = e^{-\beta E_n}$$

$$C^{>}_{AB}(t) = \langle e^{iHt} A e^{-iHt} B \rangle = \sum_{nm} p_n A_{nm} B_{mn} e^{i(E_n - E_m)t}$$

$$C^{>}_{AB}(\omega) = \sum_{nm} p_n A_{nm} B_{mn} 2\pi\delta(\omega + E_n - E_m)$$

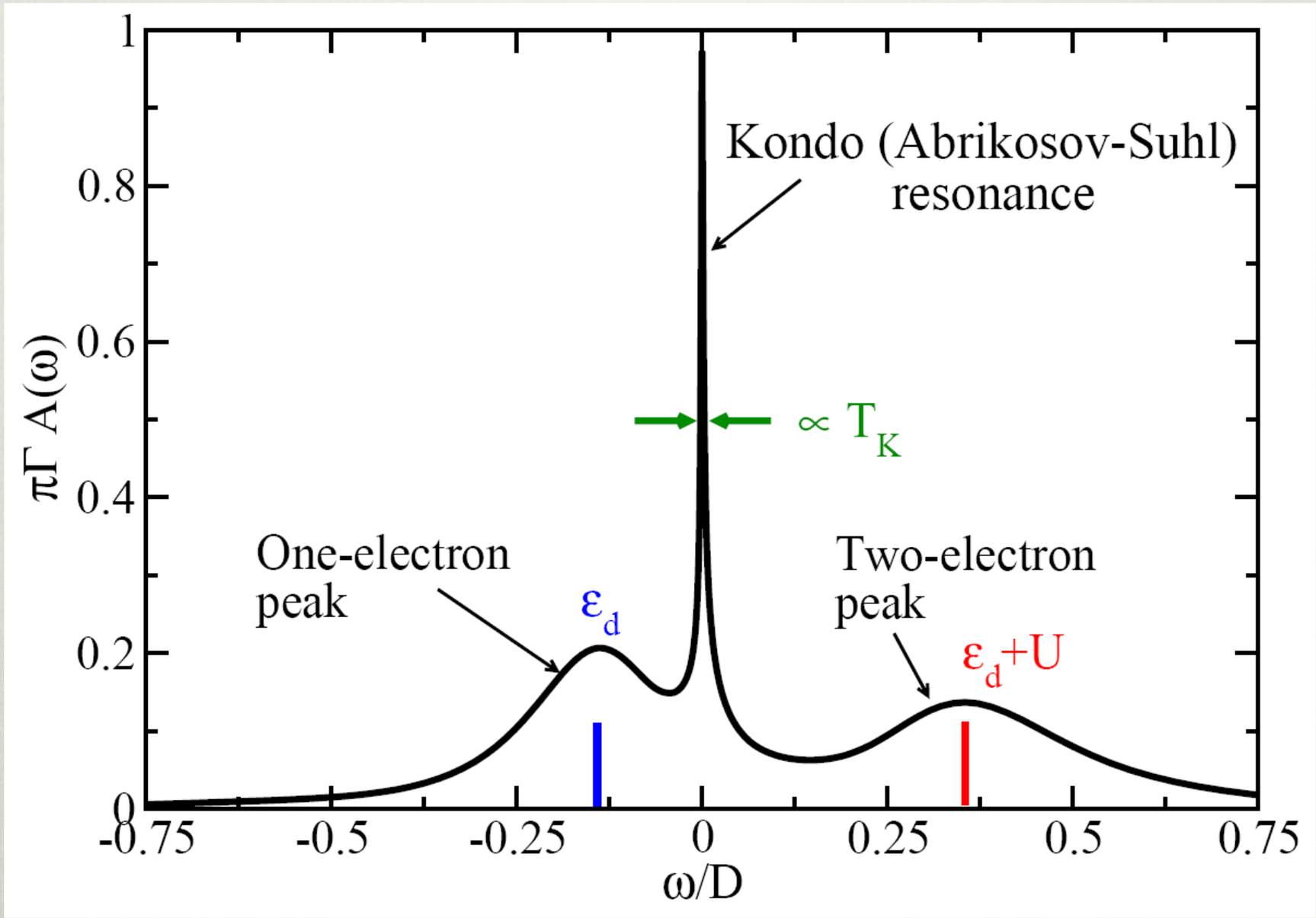
$$C^{<}_{AB}(\omega) = \sum_{nm} p_m A_{nm} B_{mn} 2\pi\delta(\omega + E_n - E_m)$$

$$G''_{AB}(\omega) = -\pi \sum_{nm} p_n A_{nm} B_{mn} \delta(\omega + E_n - E_m)\left(1 + \epsilon e^{-\beta\omega}\right)$$

$$\rho_{AB}(\omega) = -\frac{1}{\pi} G''_{AB}(\omega)$$

Lehmann representation for impurity spectral function

$$A(\omega) = \sum_{nm} \left| \langle m | d^\dagger | n \rangle \right|^2 \delta(\omega - E_m - E_n) \frac{e^{-\beta E_m} + e^{-\beta E_n}}{Z}$$



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

Anatomy of impurity Green's function

$$G(z) = \frac{1}{z - \epsilon - \Delta(z) - \Sigma(z)}$$

hybridisation function

self-energy function

Hybridisation function

$$\Delta(z) = \sum_k |V_k|^2 \frac{1}{z - \epsilon_k}$$

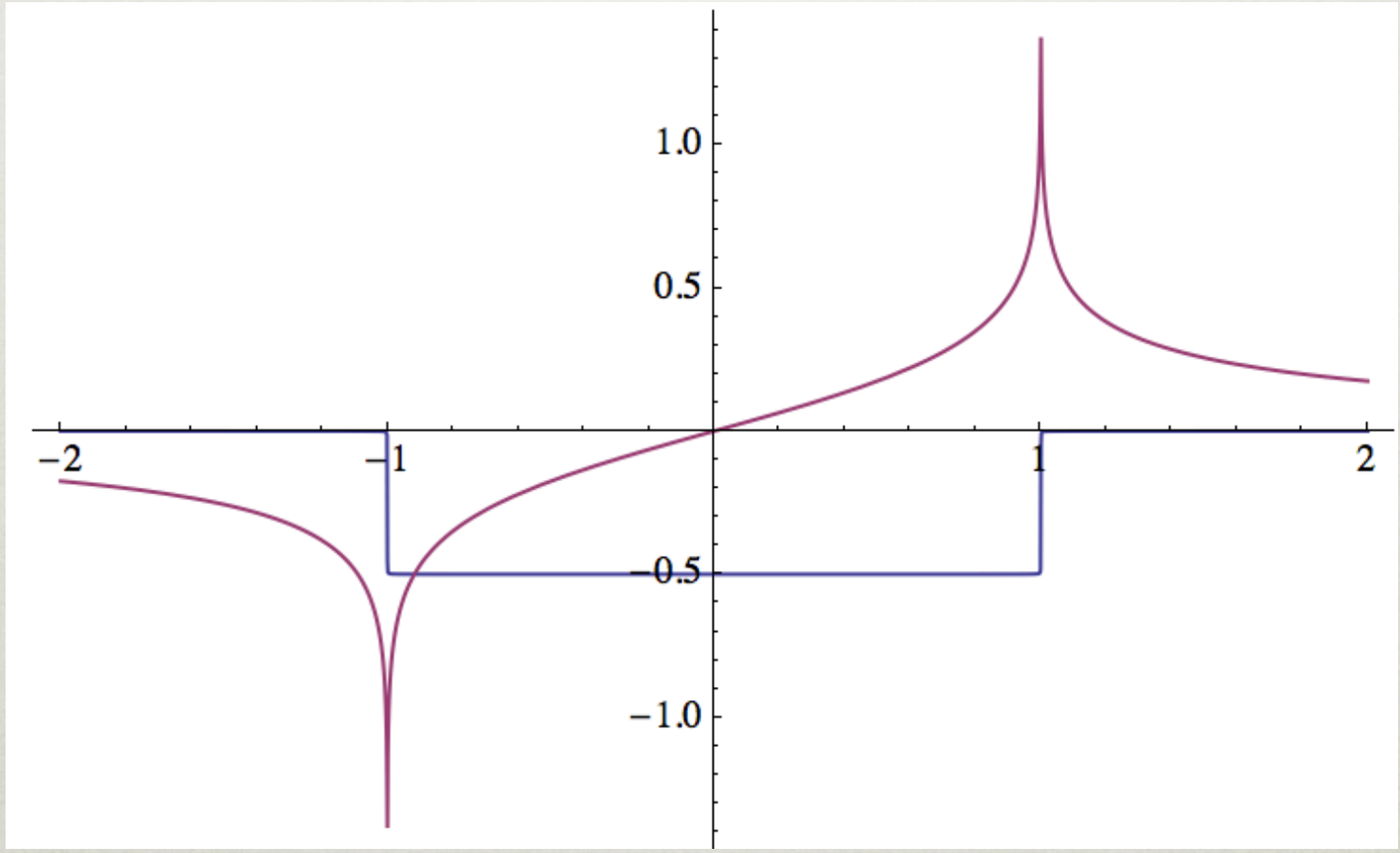
$$\Gamma(\omega) = -\mathrm{Im}\,\Delta(z + i0^+)$$

$$\Gamma(\omega) = \pi \sum_k |V_k|^2 \delta(\omega - \epsilon_k) \approx \pi \rho_0 |V_{k_F}|^2$$

Hybridization function fully describes the effect of the conduction band on the impurity.
This is possible because the band is non-interacting.

HYBRIDISATION FUNCTION FOR FLAT BAND

$$\Delta(z) = \frac{\Gamma}{2\pi} \ln \frac{z+1}{z-1}$$



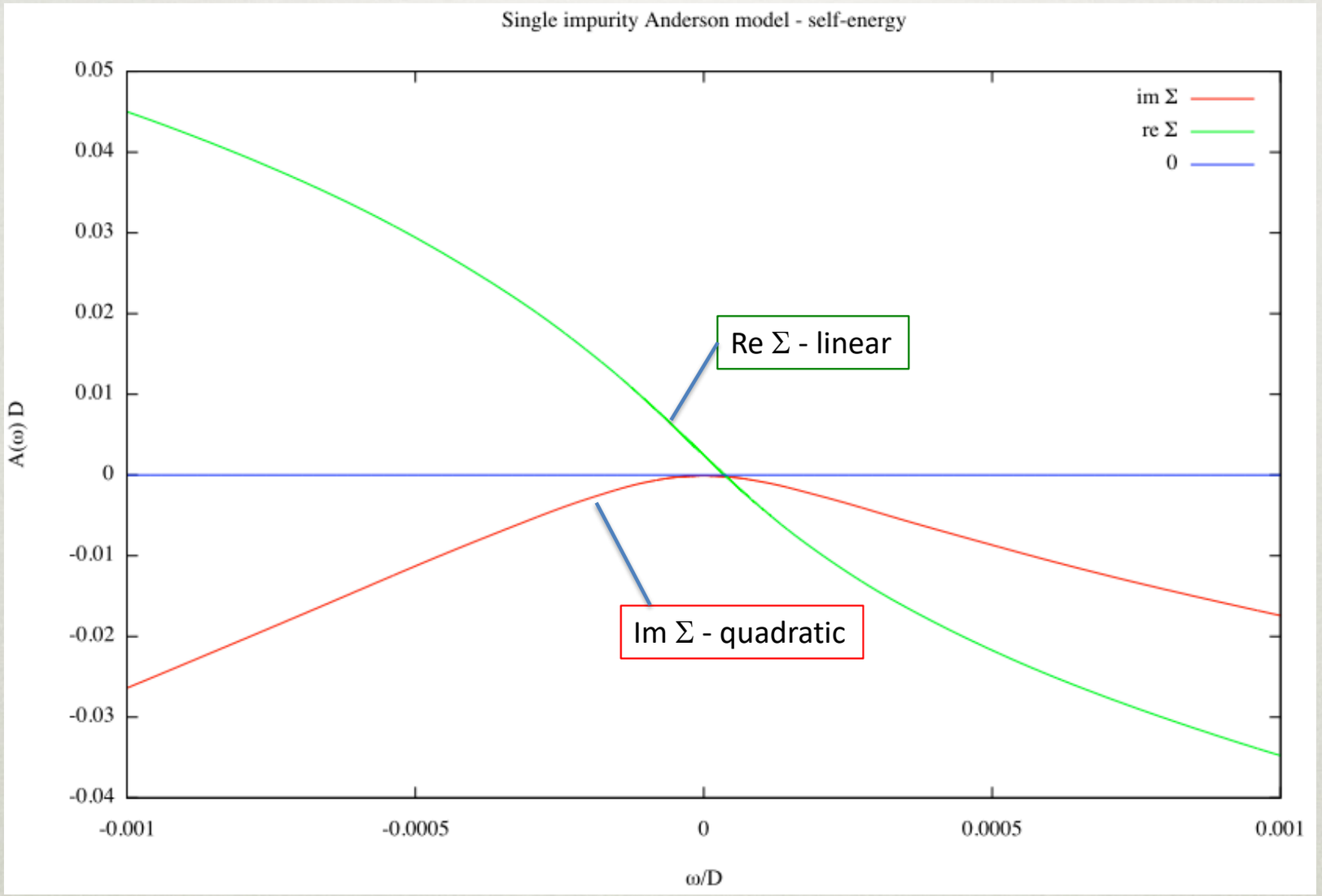
Self-energy

$$\Sigma(\omega) = \frac{\langle\langle [d, H_{\mathrm{imp}}]; d^\dagger \rangle\rangle}{\langle\langle d; d^\dagger \rangle\rangle}$$

SIAM: $$\Sigma_\sigma(\omega) = \frac{\langle\langle U n_{\bar{\sigma}} d_\sigma; d_\sigma^\dagger \rangle\rangle}{\langle\langle d_\sigma; d_\sigma^\dagger \rangle\rangle}$$

Self-energy function describes the effect of the local interaction on the impurity at the level of single-particle excitations.

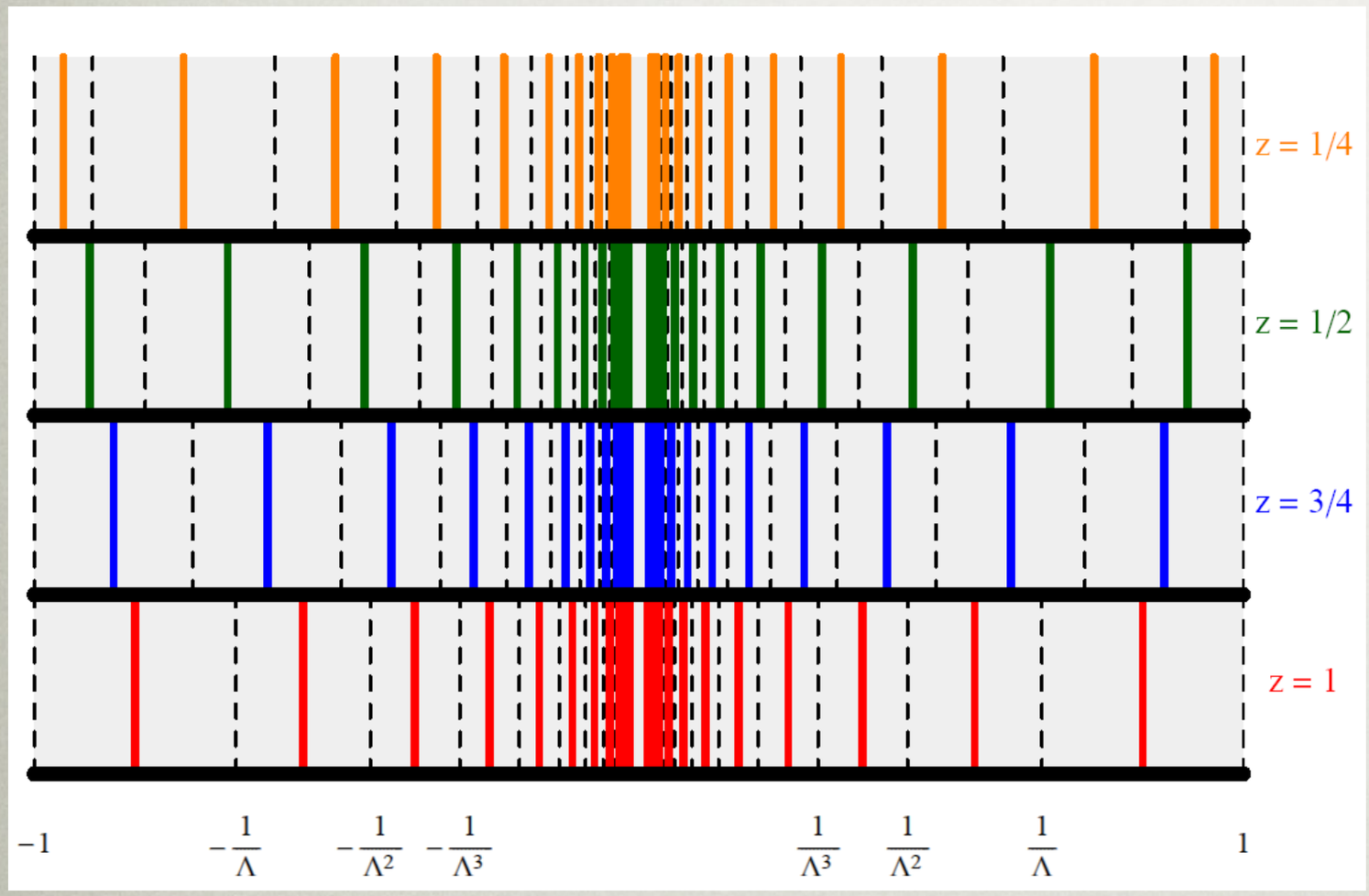
Σ AT LOW FREQUENCIES



Characteristic behavior of Fermi-liquid systems.

$$\mathrm{Im}\,\Sigma(\omega, T) = a(\omega^2 + \pi^2 T^2) + b\omega^3 + c\omega T^2 + \ldots$$

Z-AVERAGING



$$\epsilon_1^z = D$$

$$\epsilon_j^z = D\Lambda^{2-j-z}$$

$$z \in (0:1]$$

works best for $N_z=2^N$

similar to *twist averaging* over different boundary conditions in finite clusters to reduce the finite-size effects (better k-space sampling)

Frota, Oliveira, PRB 33, 7871 (1986)
Oliveira, Oliveira, PRB 49, 11986 (1994)

Discretization schemes

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)

$$A_\Lambda = \frac{1}{2}\frac{1+1/\Lambda}{1-1/\Lambda}\ln\Lambda$$

$$A_\Lambda \approx 1.04 \text{ for } \Lambda = 2$$

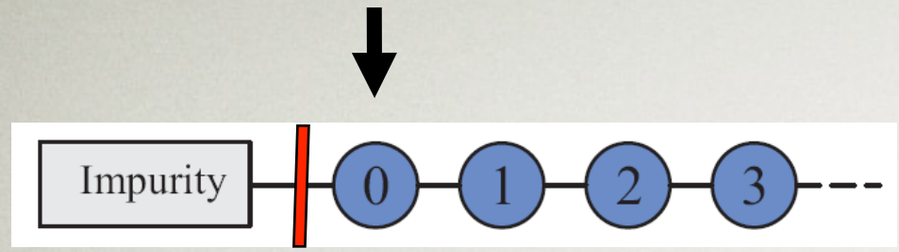
$$A_\Lambda \approx 1.16 \text{ for } \Lambda = 4$$

2) Campo-Oliveira scheme

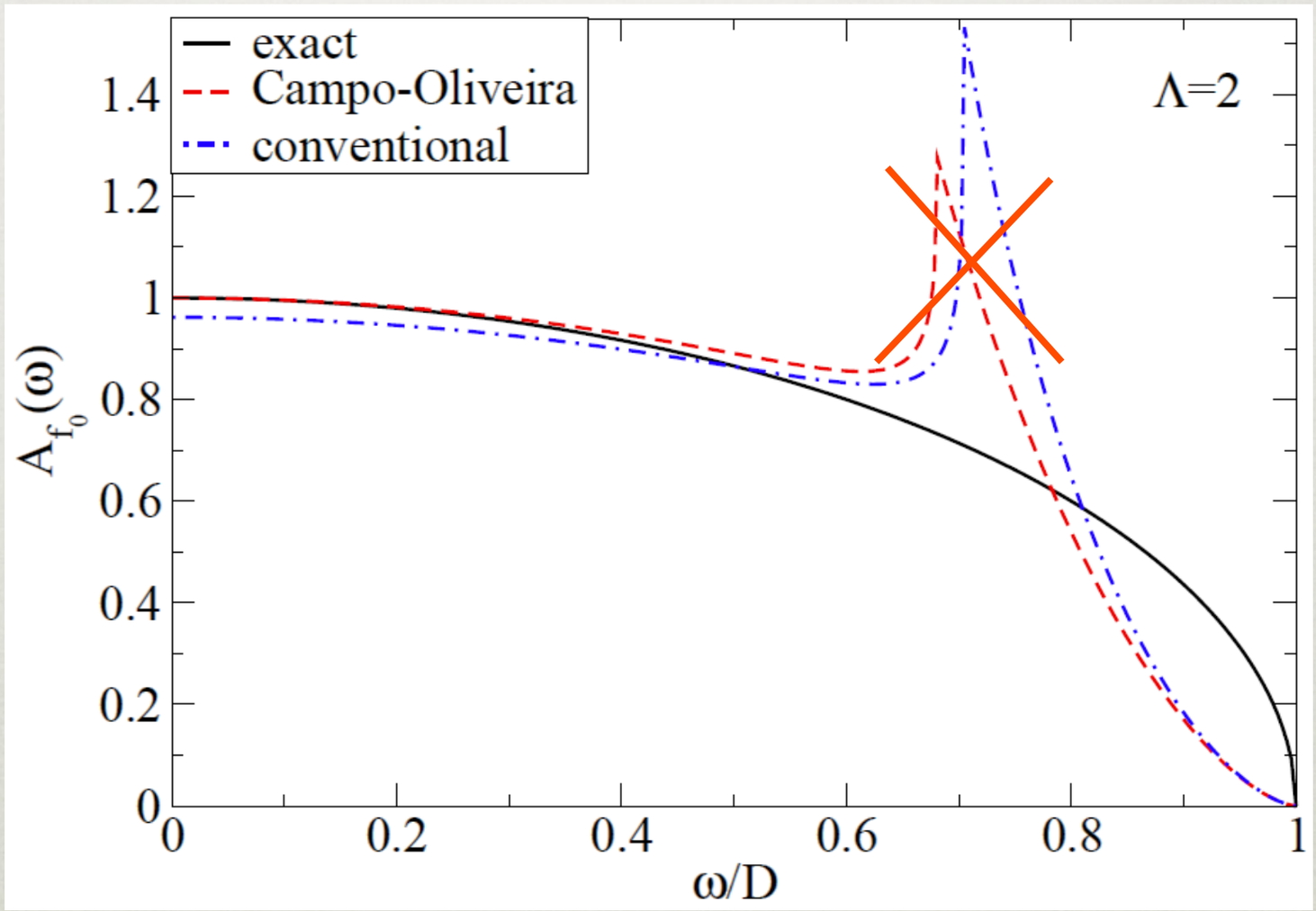
$$\mathcal{E}_j^z = \frac{\int_{I_j} \rho(\epsilon) d\epsilon}{\int_{I_j} \rho(\epsilon)\frac{1}{\epsilon}\,d\epsilon}$$

Campo, Oliveira, PRB 72, 104432 (2005)

$\mathcal{E}_j^z$: representative energy for interval $I_j = [\epsilon_{j+1}^z : \epsilon_j^z]$



$$\rho(\omega) = \rho_0 \sqrt{1 - \left(\frac{\omega}{D}\right)^2}$$



Spectral function of the first site of the Wilson chain

Flat band: $$A_{f_0}(\omega) = \frac{\epsilon_j^z - \epsilon_{j+1}^z}{2D|d\mathcal{E}_j^z/dz|} \qquad \mathcal{E}_j^z = \omega$$

Campo, Oliveira, PRB 72, 104432 (2005)

Generally: $$A_{f_0}(\omega) = \frac{\int_{I_j} \rho(\epsilon)\mathrm{d}\epsilon}{|d\mathcal{E}_j^z/dz|}$$

Can we do better?

Yes! We demand $A_{f_0}(\omega) = \rho(\omega)$

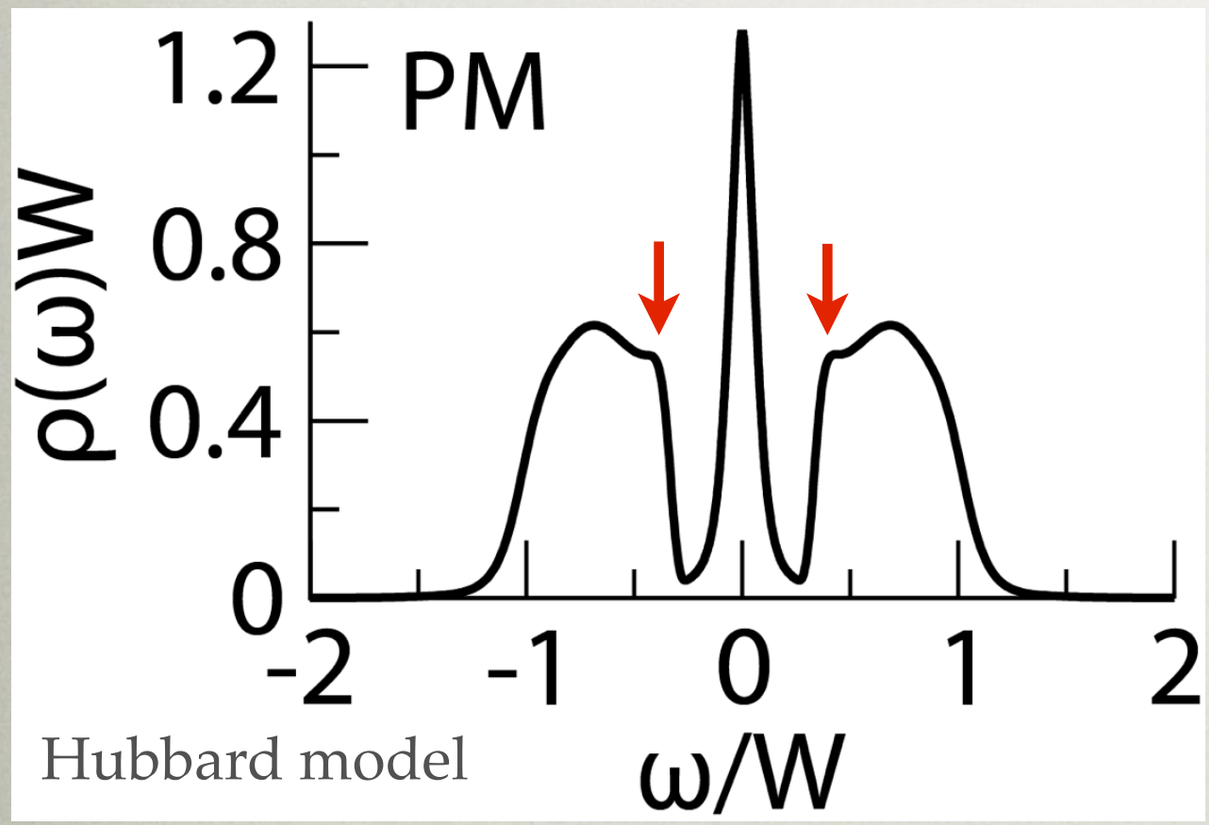
$$\frac{\int_{I_j} \rho(\epsilon) d\epsilon}{|d\mathcal{E}_j^z / dz|} = \rho(\omega)$$

$$x = j + z \qquad\qquad \mathcal{E}(x) = D f(x) \Lambda^{2-x}$$

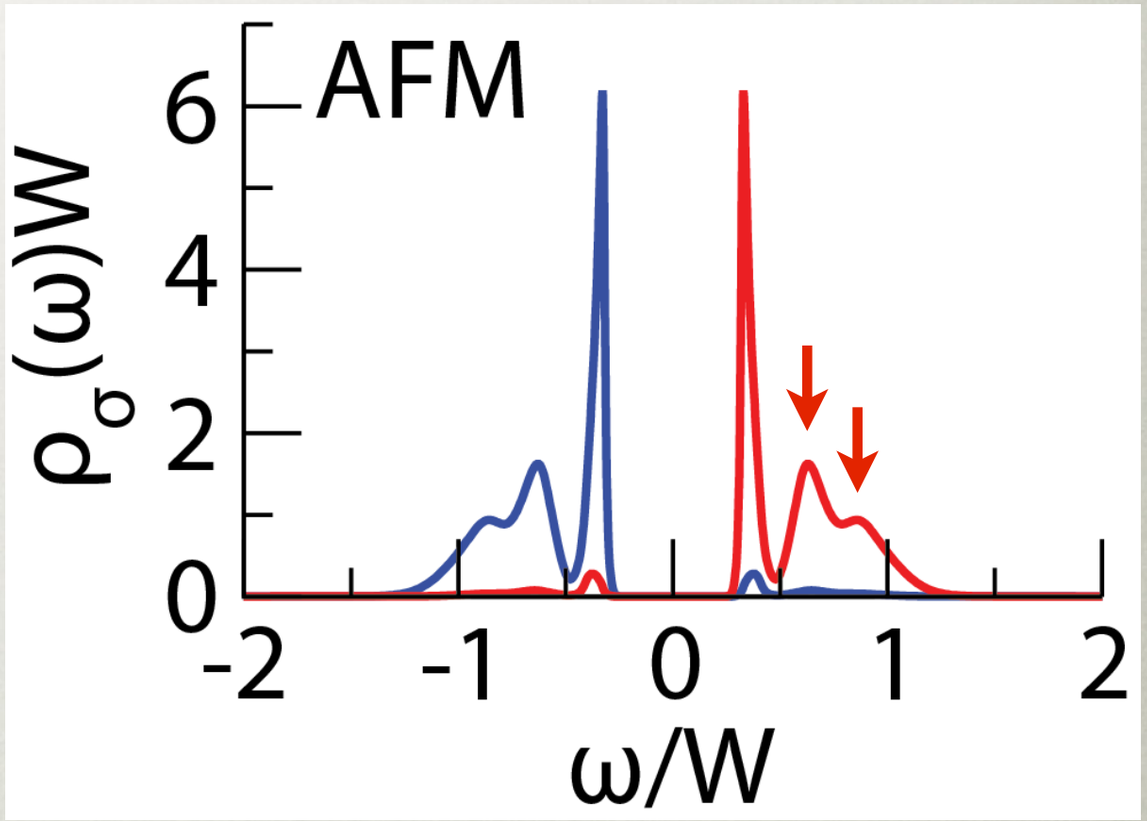
$$\frac{df(x)}{dx} = \ln \Lambda \, f(x) - \frac{\int_{\epsilon(x+1)}^{\epsilon(x)} \rho(\omega) d\omega}{\Lambda^{2-x} \rho[\mathcal{E}(x)]}$$

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

High-resolution spectra



Hubbard model



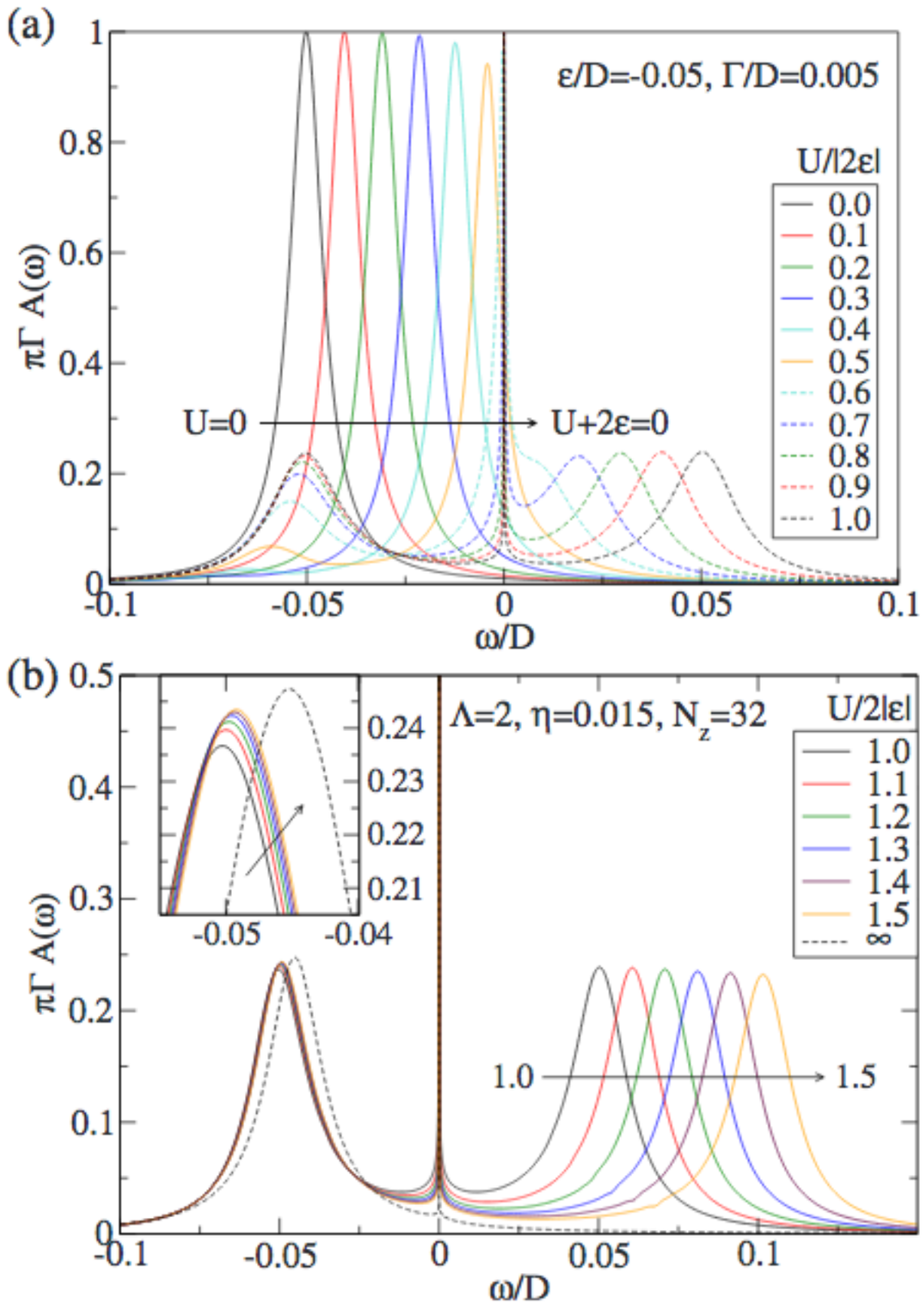


FIG. 14. (Color online) Spectral functions of the Anderson model for increasing U.

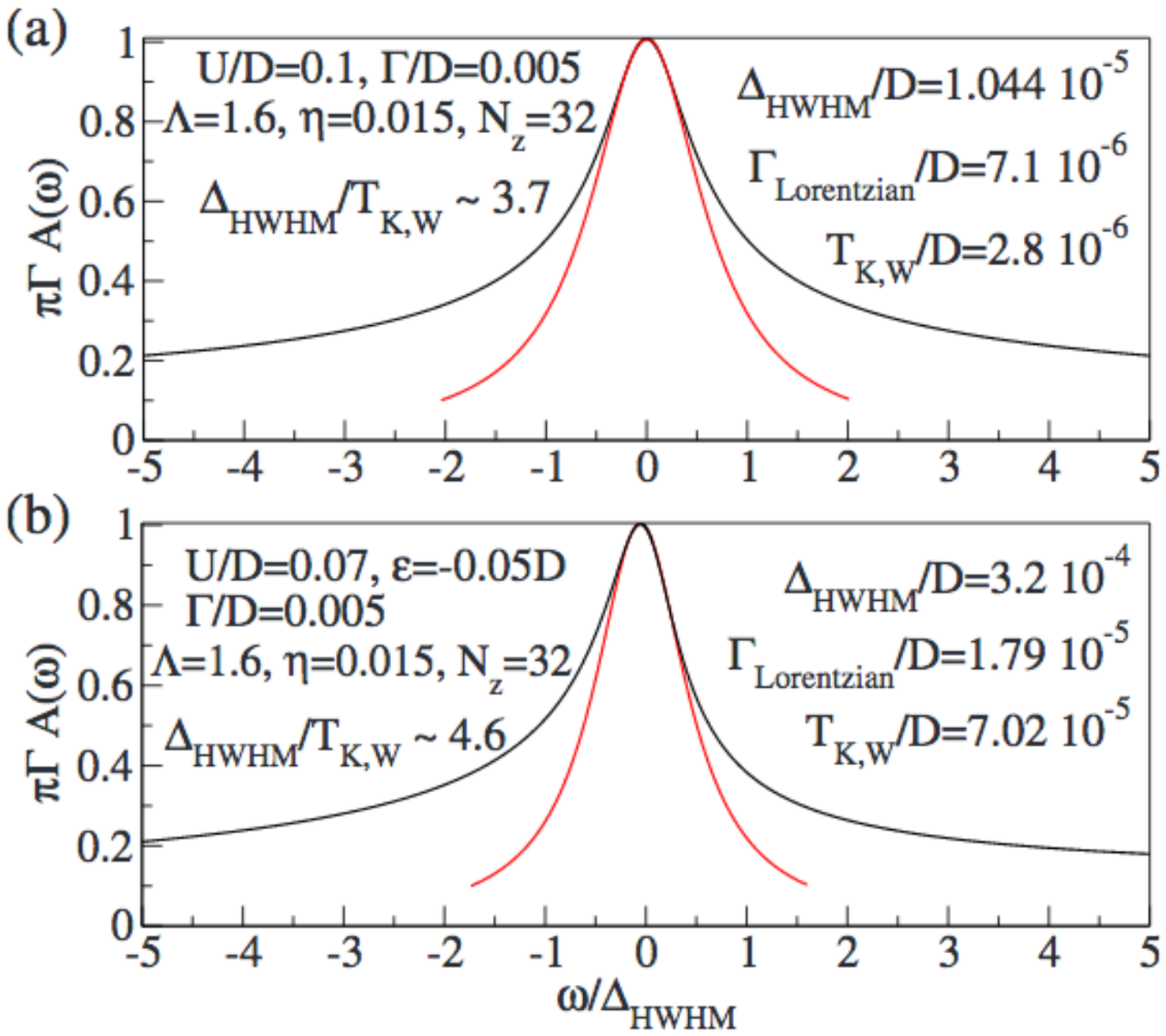
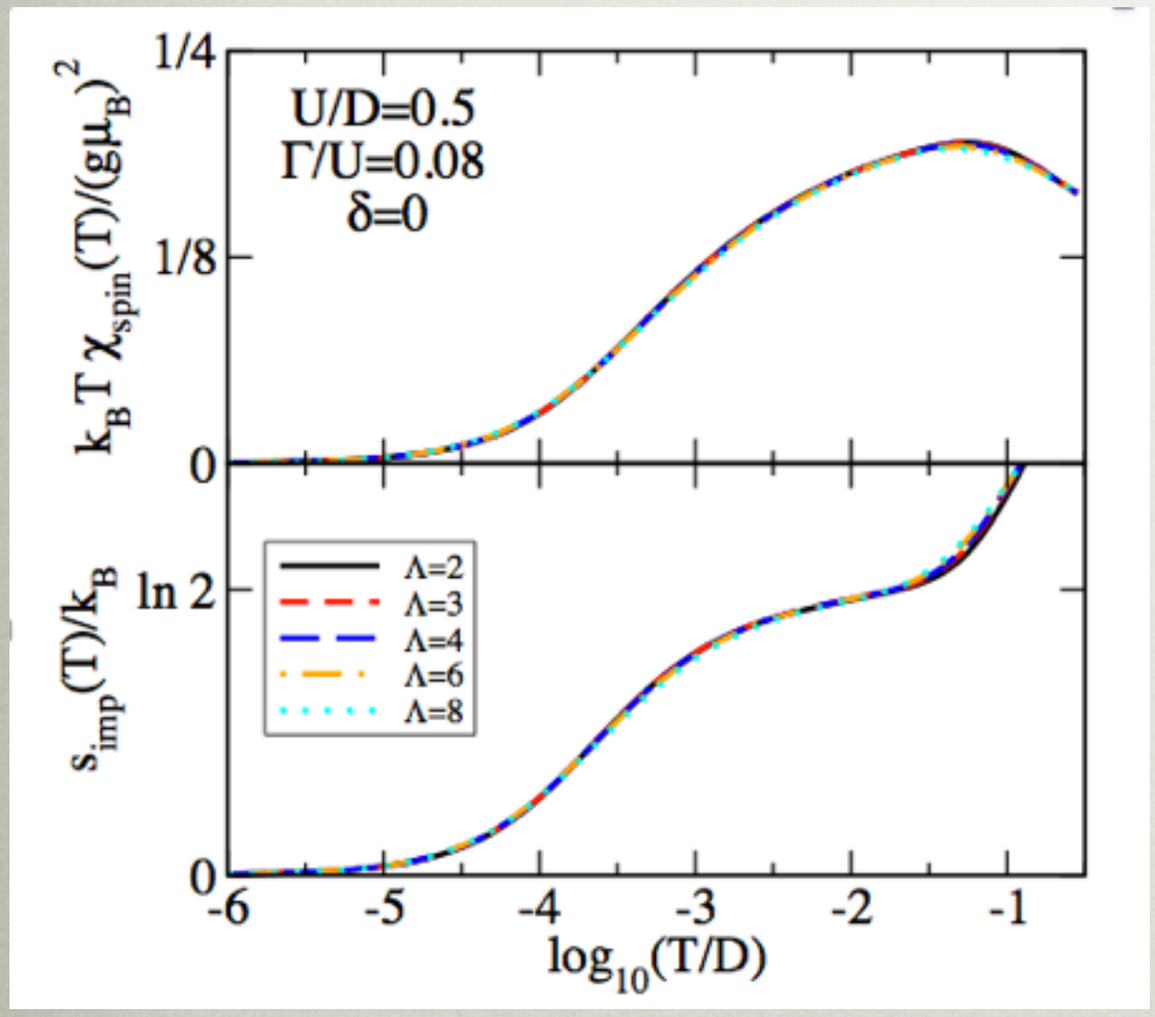
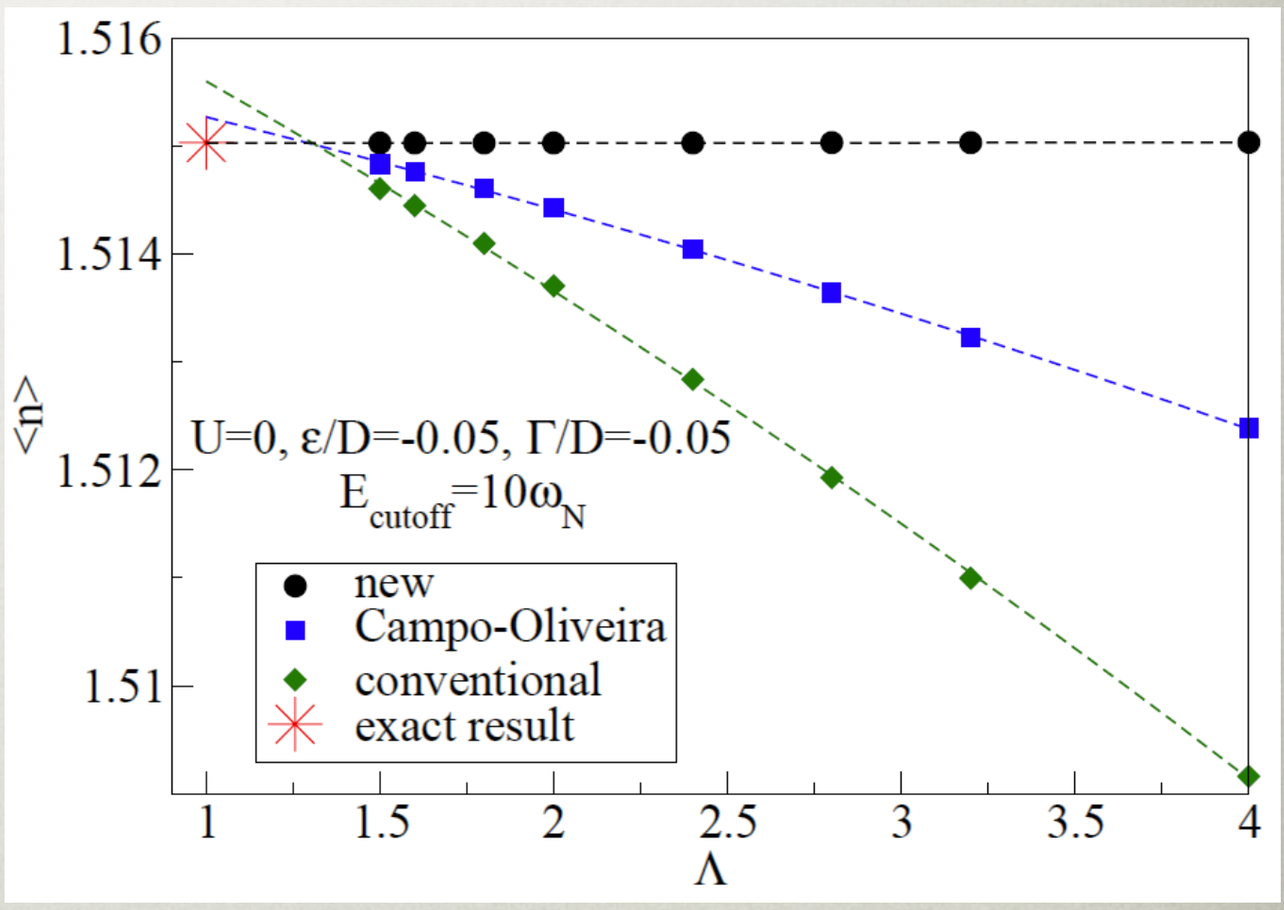


FIG. 15. (Color online) Close-up on the Kondo resonance of (a) symmetric and (b) asymmetric Anderson impurity model and a fit to a Lorentzian (red/gray curve) in the Fermi-liquid regime for $\omega \ll T_K$.

Choice of Λ


U/D=0.5
Γ/U=0.08
δ=0
1/4
1/8
0
$k_B T \chi_{spin}(T)/(g\mu_B)^2$
ln 2
0
$s_{imp}(T)/k_B$
Λ=2
Λ=3
Λ=4
Λ=6
Λ=8
-6
-5
-4
-3
-2
-1
$\log_{10}(T/D)$


1.516
1.514
1.512
1.51
<n>
U=0, ε/D=-0.05, Γ/D=-0.05
$E_{cutoff}=10\omega_N$
new
Campo-Oliveira
conventional
exact result
1
1.5
2
2.5
3
3.5
4
Λ

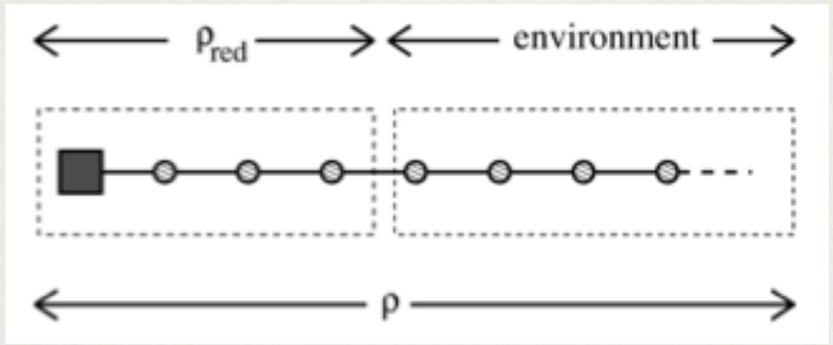
Density-matrix NRG

Problem: Higher-energy parts of the spectra calculated without knowing the true ground state of the system

Solution:

1) Compute the density matrix at the temperature of interest. It contains full information about the ground state.
2) Evaluate the spectral function in an additional NRG run using the *reduced density matrix* instead of the simple Boltzmann weights.

$$T = 0 \quad \rightarrow \quad \rho = |0\rangle\langle 0|$$



$$\hat{\rho} = \sum_{m_1,m_2,n_1,n_2} \rho_{m_1 n_1 m_2 n_2} |m_1\rangle_{\mathrm{env}} |n_1\rangle_{\mathrm{sys}} \langle n_2| \langle m_2|$$

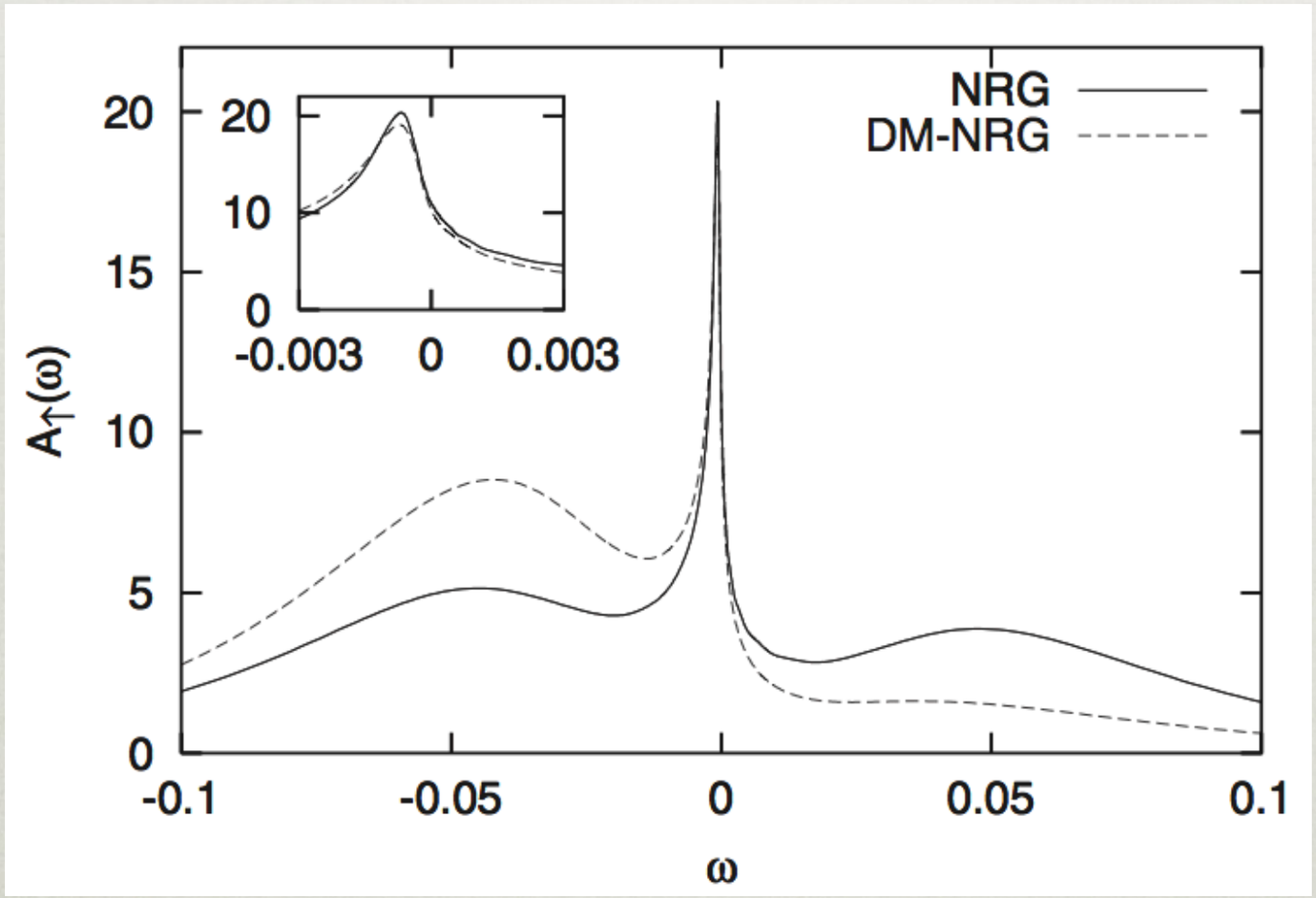
$$\hat{\rho}^{\mathrm{red}} = \sum_{n_1,n_2} \rho^{\mathrm{red}}_{n_1 n_2} |n_1\rangle_{\mathrm{sys}} \langle n_2| \qquad \rho^{\mathrm{red}}_{n_1 n_2} = \sum_m \rho_{m n_1, m n_2}$$

W. Hofstetter, PRL 2000

DMNRG for non-Abelian symmetries: Zitko, Bonca, PRB 2006

Spectral function computed as:

$$A_\mu^N(\omega) = \sum_{ijm} \left(\langle j|d_\mu^\dagger|m\rangle\langle j|d_\mu^\dagger|i\rangle \rho_{im}^{\text{reduced}} + \langle j|d_\mu^\dagger|m\rangle\langle i|d_\mu^\dagger|m\rangle \rho_{ji}^{\text{reduced}} \right) \delta(\omega - (E_j - E_m))$$



W. Hofstetter, PRL 2000

BIG PROBLEMS

- orbital degeneracy: big local Hilbert space, big Hilbert space at each shell of Wilson chains
- multiple quantum dots with multiple conduction leads
- lack of symmetry: diagonalization of big matrices scales as N^3

Recalculation of operators

$$\langle QS\omega \| \hat{O} \| Q'S'\omega' \rangle_{N+1} = \frac{\langle QSS_z\omega | \hat{O}_\mu | Q'S'S'_z\omega' \rangle_{N+1}}{\langle S'S'_z; M\mu | SS_z \rangle}$$

$$\langle QS\omega \| \hat{O} \| Q'S'\omega' \rangle_{N+1} = \sum_{ii'} C(QS, Q'S', ii') \sum_{rr'} U_{QS}(\omega, ri) U_{Q'S'}(\omega', r'i') \langle F_i(QS)r \| \hat{O} \| F_{i'}(Q'S')r' \rangle_N$$

Important to be efficiently implemented! We use BLAS routine **GEMM** (general matrix multiply). (GEMM from Intel MKL library has >80% efficiency on Xeon processors.)

Level	Data Movement	Floating-Point Operations	Example
Level 1 BLAS	O(N)	O(N)	DDOT
Level 2 BLAS	$O(N^2)$	$O(N^2)$	DGEMV
Level 3 BLAS	$O(N^2)$	$O(N^3)$	DGEMM

Parallelization

- Make use of multithreaded LAPACK routines, e.g. Intel MKL. Controlled by environment variables `MKL_NUMTHREADS`, `MKL_DYNAMIC`. Diagonalisation does not scale linearly, but the speed-up is substantial.
- Run diagonalisations in parallel using multithreading (OpenMP) on the same compute node, or using message-passing (MPI) across several compute nodes.

Note: nested OpenMP parallelism needs to be enabled using `OMP_NESTED=TRUE`. Often difficult to make it work (segmentation faults).

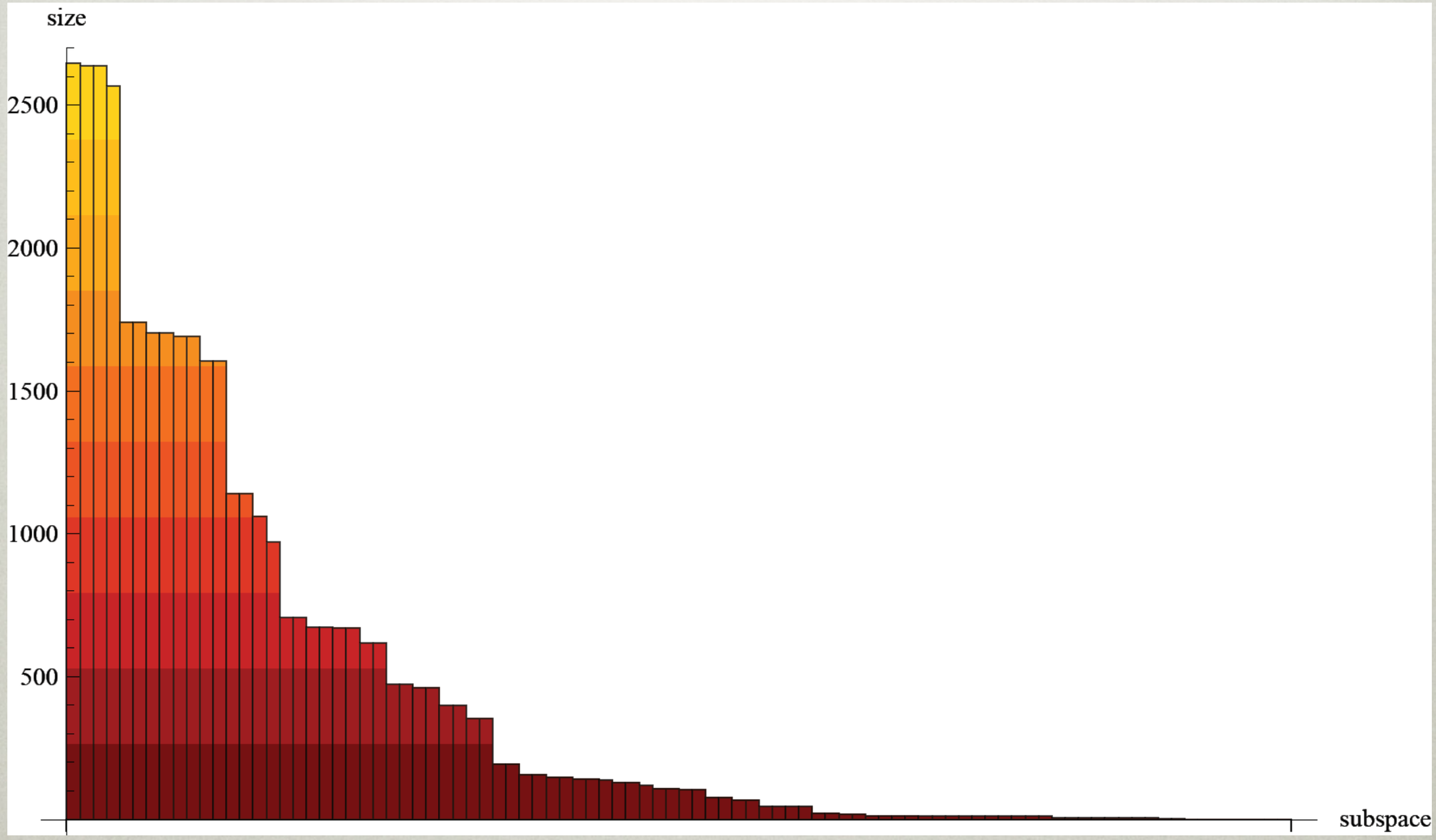
log

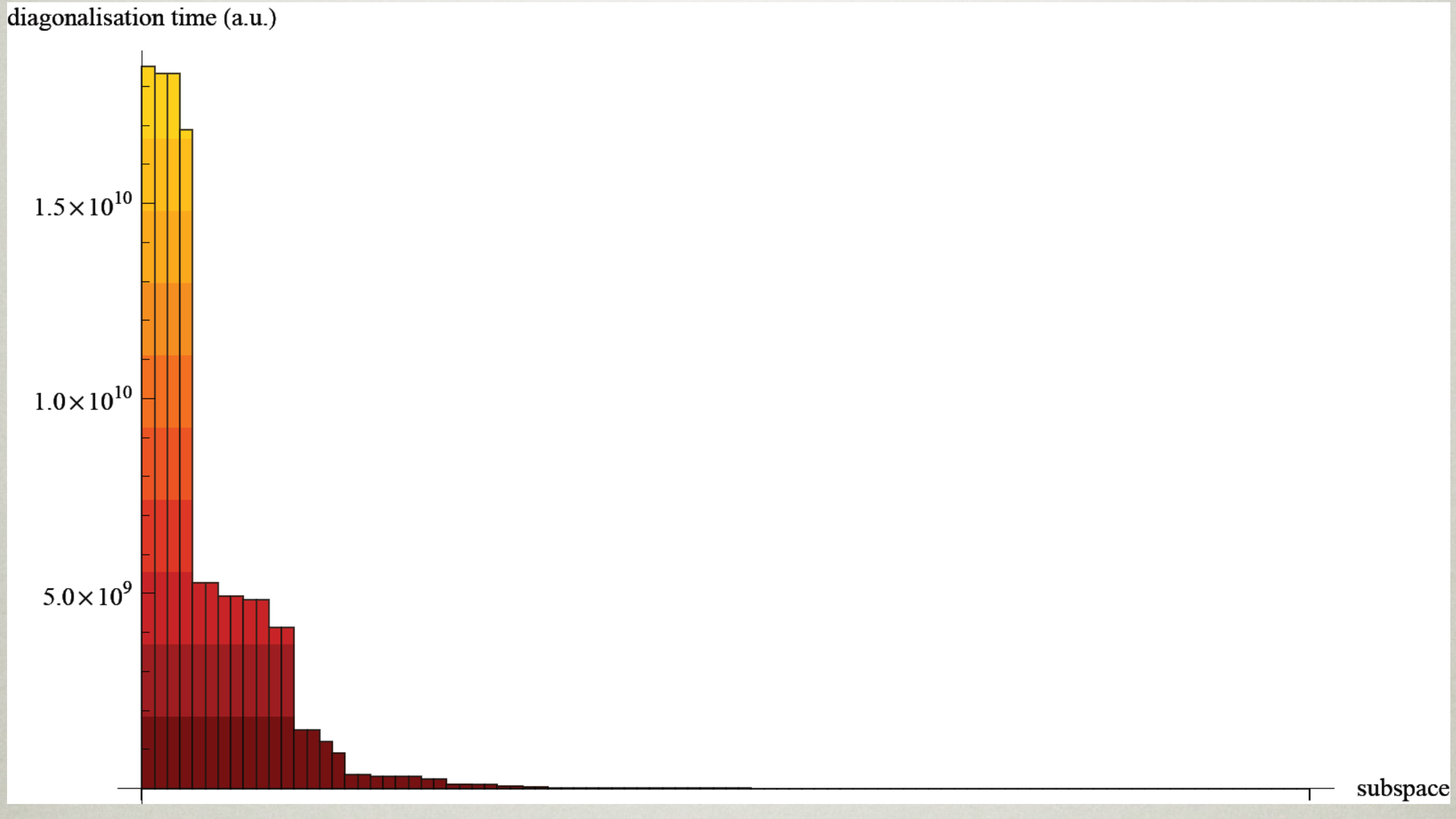
```
NRG Ljubljana 2.4.3.31 - (c) Rok Zitko <rok.zitko@ijs.si>
Timestamp: Mon Nov 13 12:55:52 2017
Compiled on Aug 14 2018 at 10:37:37
Compiled-in symmetry types: ANYJ DBLISOSZ DBLSU2 ISO ISO2 ISO2LR
ISOLR ISOSZ ISOSZLR NONE P PP QJ QS QSC3 QSLR QST QSTZ QSZ QSZLR
QSZTZ SL SL3 SPSU2 SPSU2C

No MPI: single node calculation.

[OMP] Max. number of threads: 1
[OMP] Number of processors: 32
[OMP] Dynamic thread adjustment: 0
[OMP] Nested parallelism: 0

Using Intel MKL library 11.3.2
Processor optimization: Intel(R) Advanced Vector Extensions 2
(Intel(R) AVX2) enabled processors
max_threads=8 blas_max_threads=8 dynamic=0
```

export MKL_NUM_THREADS=8

export MKL_DYNAMIC=FALSE

Matrix dimensions in different invariant subspaces.



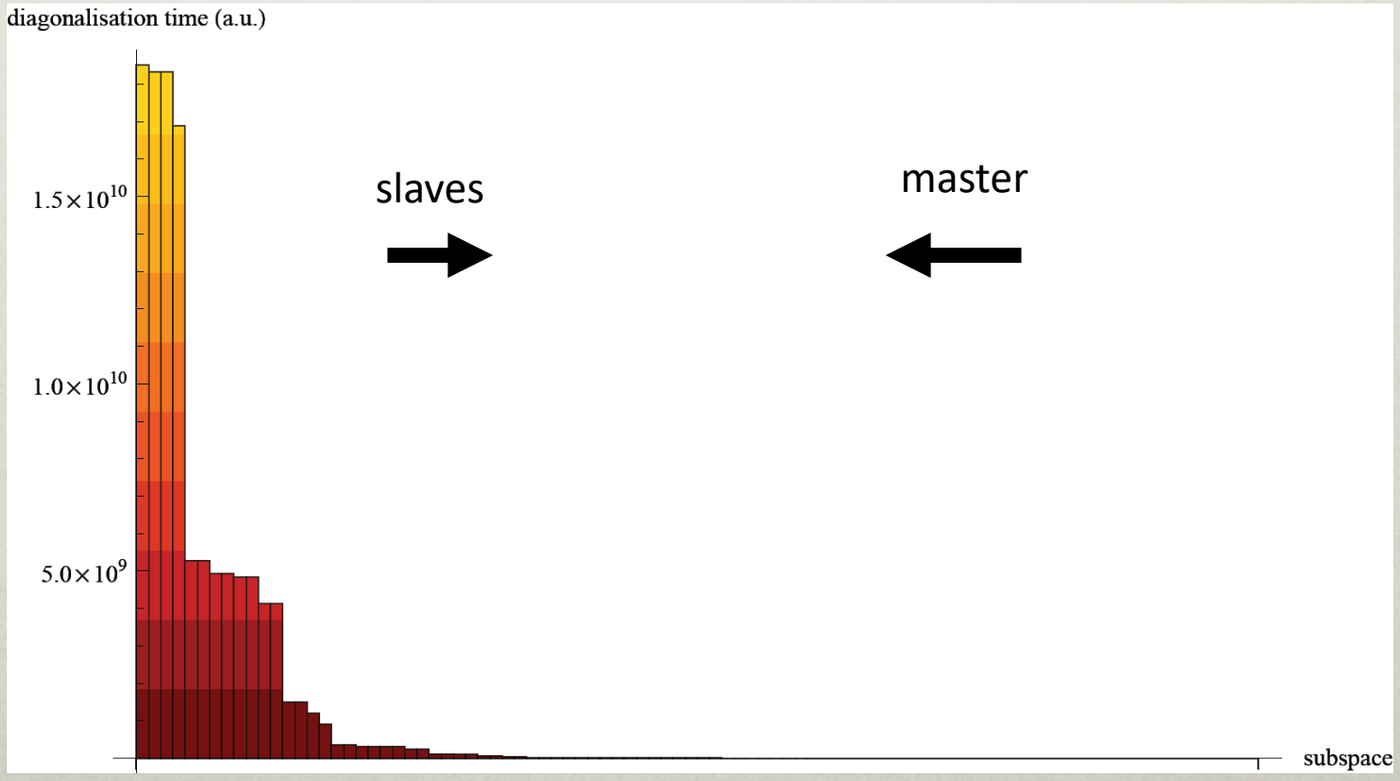


Conclusion: up to ~5-6 simultaneous diagonalisations.

controller agent

~~Master-slave~~ strategy

1. Master delegates diagonalisations of large matrices to slave nodes.
2. Master diagonalizes small matrices locally.



Real vs. complex numerics

Choice depends on the Hamiltonian
and all operators of interest.

Examples:
- magnetic field along the y-axis
- two superconducting leads with phase difference
- calculations of transverse magnetic susceptibility

Significant (almost an order of magnitude)
difference in performance!