Magnetic impurities in metals: Kondo effect and the numerical renormalization group

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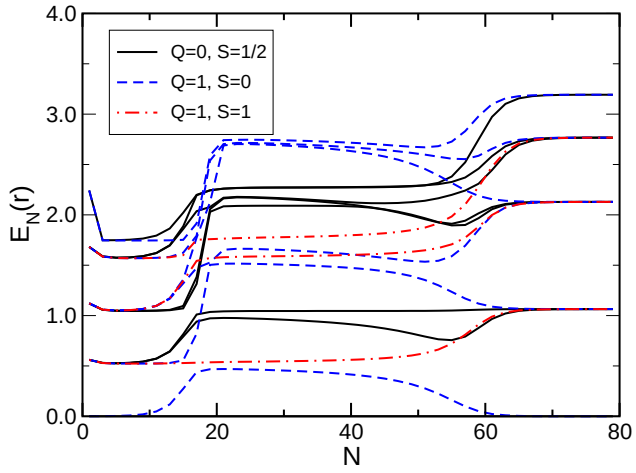

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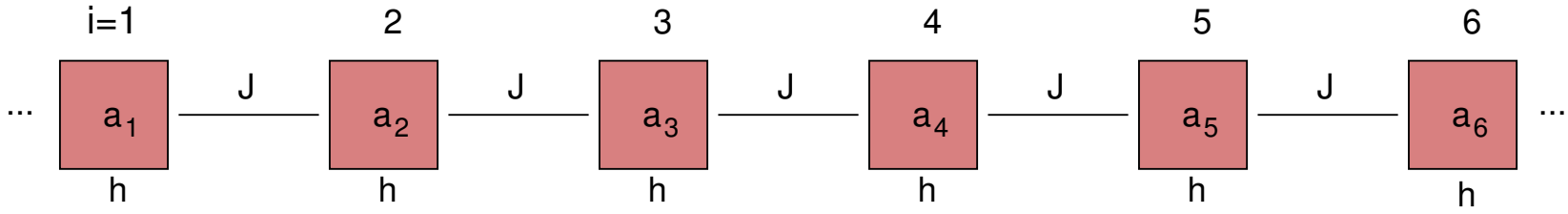
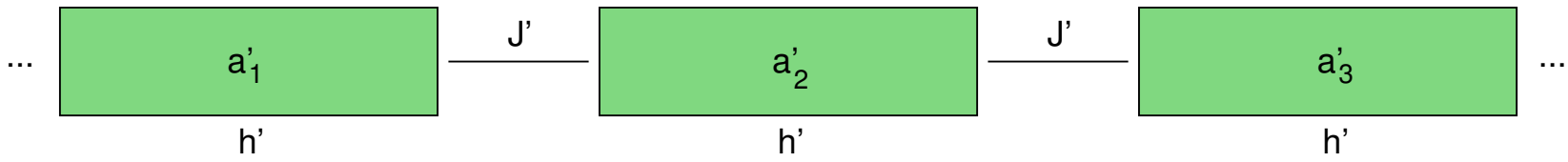
2. introduction to quantum impurity physics
3. the Numerical Renormalization Group
   $\rightarrow$ application to the single-impurity Anderson model
4. fixed points in quantum impurity models
5. calculation of physical properties and applications

1. introduction to basic rg concepts

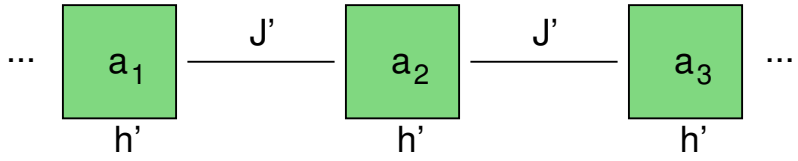
consider a model on a one-dimensional lattice, with operators a_i (i: lattice site), parameters $J, h, \ldots$, and Hamiltonian $H(J, h, \ldots)$.



combine two sites to give (effectively) one site with operators a'_i and parameters $J', h', \ldots$.



we assume that the Hamiltonian H' of the effective model is of the same form, with renormalized parameters: $H' = H(J', h', \ldots)$.
then rescale the model to the original lattice spacing:



the mapping $H \to H'$ is a renormalization group transformation

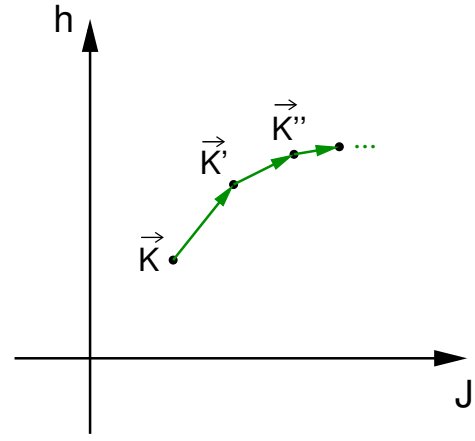
$$H(J', h', \ldots) = R\{H(J, h, \ldots)\}$$

with $\vec{K} = (J, h, \ldots)$: $R(\vec{K}) = \vec{K}'$

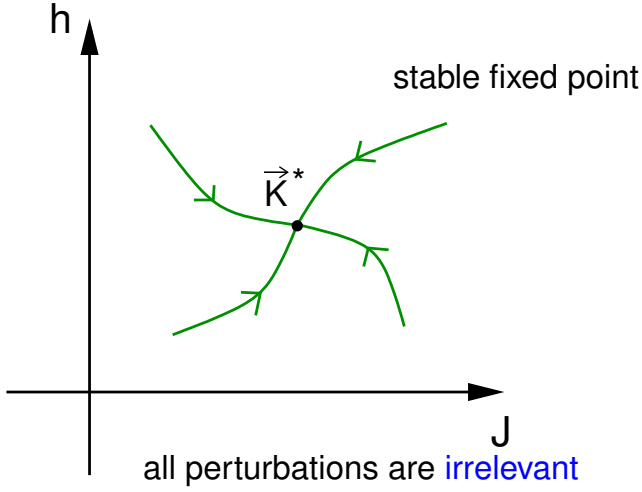
now consider a sequence of transformations:

$$\vec{K} \xrightarrow{R} \vec{K}' \xrightarrow{R} \vec{K}''$$

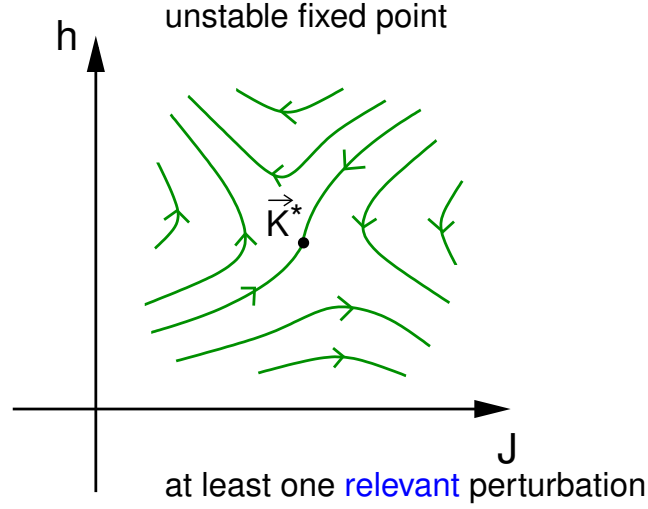
this results in a trajectory in parameter space:



flow diagrams and fixed points



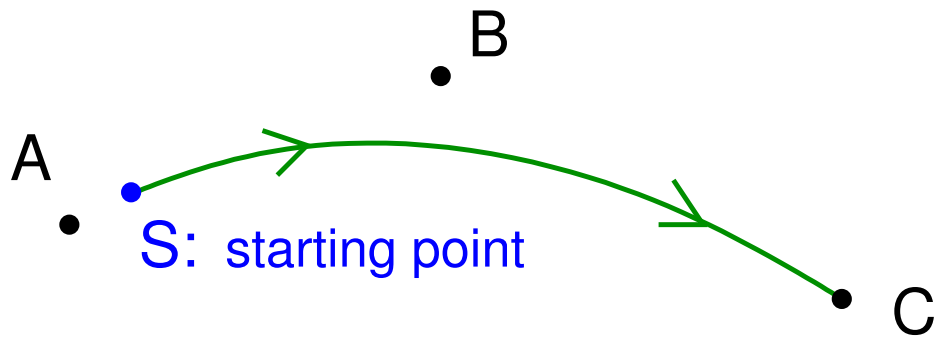
$$R(\vec{K}^*) = \vec{K}^*$$



the central issue:

How does the behaviour of the system change under a scale transformation?

$\rightarrow$ the physics of the problem described as a flow between fixed points.



- identify the fixed points of the model (and their physical meaning)
- identify the relevant/irrelevant perturbations
- if possible: describe the full flow from S to C

and finally: calculate physical properties

some technical issues:

- how to perform the mapping $H \to H'$ for a given model?
  - Ising model:(1d) in the partition function Z, sum over every second spin
- but: the whole strategy depends on the details of the model
  - spins/fermions/bosons
  - dimension, lattice structure, etc.

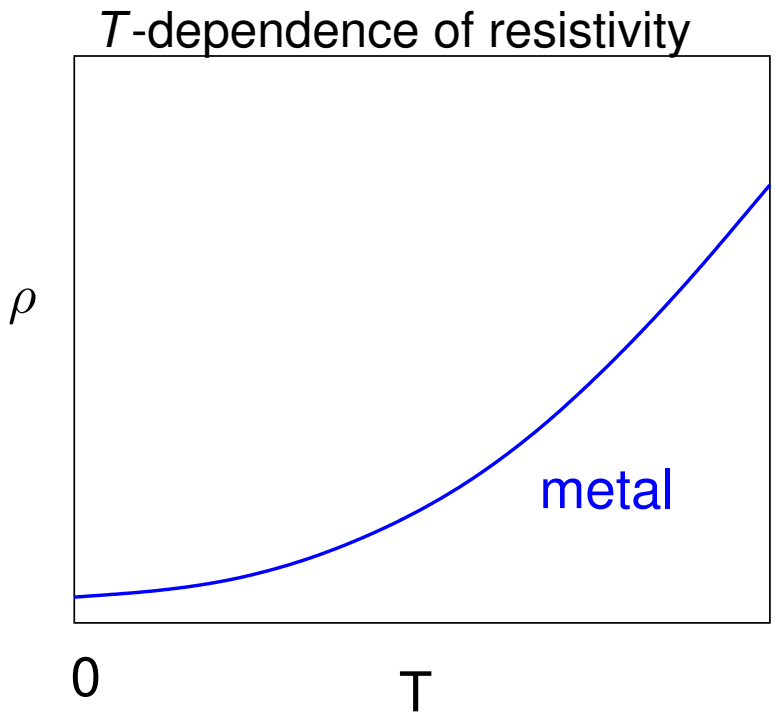
$\Longrightarrow$ for a given model, it is a priori not clear whether a successful rg scheme can be developed at all

in the following:

- (numerical) renormalization group for quantum impurity models
  - Wilson's NRG for the single-impurity Anderson model
- interpretation of fixed points and flow diagrams

2. introduction to quantum impurity physics

the Kondo effect: magnetic impurities in metals



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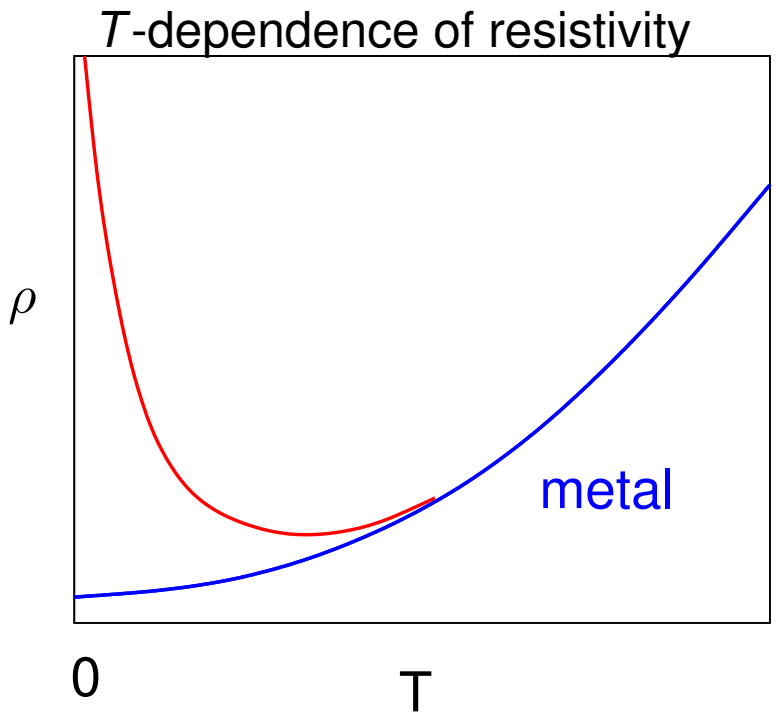
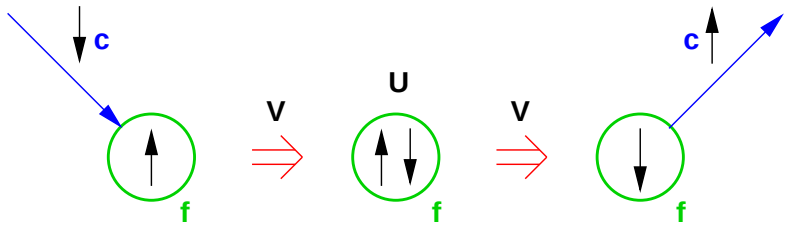
the Kondo effect: magnetic impurities in metals

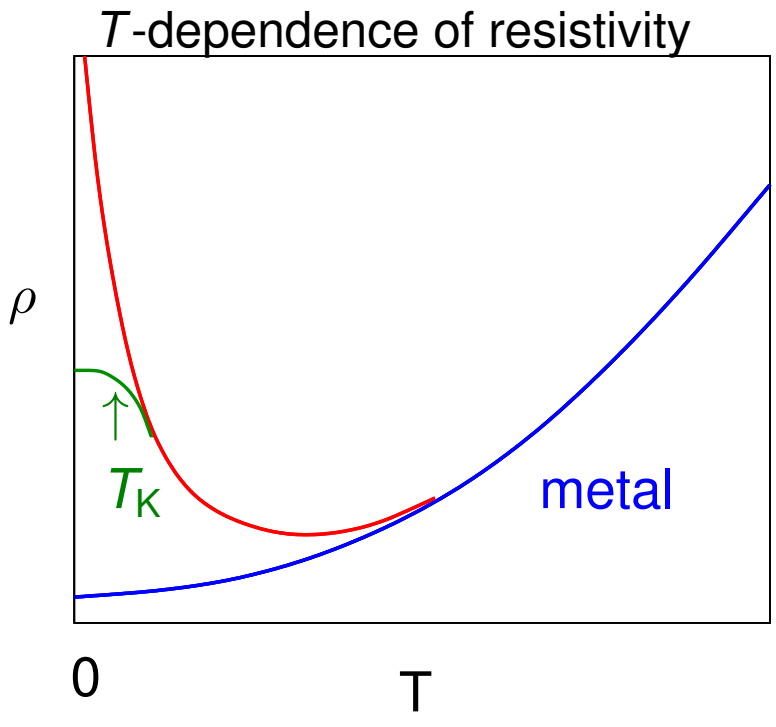


scattering processes of conduction electrons at magnetic impurities

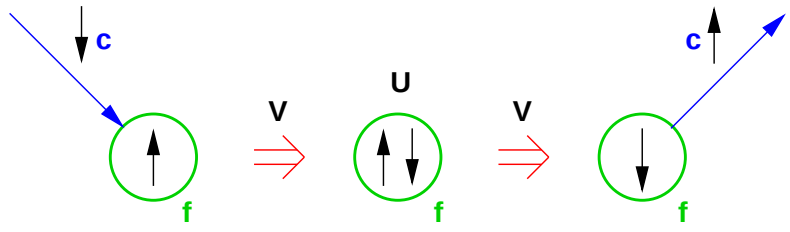


2. introduction to quantum impurity physics

the Kondo effect: magnetic impurities in metals



scattering processes of conduction electrons at magnetic impurities



screening of magnetic moments due to singlet formation

$$\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_f|\downarrow\rangle_c - |\downarrow\rangle_f|\uparrow\rangle_c\right)$$

modelling of magnetic impurities in metals

here: single-impurity Anderson model

[A.C. Hewson, *The Kondo Problem To Heavy Fermions*, CUP 1993]

$$H = \varepsilon_f \sum_\sigma f_\sigma^\dagger f_\sigma + U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow$$
$$+ \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + V \sum_{k\sigma} \left(f_\sigma^\dagger c_{k\sigma} + c_{k\sigma}^\dagger f_\sigma \right)$$

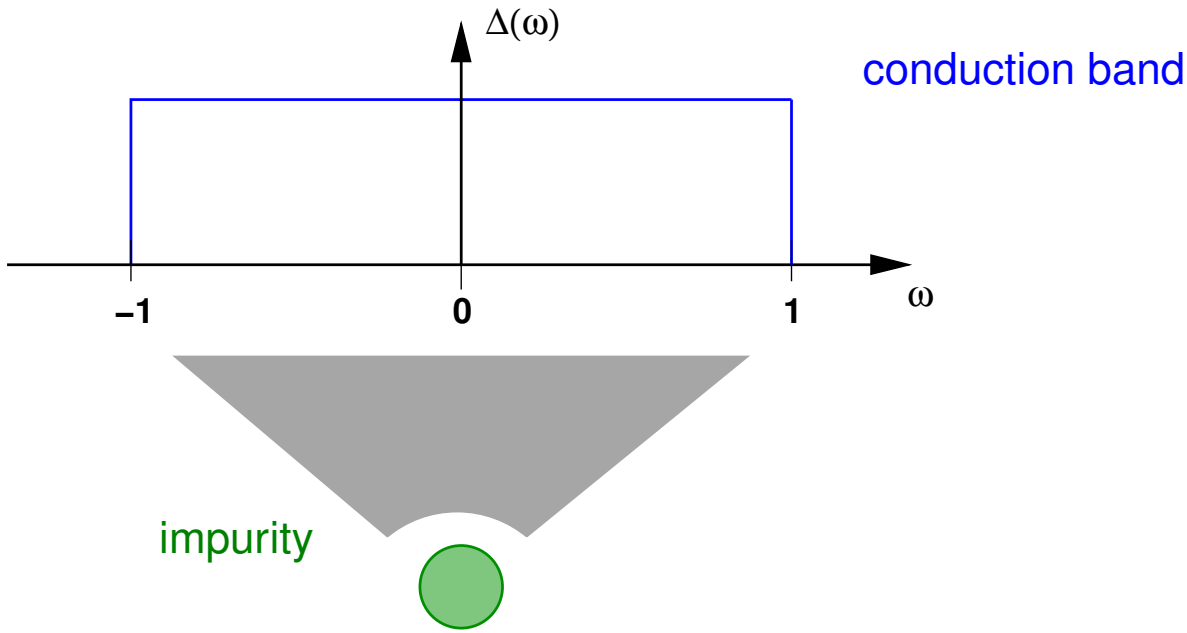
the model describes:

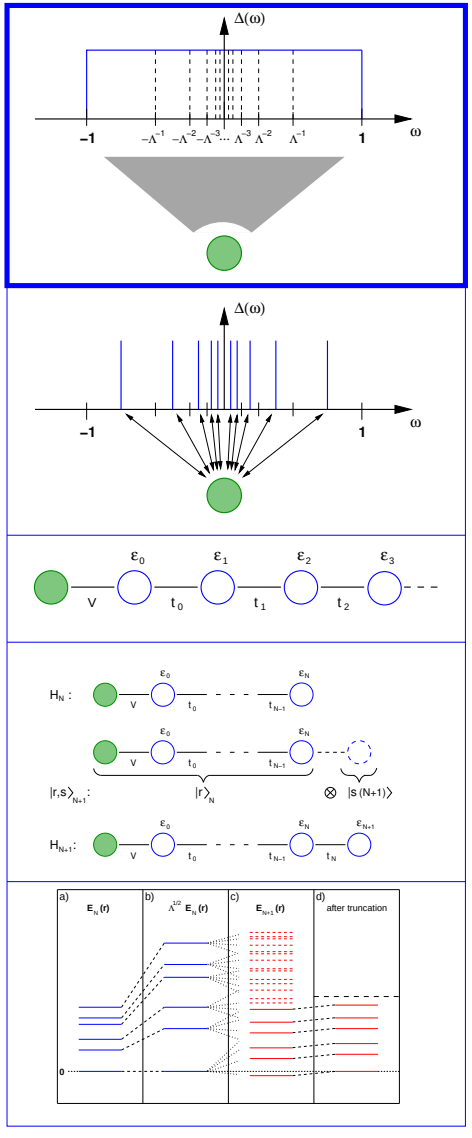
- formation of local moments: $|\uparrow\rangle_f$, $|\downarrow\rangle_f$
- scattering of conduction electrons
- screening of local moments below temperature scale T_K

3. the numerical renormalization group

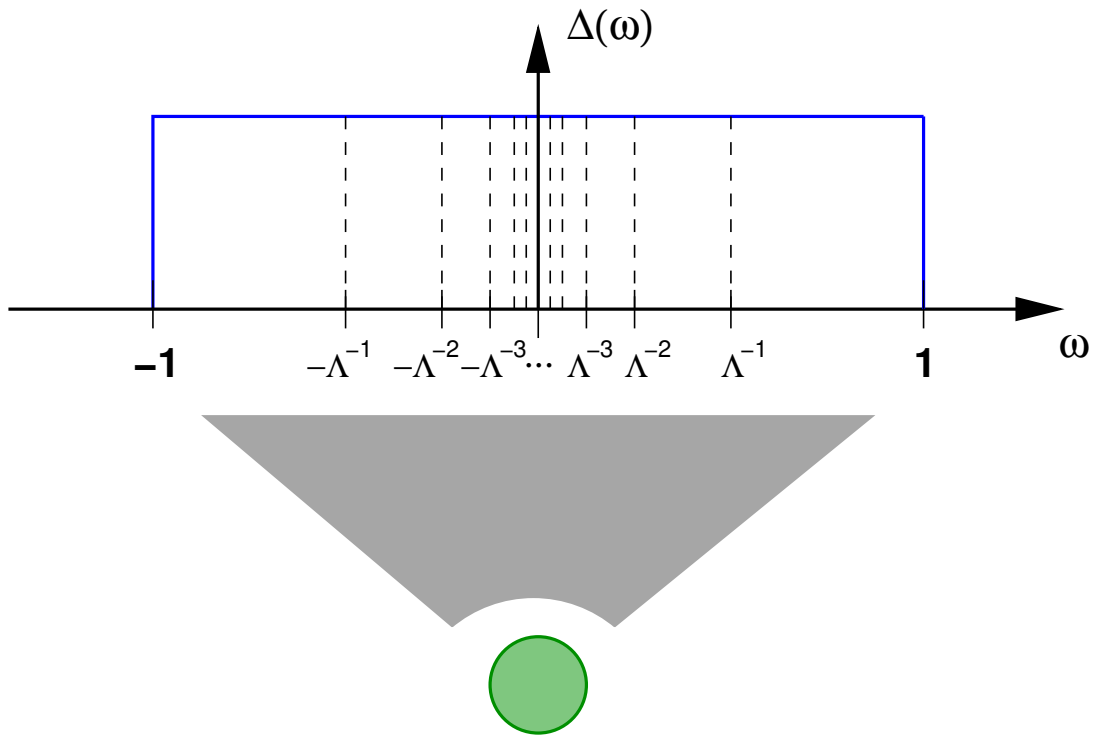
K.G. Wilson, Rev. Mod. Phys. **47**, 773 (1975) $\rightarrow$ Kondo problem

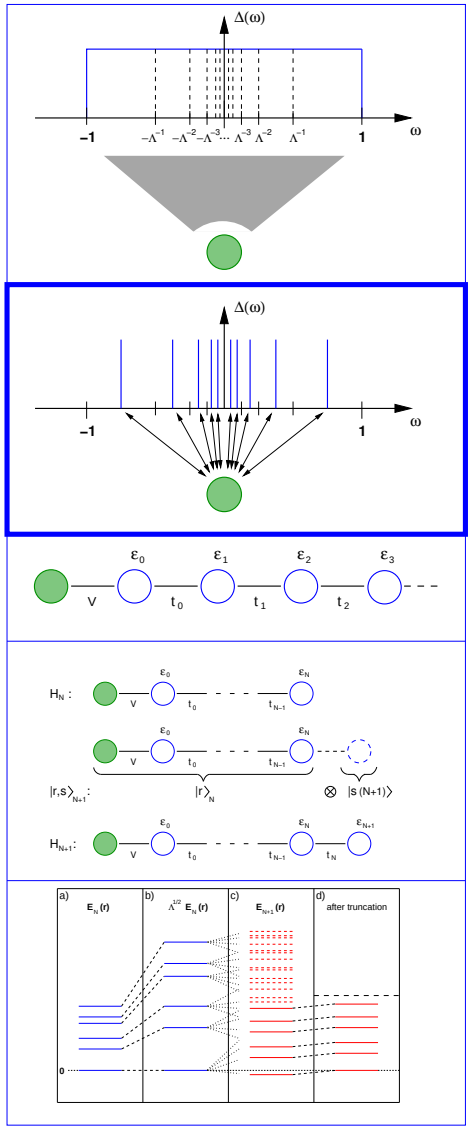
review: R. Bulla, T. Costi, and Th. Pruschke, Rev. Mod. Phys. **80**, 395 (2008)



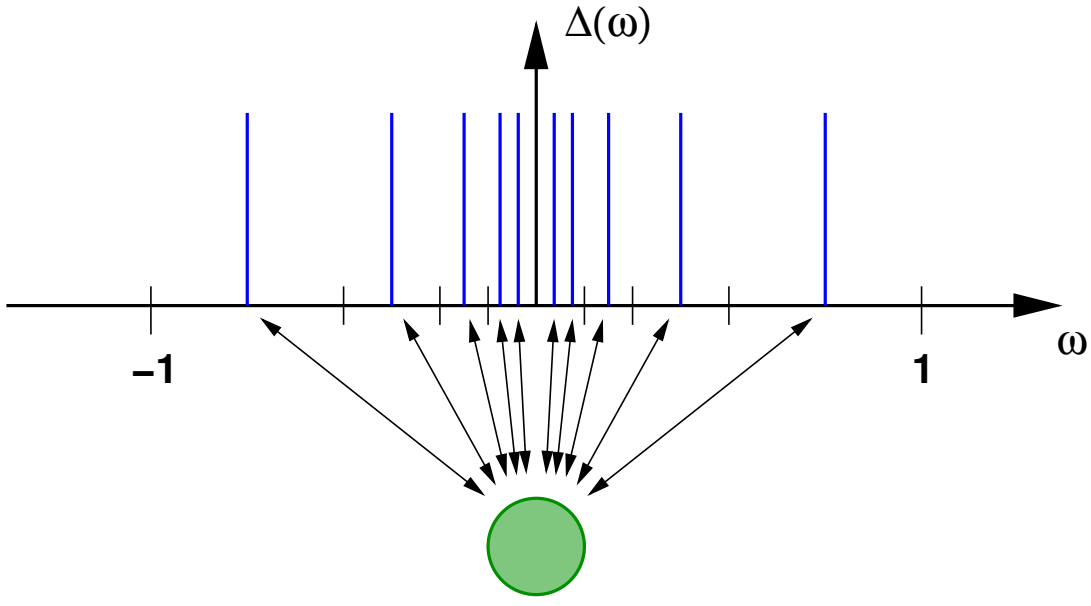


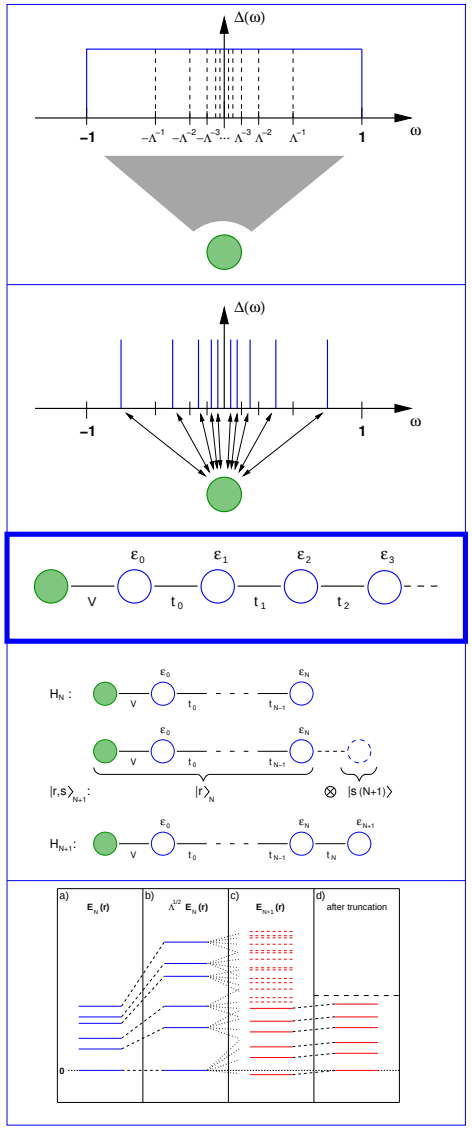
1. NRG-discretization parameter $\Lambda > 1$



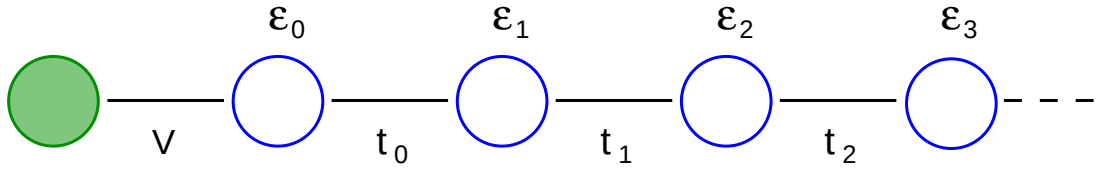


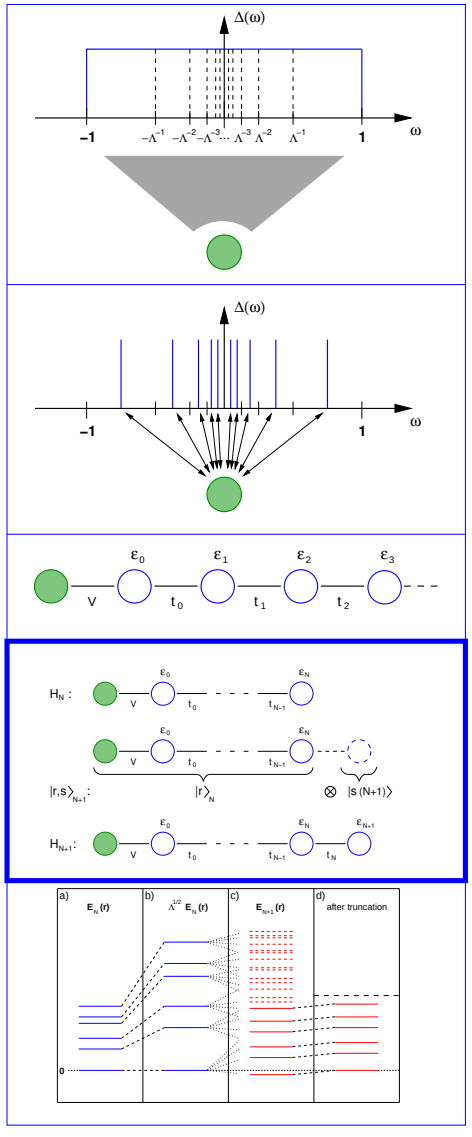
2. logarithmic discretization



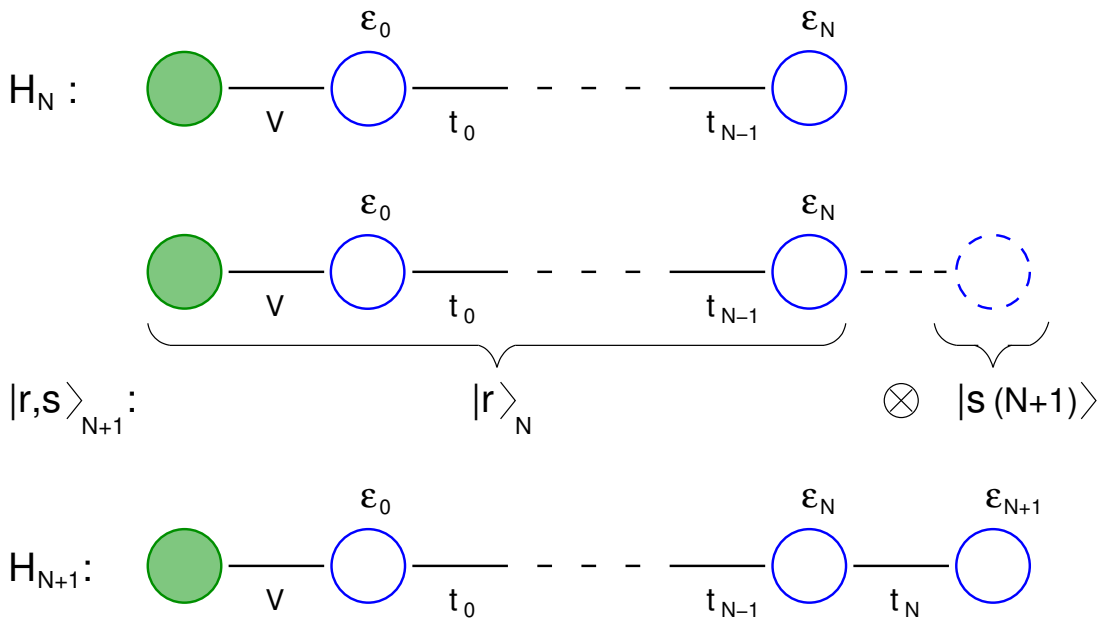


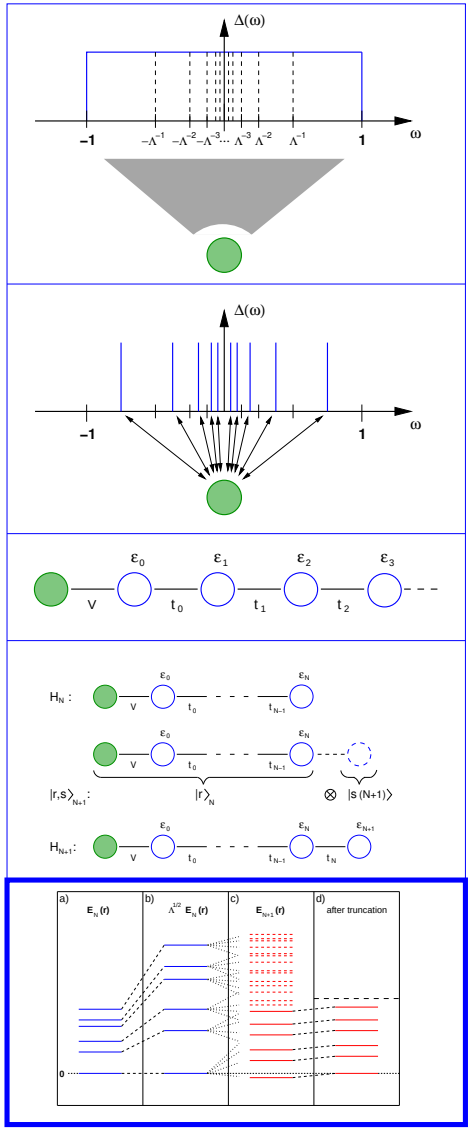
3. mapping on semi-infinite chain



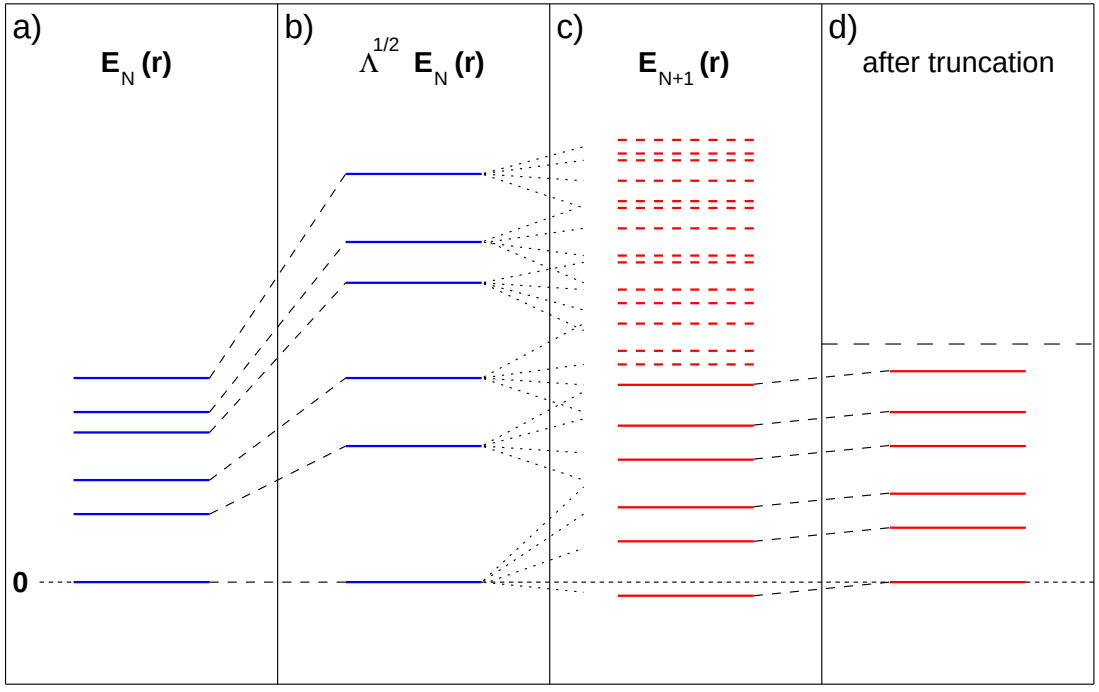


4. iterative diagonalization





5. truncation



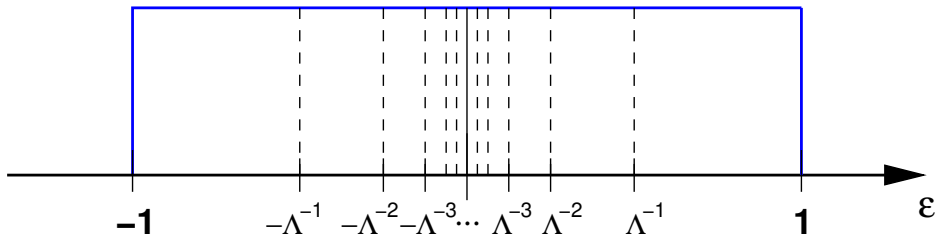
logarithmic discretization

starting point: siAm in the integral representation:

$$
\begin{aligned}
H_{\text{imp}} &= \sum_{\sigma} \varepsilon_{\text{f}} f_{\sigma}^{\dagger} f_{\sigma} + U f_{\uparrow}^{\dagger} f_{\uparrow} f_{\downarrow}^{\dagger} f_{\downarrow} \ , \\
H_{\text{bath}} &= \sum_{\sigma} \int_{-1}^{1} \mathrm{d}\varepsilon \, g(\varepsilon) a_{\varepsilon\sigma}^{\dagger} a_{\varepsilon\sigma} \ , \\
H_{\text{imp}-\text{bath}} &= \sum_{\sigma} \int_{-1}^{1} \mathrm{d}\varepsilon \, h(\varepsilon) \left(f_{\sigma}^{\dagger} a_{\varepsilon\sigma} + a_{\varepsilon\sigma}^{\dagger} f_{\sigma} \right).
\end{aligned}
$$

$\Lambda > 1$ defines a set of intervals with discretization points

$$\pm x_n = \Lambda^{-n} \ , \quad n = 0, 1, 2, \ldots \ .$$



width of the intervals: $d_n = \Lambda^{-n}(1-\Lambda^{-1})$

within each interval: introduce a complete set of orthonormal functions

$$\psi^{\pm}_{np}(\varepsilon) = \begin{cases} \frac{1}{\sqrt{d_n}} e^{\pm i\omega_n p\varepsilon} & \text{for } x_{n+1} < \pm\varepsilon < x_n \\ 0 & \text{outside this interval .} \end{cases}$$

expand the conduction electron operators $a_{\varepsilon\sigma}$ in this basis

$$a_{\varepsilon\sigma} = \sum_{np} \left[a_{np\sigma}\psi^{+}_{np}(\varepsilon) + b_{np\sigma}\psi^{-}_{np}(\varepsilon) \right] ,$$

assumption:

$$h(\varepsilon) = h^{\pm}_n \quad , \quad x_{n+1} < \pm\varepsilon < x_n \, ,$$

the hybridization term then takes the form:

$$\int_{-1}^{1} \mathrm{d}\varepsilon \, h(\varepsilon) f^{\dagger}_{\sigma} a_{\varepsilon\sigma} = \frac{1}{\sqrt{\pi}} f^{\dagger}_{\sigma} \sum_{n} \left[\gamma^{+}_{n} a_{n0\sigma} + \gamma^{-}_{n} b_{n0\sigma} \right]$$

the impurity couples only to the
$p = 0$ components of the conduction band states!

the conduction electron term transforms to:

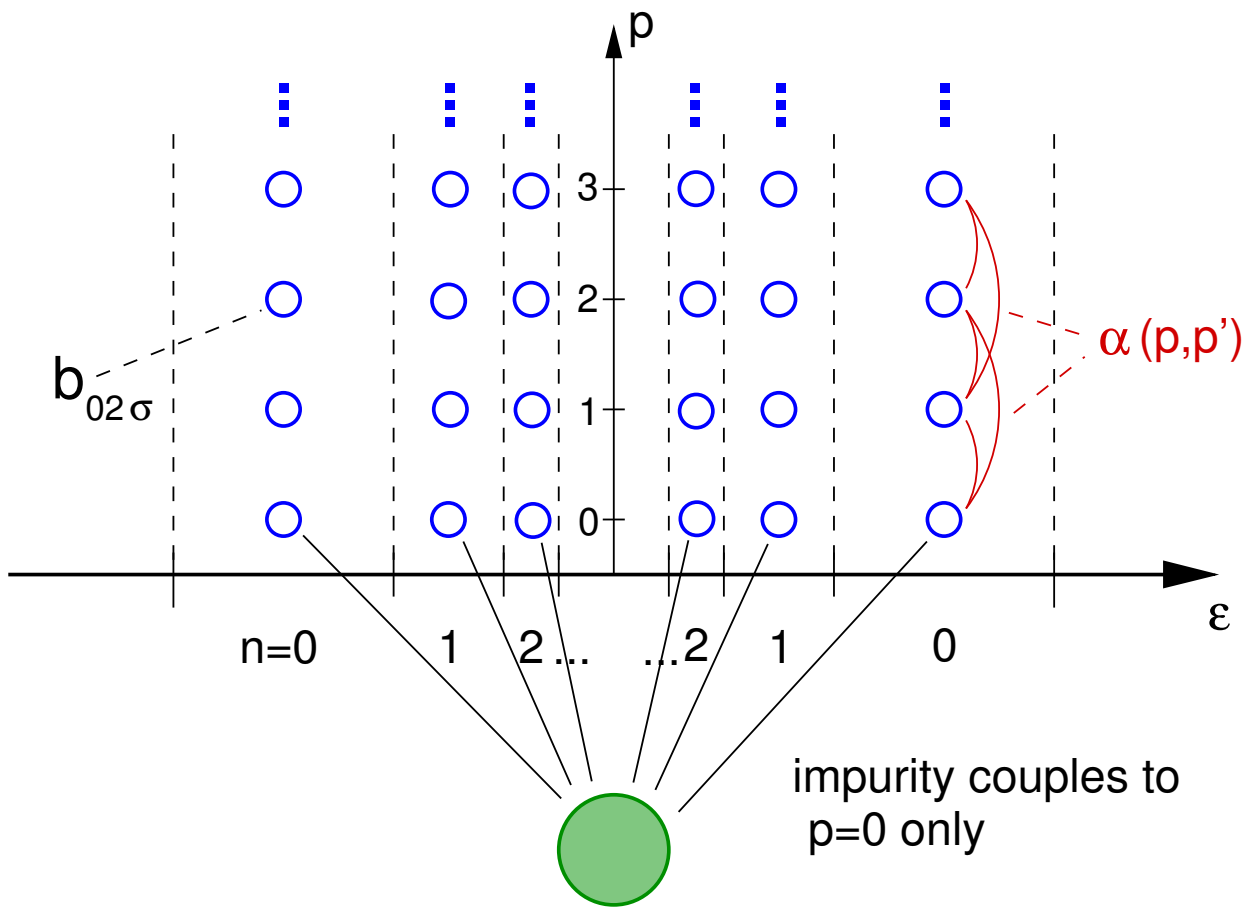
$$\int_{-1}^{1} \mathrm{d}\varepsilon\, g(\varepsilon) a^{\dagger}_{\varepsilon\sigma} a_{\varepsilon\sigma} = \sum_{np} \left(\xi^{+}_{n} a^{\dagger}_{np\sigma} a_{np\sigma} + \xi^{-}_{n} b^{\dagger}_{np\sigma} b_{np\sigma} \right)$$
$$+ \sum_{n,p\neq p'} \left(\alpha^{+}_{n}(p,p') a^{\dagger}_{np\sigma} a_{np'\sigma} - \alpha^{-}_{n}(p,p') b^{\dagger}_{np\sigma} b_{np'\sigma} \right) .$$

For a linear dispersion, $g(\varepsilon) = \varepsilon$, one obtains:

$$\xi^{\pm}_{n} = \pm \frac{1}{2} \Lambda^{-n} (1 + \Lambda^{-1}) ,$$

$$\alpha^{\pm}_{n}(p,p') = \frac{1 - \Lambda^{-1}}{2\pi i} \frac{\Lambda^{-n}}{p' - p} \exp\left[\frac{2\pi i (p' - p)}{1 - \Lambda^{-1}} \right] .$$

structure of the Hamiltonian

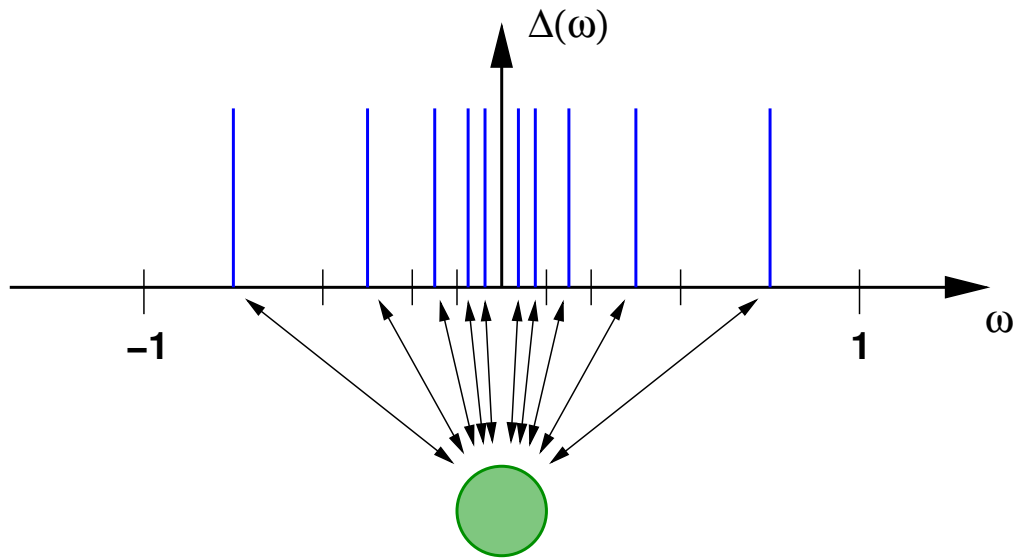


discretization of the Hamiltonian:

drop the terms with $p \neq 0$ in the conduction band

now: relabel the operators $a_{n0\sigma} \equiv a_{n\sigma}$, etc.,
the discretized Hamiltonian takes the form:

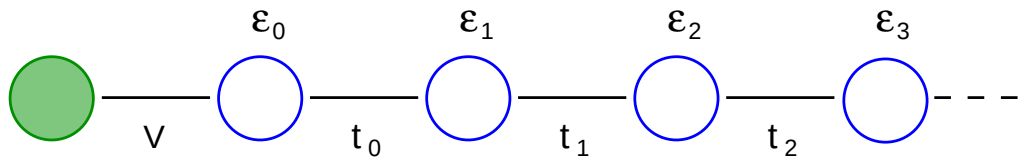
$$
\begin{aligned}
H &= H_{\text{imp}} + \sum_{n\sigma} \left[\xi_n^+ a_{n\sigma}^\dagger a_{n\sigma} + \xi_n^- b_{n\sigma}^\dagger b_{n\sigma} \right] \\
&+ \frac{1}{\sqrt{\pi}} \sum_\sigma f_\sigma^\dagger \left[\sum_n \left(\gamma_n^+ a_{n\sigma} + \gamma_n^- b_{n\sigma} \right) \right] \\
&+ \frac{1}{\sqrt{\pi}} \sum_\sigma \left[\sum_n \left(\gamma_n^+ a_{n\sigma}^\dagger + \gamma_n^- b_{n\sigma}^\dagger \right) \right] f_\sigma
\end{aligned}
$$



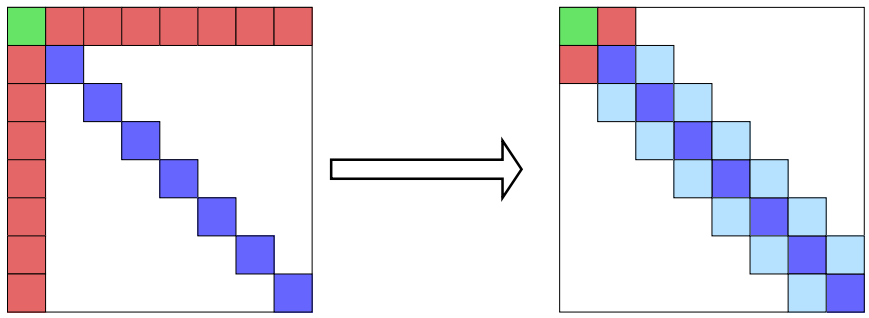
mapping on a semi-infinite chain

orthogonal transformation of the operators $\{a_{n\sigma}, b_{n\sigma}\}$ to a new set of operators $\{c_{n\sigma}\}$ such that the discretized Hamiltonian takes the form:

$$
\begin{aligned}
H &= H_{\text{imp}} + V \sum_{\sigma} \left[f_{\sigma}^{\dagger} c_{0\sigma} + c_{0\sigma}^{\dagger} f_{\sigma} \right] \\
&+ \sum_{\sigma n=0}^{\infty} \left[\varepsilon_n c_{n\sigma}^{\dagger} c_{n\sigma} + t_n \left(c_{n\sigma}^{\dagger} c_{n+1\sigma} + c_{n+1\sigma}^{\dagger} c_{n\sigma} \right) \right]
\end{aligned}
$$



the mapping is equivalent to the tridiagonalization of a matrix



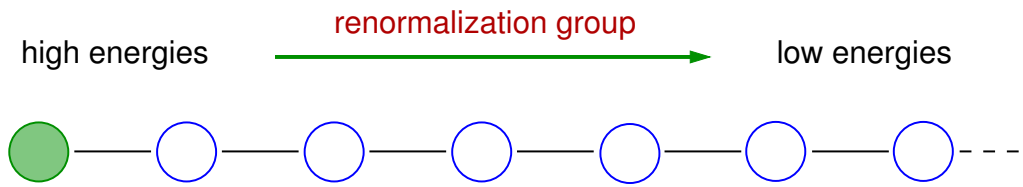
for a constant density of states

$$t_n = \frac{\left(1+\Lambda^{-1}\right)\left(1-\Lambda^{-n-1}\right)}{2\sqrt{1-\Lambda^{-2n-1}}\sqrt{1-\Lambda^{-2n-3}}}\,\Lambda^{-n/2}\,.$$

In the limit of large n this reduces to

$$t_n \longrightarrow \frac{1}{2}\left(1+\Lambda^{-1}\right)\Lambda^{-n/2}\,.$$

this means: in moving along the chain we start from high energies (U, V, D)
and go to arbitrary low energies



in real space: double the system size by adding two sites to the chain
(for $\Lambda = 2$)

iterative diagonalization

the chain Hamiltonian can be viewed as a series of Hamiltonians H_N ($N = 0, 1, 2, \ldots$) which approaches H in the limit $N \to \infty$:

$$H = \lim_{N\to\infty} \Lambda^{-(N-1)/2} H_N \ ,$$

with

$$H_N = \Lambda^{(N-1)/2} \Bigg[H_{\rm imp} + \sqrt{\frac{\xi_0}{\pi}} \sum_\sigma \left(f_\sigma^\dagger c_{0\sigma} + c_{0\sigma}^\dagger f_\sigma \right)$$
$$+ \sum_{\sigma\, n=0}^{N} \varepsilon_n c_{n\sigma}^\dagger c_{n\sigma} + \sum_{\sigma\, n=0}^{N-1} t_n \left(c_{n\sigma}^\dagger c_{n+1\sigma} + c_{n+1\sigma}^\dagger c_{n\sigma} \right) \Bigg] \ .$$

two successive Hamiltonians are related by

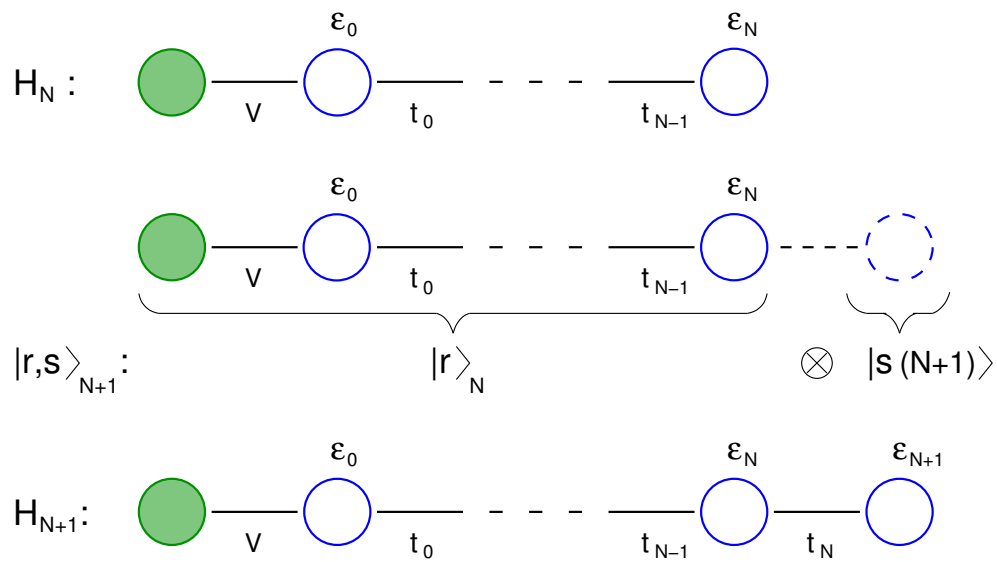
$$H_{N+1} = \sqrt{\Lambda} H_N + \Lambda^{N/2} \sum_\sigma \varepsilon_{N+1} c_{N+1\sigma}^\dagger c_{N+1\sigma}$$
$$+ \Lambda^{N/2} \sum_\sigma t_N \left(c_{N\sigma}^\dagger c_{N+1\sigma} + c_{N+1\sigma}^\dagger c_{N\sigma} \right) \ ,$$

starting point:

$$H_0 = \Lambda^{-1/2}\left[H_{\rm imp} + \sum_\sigma \varepsilon_0 c^\dagger_{0\sigma} c_{0\sigma} + \sqrt{\frac{\xi_0}{\pi}} \sum_\sigma \left(f^\dagger_\sigma c_{0\sigma} + c^\dagger_{0\sigma} f_\sigma \right) \right] .$$

renormalization group transformation:

$$H_{N+1} = R\left(H_N\right)$$

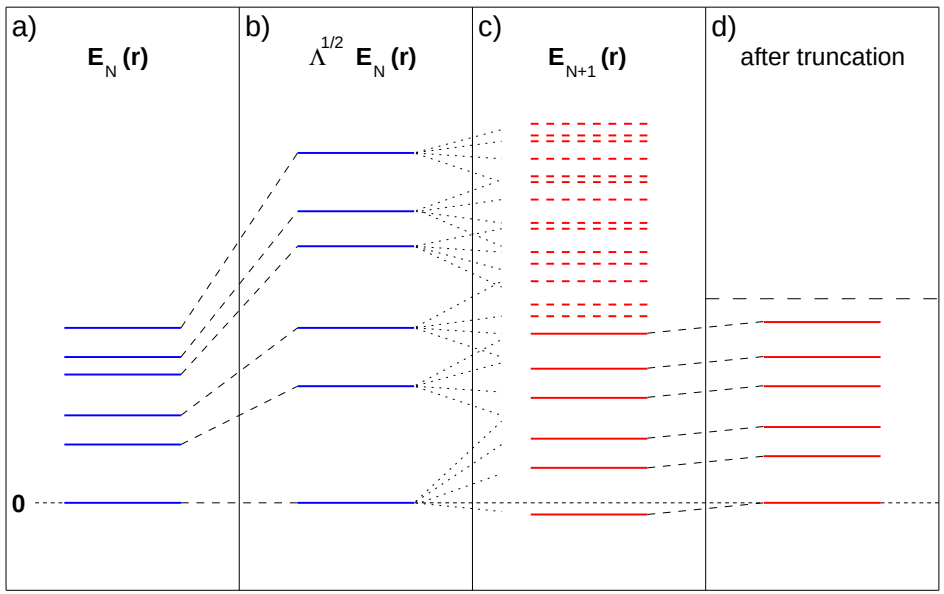


set up an iterative scheme for the diagonalization of H_N
$\rightarrow$ construct a basis for H_{N+1}

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

diagonalization: new eigenenergies $E_{N+1}(w)$ and eigenstates $|w\rangle_{N+1}$

truncation:

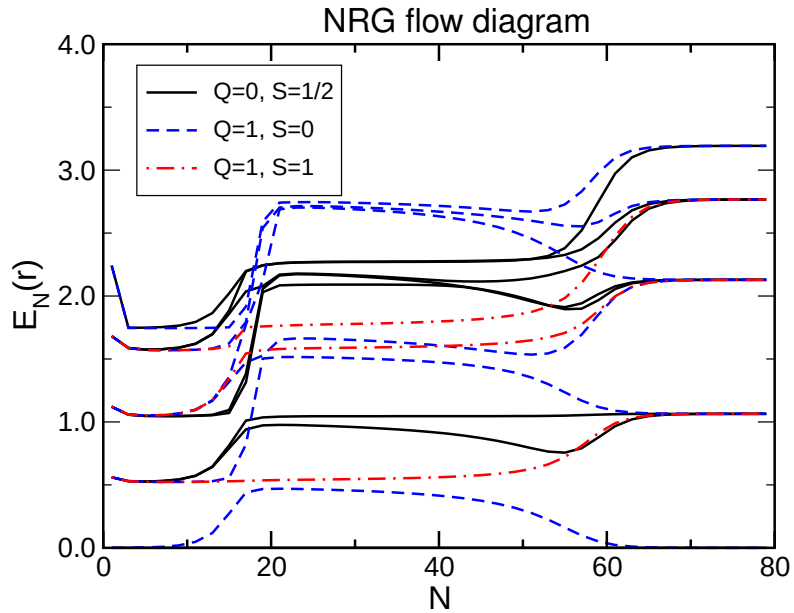


renormalization group flow and fixed points

plot the rescaled many-particle energies $E_N(r)$ as a function of N (odd N only)

fixed points of the
single-impurity Anderson model

FO: free orbital
LM: local moment
SC: strong coupling



parameters: $\varepsilon_f = -0.5 \cdot 10^{-3}$, $U = 10^{-3}$, $V = 0.004$, and $\Lambda = 2.5$

renormalization group flow and fixed points

plot the rescaled many-particle energies $E_N(r)$ as a function of N (odd N only)

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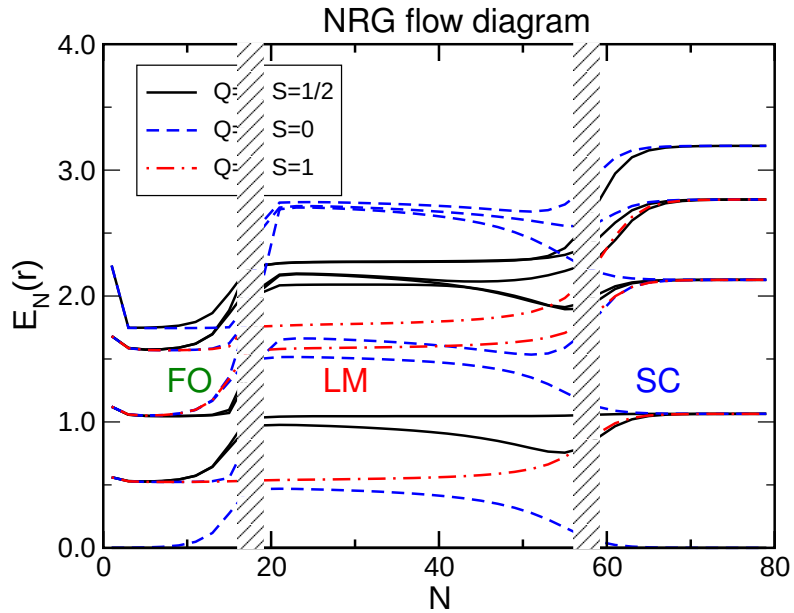


parameters: $\varepsilon_f = -0.5 \cdot 10^{-3}$, $U = 10^{-3}$, $V = 0.004$, and $\Lambda = 2.5$

4. fixed points in quantum impurity models

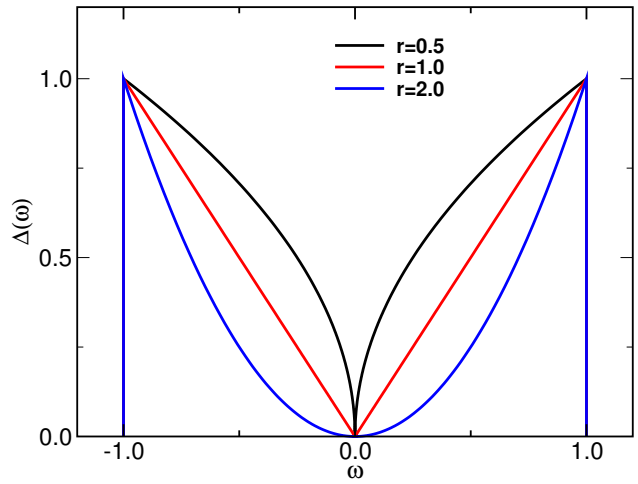
quantum impurity models show a variety of different fixed points

here:

- quantum critical point in the soft-gap Anderson model

  single-impurity Anderson model
  with hybridization function
  $\Delta(\omega) = \Delta|\omega|^r$

  $\longrightarrow$ interacting fixed point

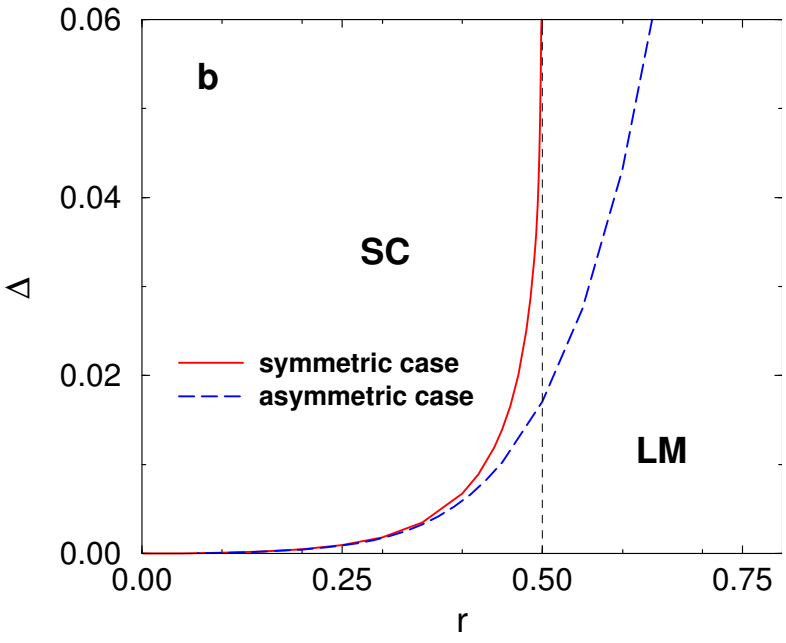


- non-Fermi liquid fixed point in the two-channel Kondo model

  $\longrightarrow$ Majorana fermions

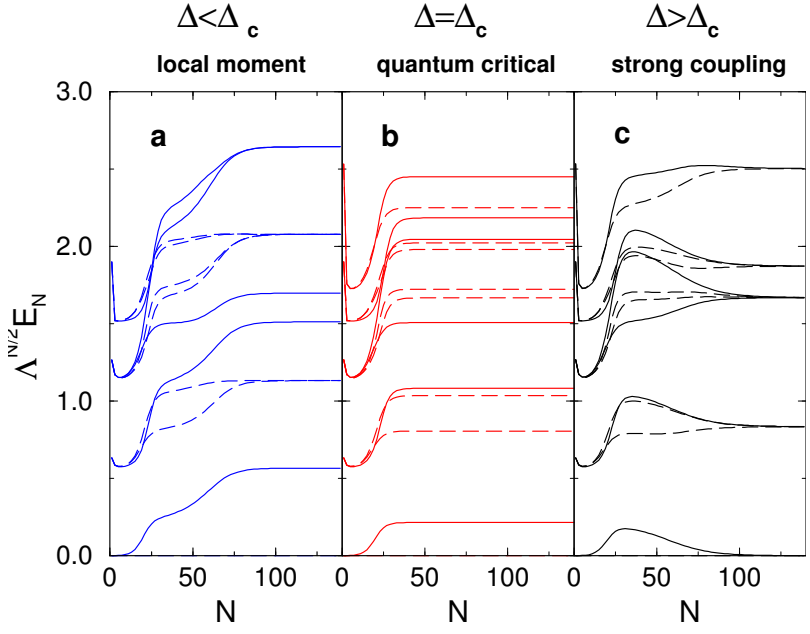
soft-gap Anderson model

phase diagram



quantum phase transition
between SC and LM phases

flow diagrams



non-trivial structure of the qcp

[H.-J. Lee, R. Bulla, M. Vojta
J. Phys.: Condens. Matter **17**, 6935 (2005)]

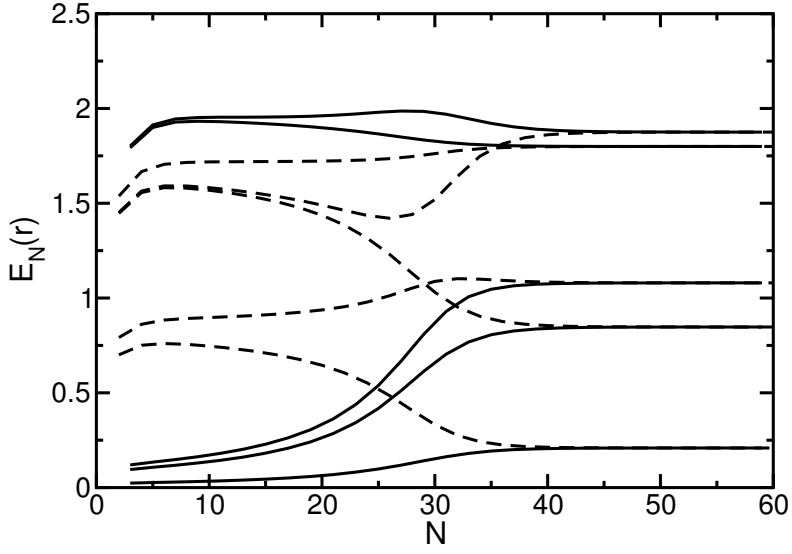
two-channel Kondo model

$$H = \sum_{k\sigma} \sum_{\alpha} \varepsilon_k c^{\dagger}_{k\sigma\alpha} c_{k\sigma\alpha} + J \sum_{\alpha} \vec{S} \cdot \vec{s_{\alpha}}$$

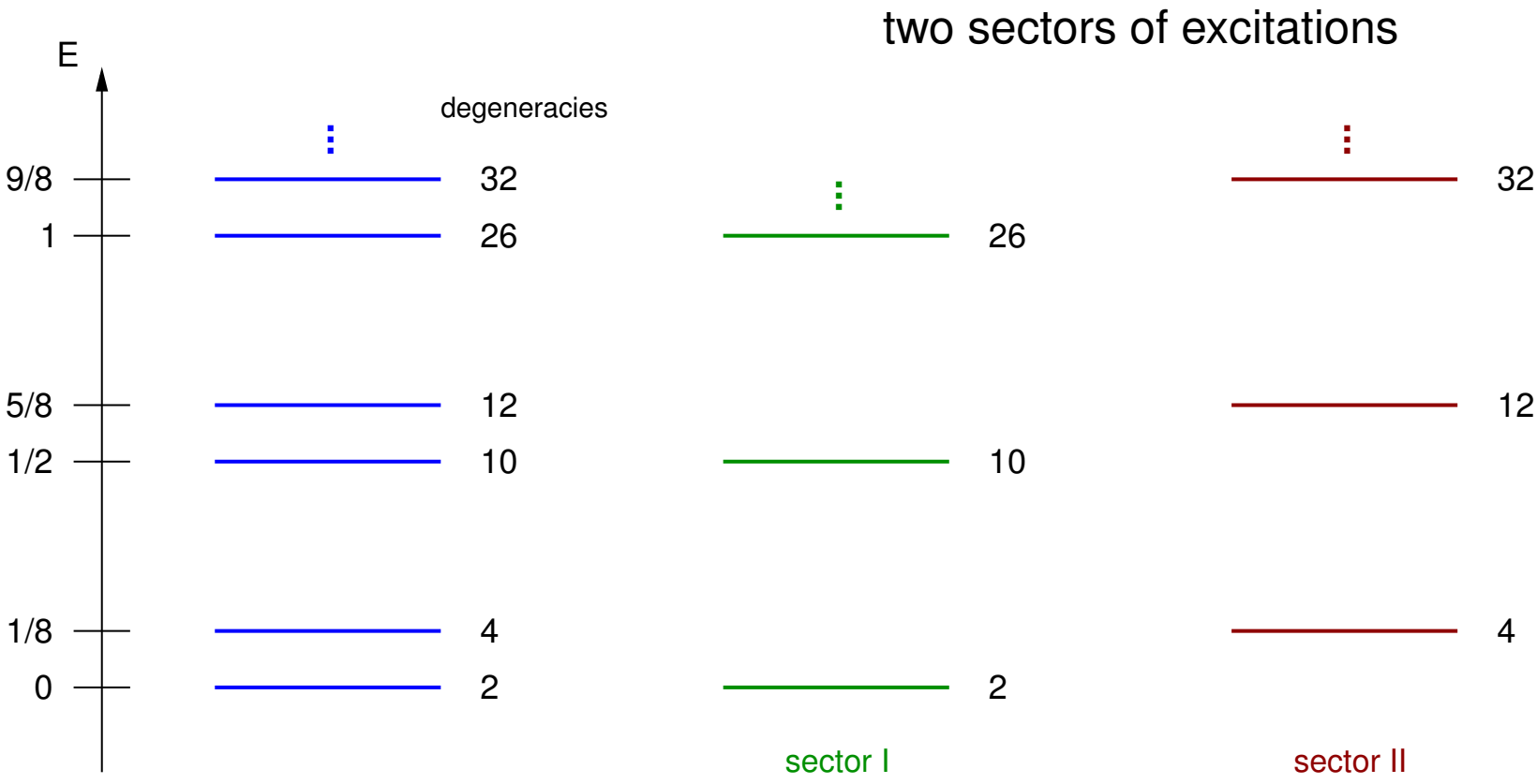
$\rightarrow$ non-Fermi liquid fixed point with residual impurity entropy $S_{\mathrm{imp}} = \frac{1}{2} \ln 2$

NRG flow diagram

$\rightarrow$ characteristic structure of the non-Fermi liquid fixed point

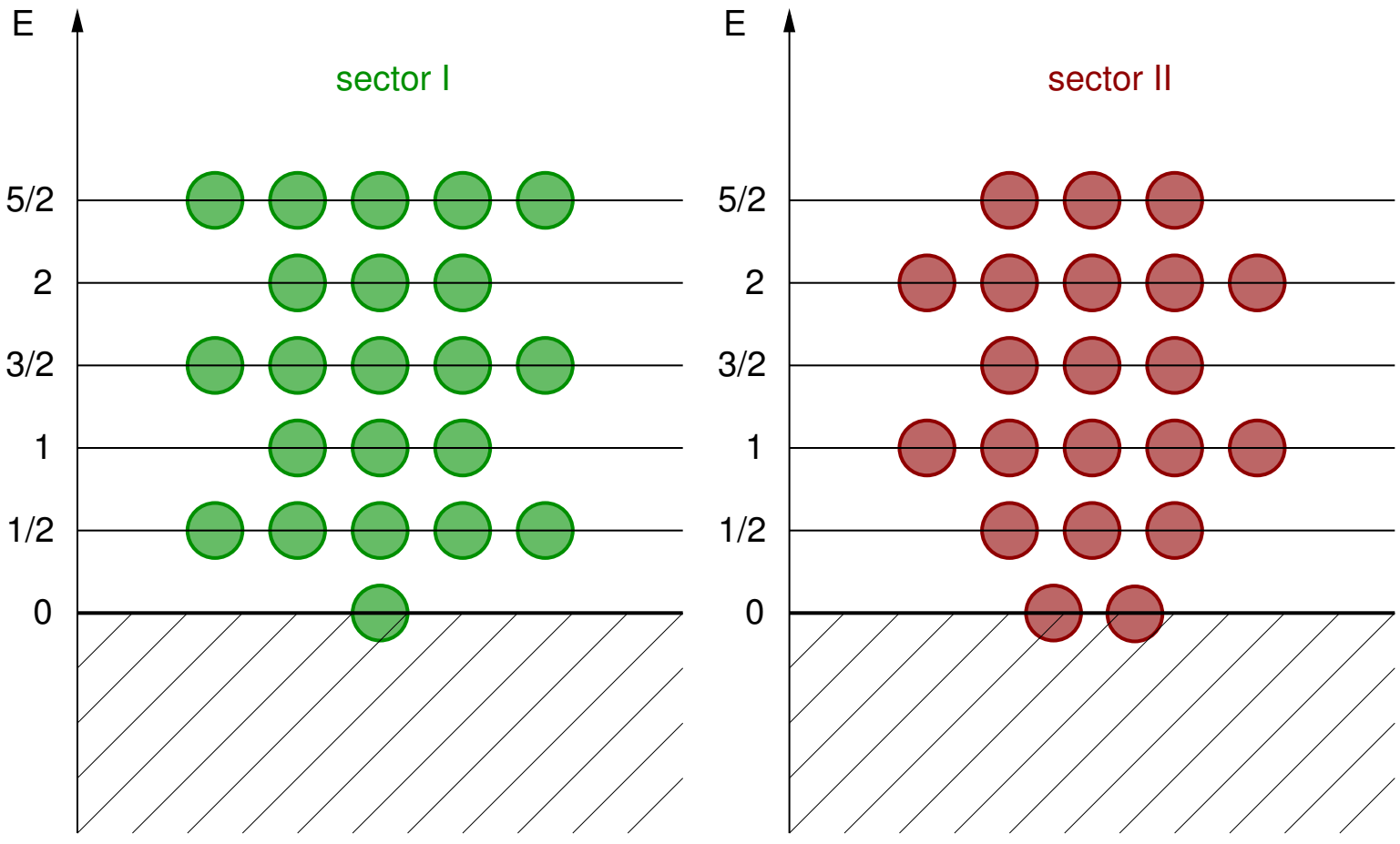


structure of the fixed point



the many-particle spectra of each sector can be constructed from single-particle spectra of Majorana fermions

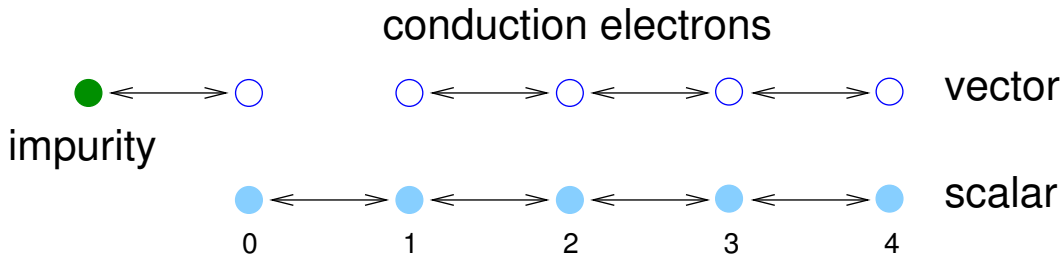
single-particle spectra



[R. Bulla, A.C. Hewson, G.-M. Zhang, Phys. Rev. B **56**, 11721 (1997)]

where does this structure come from?

$\rightarrow$ vector and scalar Majorana fermion chains with different boundary conditions



from the numerical analysis of the two-channel Anderson model we obtain

emergent fractionalized degrees of freedom (Majorana fermions) at the low-energy fixed point!

a quotation from:
Universality and Scaling in a Charge Two-Channel Kondo Device
A.K. Mitchell, L.A. Landau, L. Fritz, and E. Sela, Phys. Rev. Lett. **116**, 157202 (2016)

> *Finally, we highlight a perspective on these results, connected with the ongoing search for Majorana fermions. The quantitative agreement between theory and experiment over 9 orders of magnitude in T / T_K proves that this device realizes a non-Fermi liquid state involving a free Majorana localized on the dot, described by the 2CK critical fixed point. These results therefore unambiguously establish the existence of Majorana fermions in this frustrated strongly interacting system.*

5. calculation of physical properties and applications

What can we do with the NRG?

calculation of physical properties	of a	quantum impurity model	to explain/ understand	exp. results/ physical phenomena

- thermodynamics
- dynamic correlation functions
- non–equilibrium properties

- one or several impurities
- one or several fermionic/bosonic baths
- lattice models in DMFT

- Kondo physics
- non–Fermi liquid physics and quantum criticality
- transport in quantum dot systems

calculation of physical properties

A. thermodynamics

use the spectra of many-particle energies $E_N(r)$ at each iteration to calculate thermodynamic/static properties at a corresponding temperature

$$T_N \propto \Lambda^{-N/2}$$

$\rightarrow$ specific heat $C(T)$, susceptibility $\chi(T)$, etc.

B. dynamic properties

example: single-particle Green function

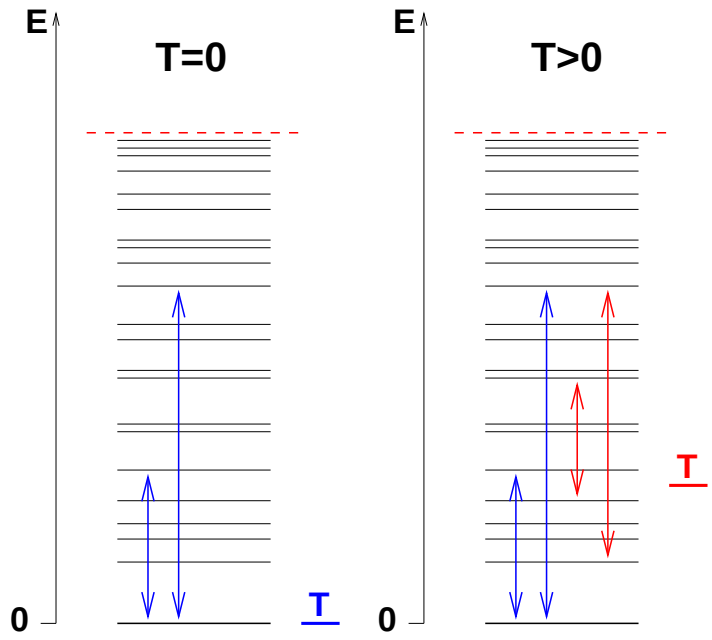
$$G_\sigma(z) = \langle\langle f_\sigma, f_\sigma^\dagger \rangle\rangle_z = i \int_0^\infty \mathrm{d}t \; e^{izt} \langle [f_\sigma(t), f_\sigma^\dagger]_+ \rangle \tag{1}$$

spectral function:

$$A(\omega) = -\frac{1}{\pi} \mathrm{Im}\; G(\omega + i\delta^+) \;, \tag{2}$$

In each iteration, calculate the spectral function for each cluster of size N via:

$$A_{\sigma N}(\omega) = \frac{1}{Z_N} \sum_{nm} \left| {}_N\left\langle n \left| f_\sigma^\dagger \right| m \right\rangle_N \right|^2 \delta\left(\omega - (E_n^N - E_m^N)\right) \left(e^{-\beta E_m^N} + e^{-\beta E_n^N}\right) \quad (3)$$

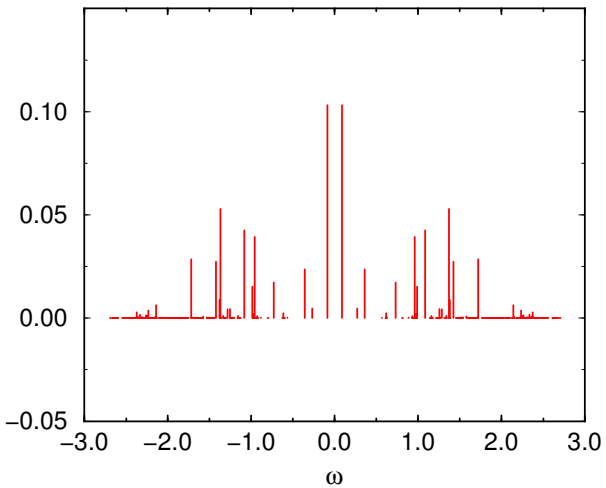


$T = 0$: transitions between ground state and all excited states

$T > 0$: in addition: transitions between excited states

effect of the truncation on the spectral functions of each iteration:

$N = 14$



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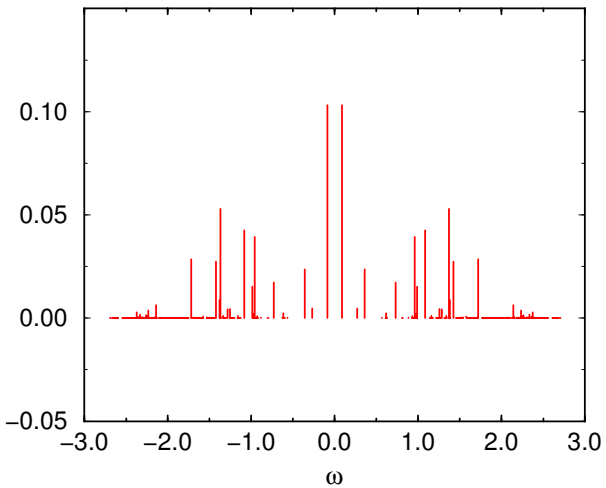
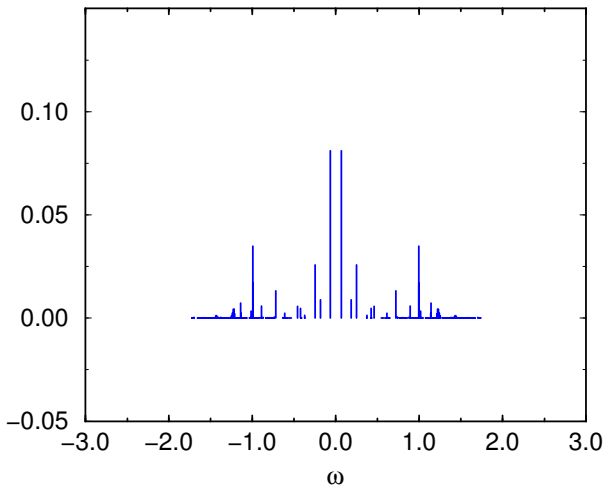


$N = 16$



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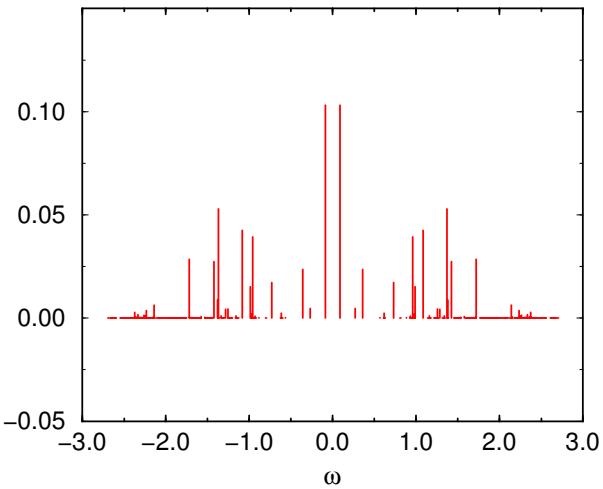
$N = 14$



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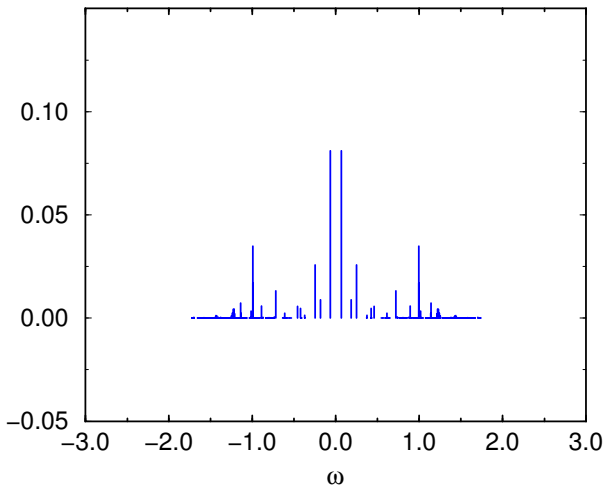
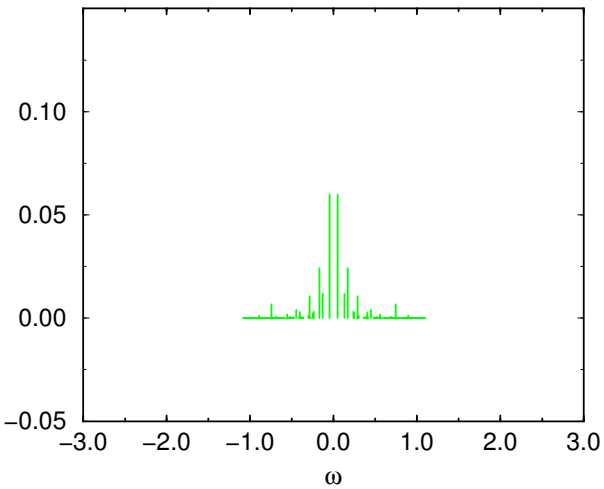


$N = 18$



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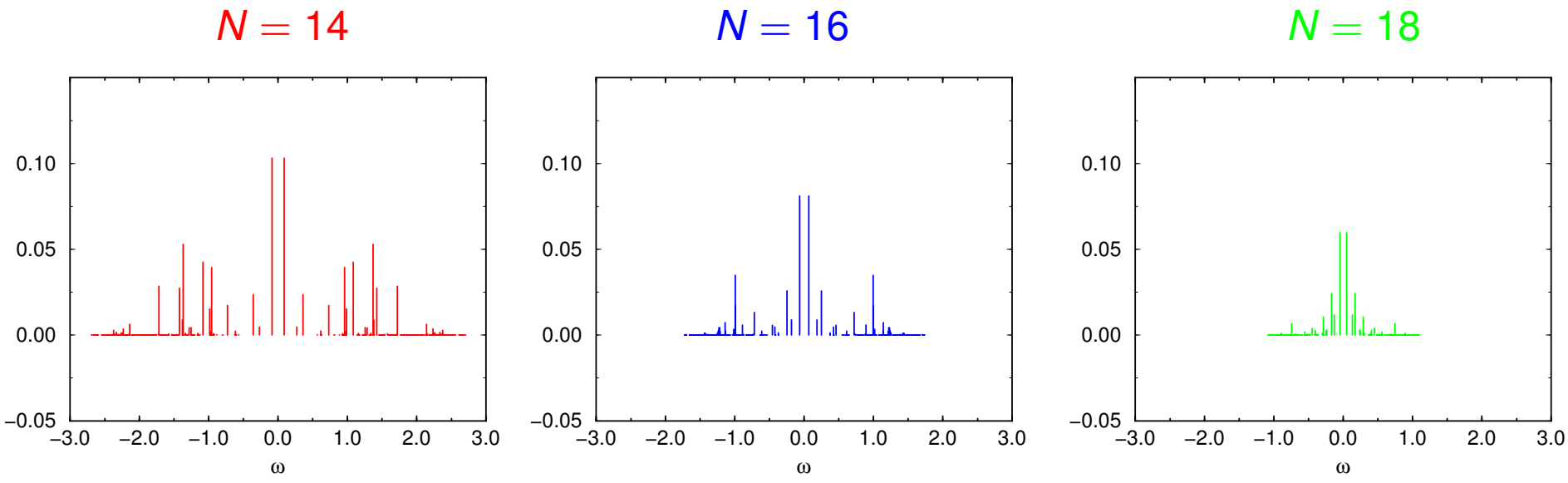
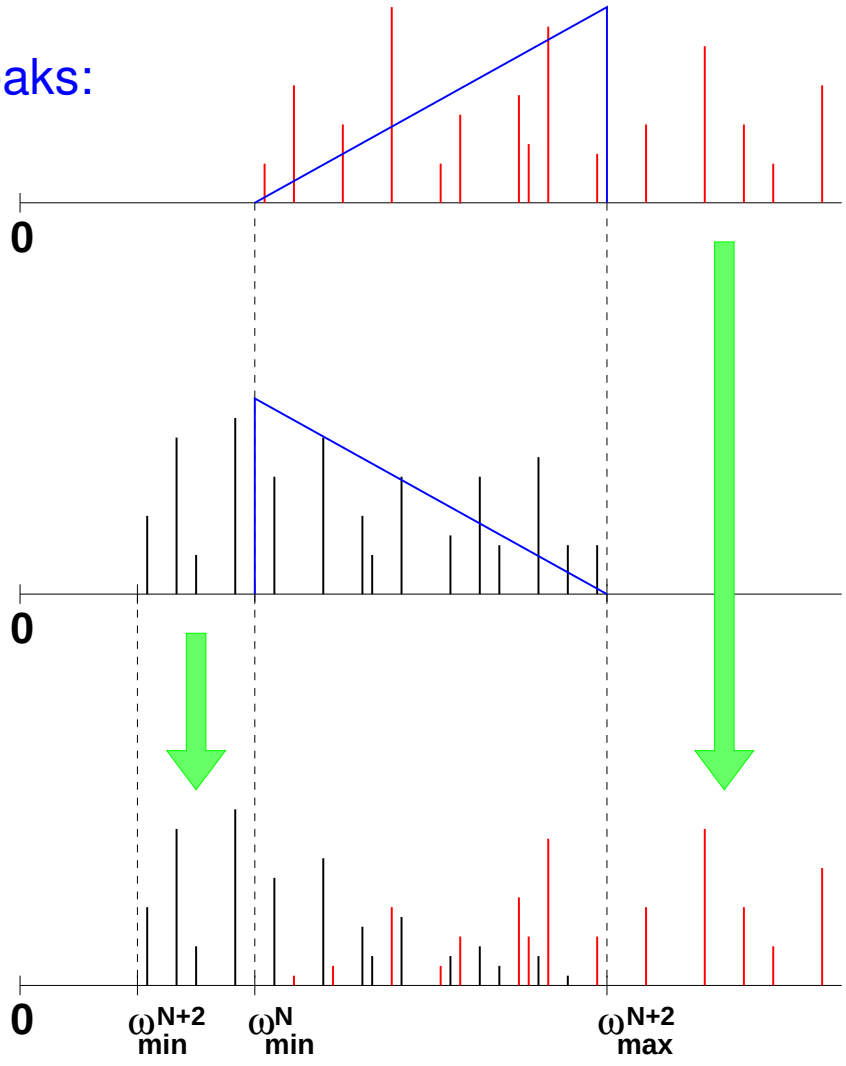


this means:
final spectral function = superposition of the data from all iterations

superposition of δ-Peaks:



finally: broadening of the δ-peaks $\longrightarrow$ Gaussian on a logarithmic scale

$$\delta(\omega - \omega_n) \to \frac{e^{-b^2/4}}{b\,\omega_n\sqrt{\pi}} \exp\left[-\frac{(\ln\omega - \ln\omega_n)^2}{b^2}\right] \tag{4}$$

results for the single-impurity Anderson model:

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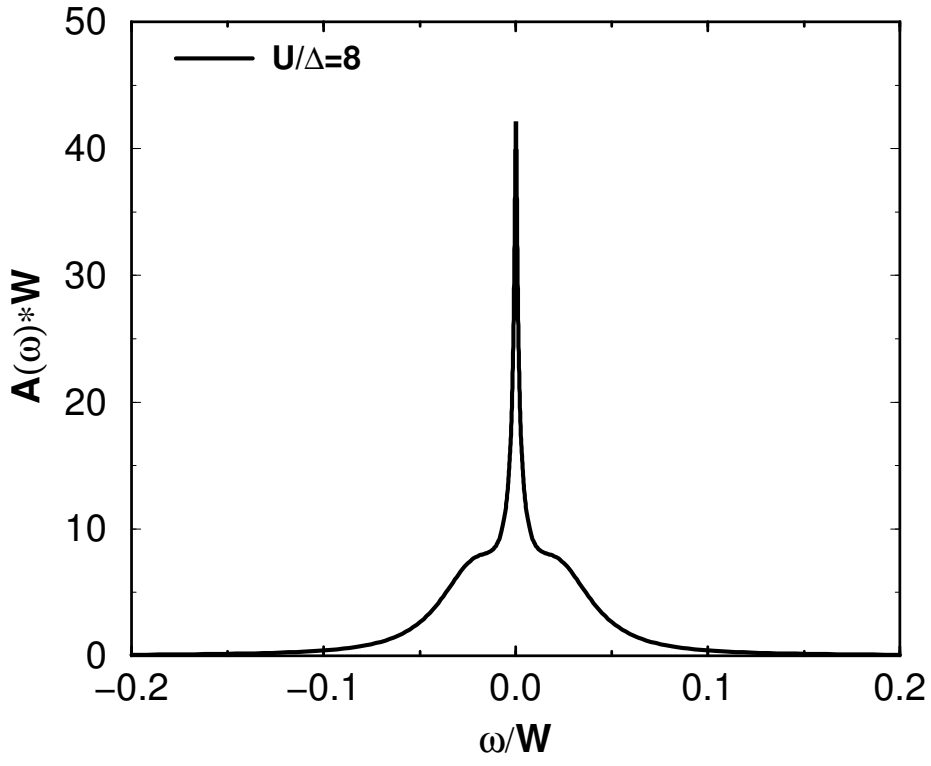

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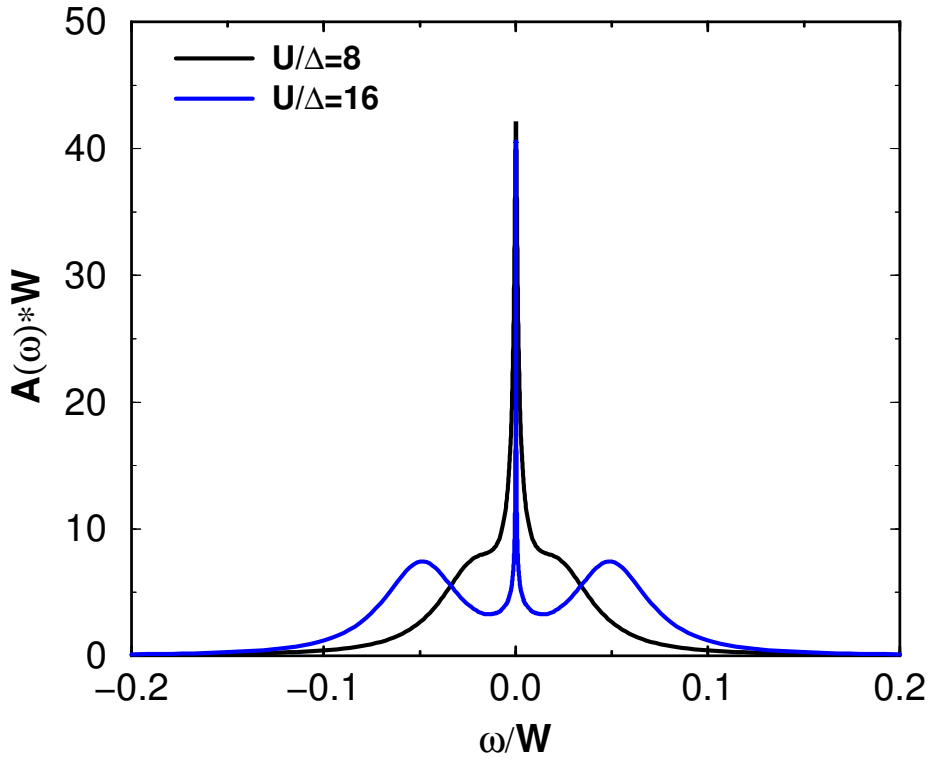

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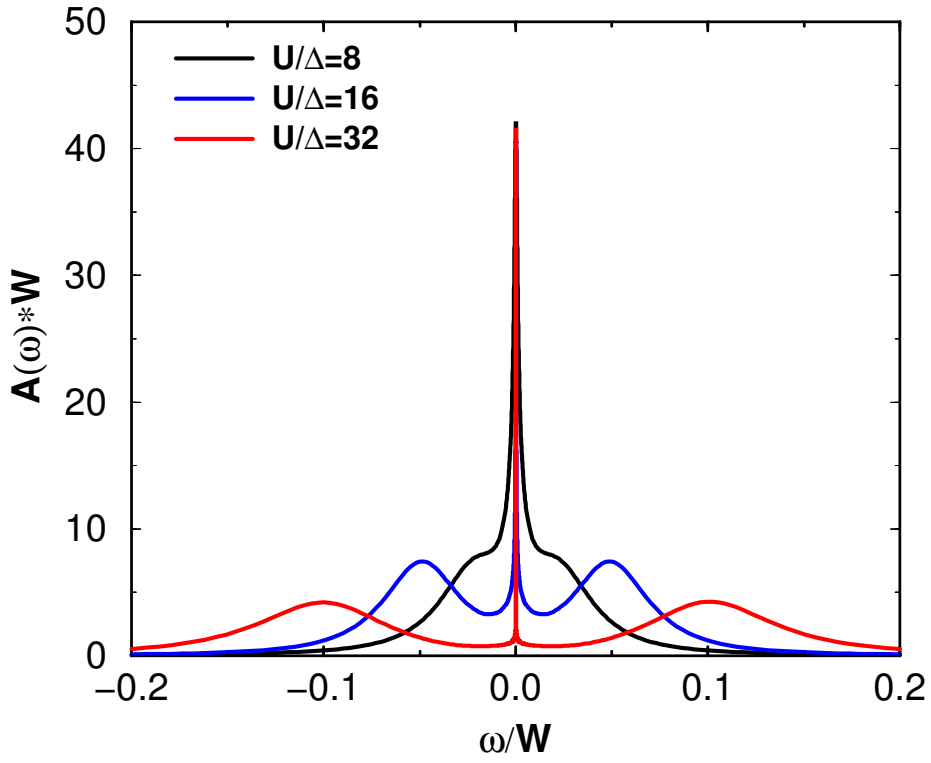
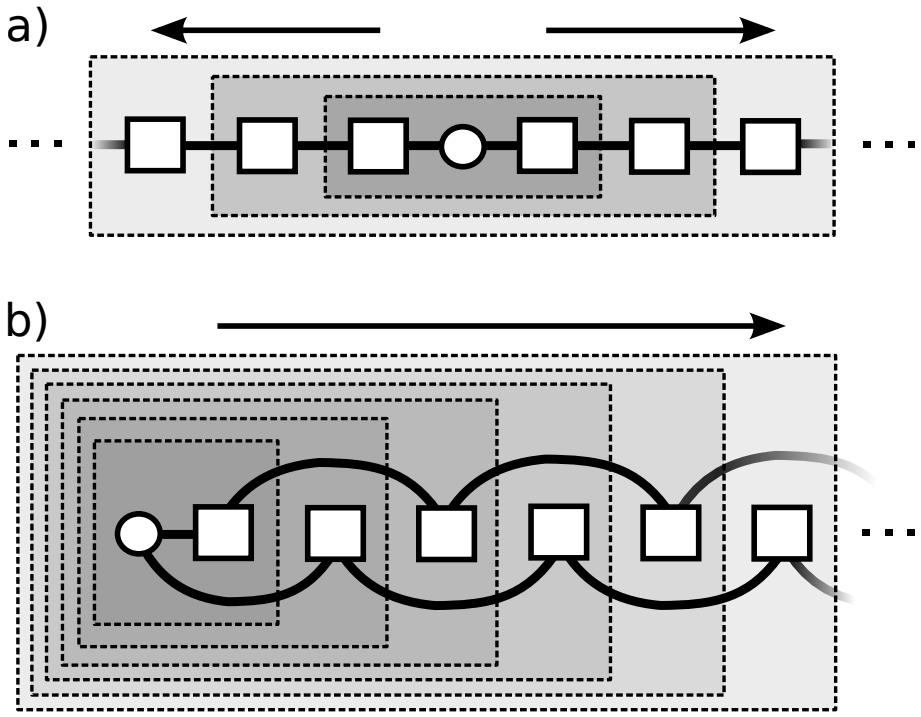


NRG for multi-channel models

A.K. Mitchell, M.R. Galpin, S. Wilson-Fletcher, D.E. Logan, and R. Bulla
Generalized Wilson chain for solving multichannel quantum impurity problems
Phys. Rev. B **89**, 121105(R) (2014)



standard approach

interleaved NRG

6. summary

in this talk:

- a short introduction to
  - the renormalization group concept
  - quantum impurity physics
  - the NRG method
    - flow diagrams and fixed points
    - calculation of physical properties

I did **not** discuss:

- quantum dots and Kondo physics
- non-equilibrium properties
- all the recent developments which considerably extended the power of the NRG method; see the work of
  - F. Anders, Th. Costi, J. von Delft, A. Mitchell, A. Weichselbaum, ...
- relation to other renormalization group methods
  - DMRG
  - fRG