The Numerical Renormalization Group

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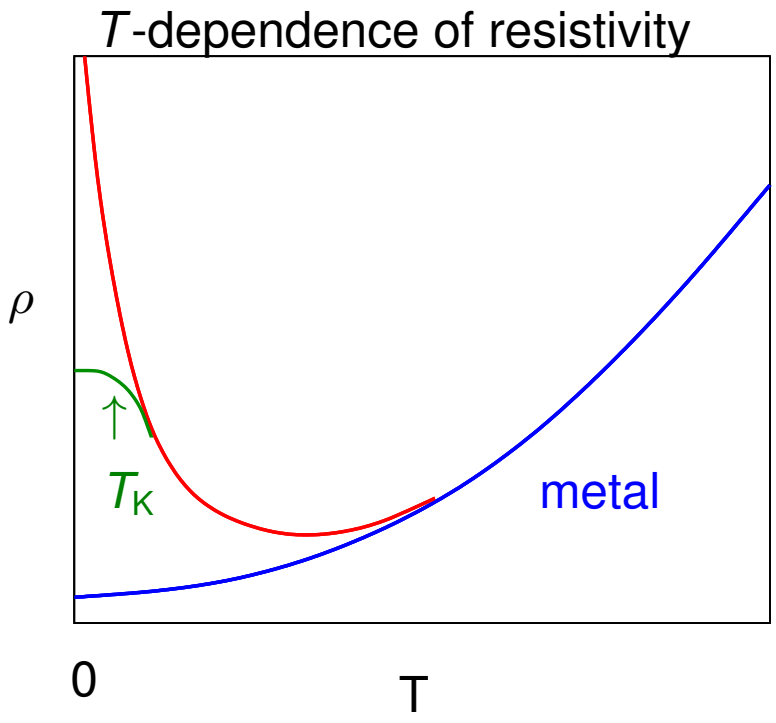
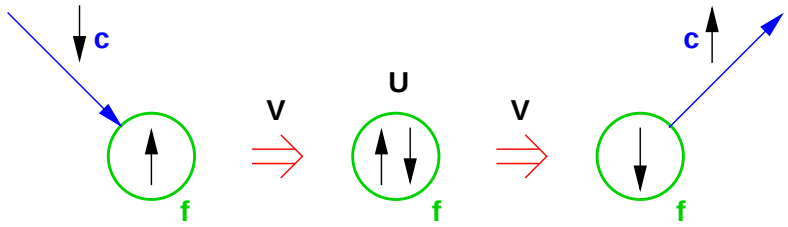
Contents

1. Introduction

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

available methods

- Bethe ansatz
- density matrix renormalization group
- equations of motion
- exact diagonalization
- local moment approach
- non-crossing approximation
- numerical renormalization group
- quantum Monte Carlo
- perturbation theory

2. The single-impurity Anderson model

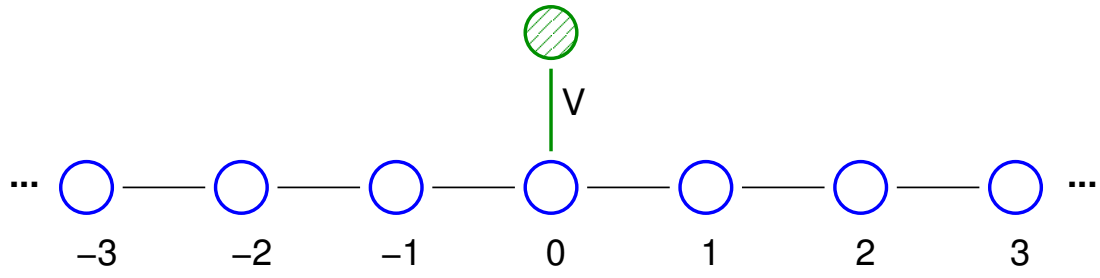
quantum impurity models

$$H = H_{\text{imp}} + H_{\text{bath}} + H_{\text{imp}-\text{bath}} \ .$$

in the single-impurity Anderson model

$$H_{\text{imp}} = \sum_{\sigma} \varepsilon_{\text{f}} f_{\sigma}^{\dagger} f_{\sigma} + U f_{\uparrow}^{\dagger} f_{\uparrow} f_{\downarrow}^{\dagger} f_{\downarrow} \ ,$$

a specific geometry



bath: one-dimensional tight-binding chain

$$H_{\text{bath}} = \sum_{\sigma} \sum_{l=-\infty}^{\infty} \varepsilon_l \, c_{l\sigma}^{\dagger} c_{l\sigma} + \sum_{\sigma} \sum_{l=-\infty}^{\infty} t_l \left(c_{l\sigma}^{\dagger} c_{l+1\sigma} + c_{l+1\sigma}^{\dagger} c_{l\sigma} \right) \ .$$

impurity-bath coupling

$$H_{\mathrm{imp-bath}} = V \sum_{\sigma} \left(f_{\sigma}^{\dagger} c_{0\sigma} + c_{0\sigma}^{\dagger} f_{\sigma} \right) \ ,$$

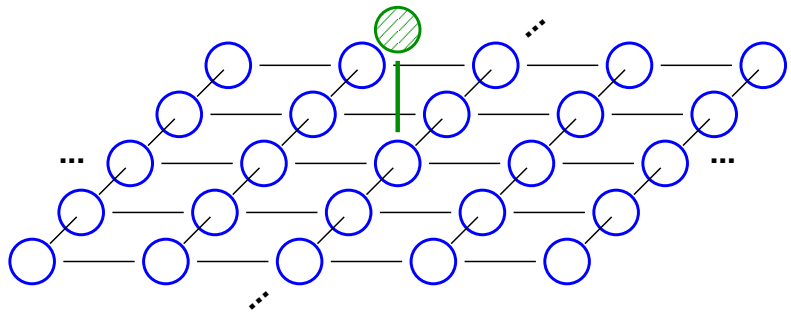
general form of the bath

$$H_{\mathrm{bath}} = \sum_{\sigma l} \varepsilon_l c_{l\sigma}^{\dagger} c_{l\sigma} + \sum_{\sigma} \sum_{ij} t_{ij} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) \ .$$

$$H_{\mathrm{bath}} = \sum_{\sigma} \vec{c_{\sigma}}^{\,\dagger} \, T \vec{c_{\sigma}} \ \text{ with } \ \vec{c_{\sigma}}^{\,\dagger} = \left(\ldots, c_{-1\sigma}^{\dagger}, c_{0\sigma}^{\dagger}, c_{1\sigma}^{\dagger}, \ldots \right) \ ,$$

site-representation of the siAm

example



diagonal form of the bath

$$H_{\text{bath}} = \sum_{\sigma k} \varepsilon_k b^{\dagger}_{k\sigma} b_{k\sigma} \ ,$$

orthogonal tranformation

$$c_{i\sigma} = \sum_{k} a_{ik} b_{k\sigma} \quad , \quad c^{\dagger}_{i\sigma} = \sum_{k} a^{*}_{ik} b^{\dagger}_{k\sigma} \ .$$

The a_{ik} are the matrix elements of the unitary matrix A which diagonalizes the matrix T

$$\left(A^{t} T A \right)_{kq} = \varepsilon_k \delta_{kq} \ .$$

hybridization term

$$H_{\text{imp}-\text{bath}} = \sum_{k\sigma} V_k \left(f^{\dagger}_{\sigma} b_{k\sigma} + b^{\dagger}_{k\sigma} f_{\sigma} \right) \ ,$$

with $V_k = V a_{0k}$.

k-representation of the siAm

single-particle Green function $G_\sigma(z) = \langle\langle f_\sigma, f_\sigma^\dagger \rangle\rangle_z$ can be written in the form

$$G_\sigma(z) = \frac{1}{z - \varepsilon_f - \bar{\Delta}(z) - \Sigma^U(z)} \quad , \quad (z = \omega + i\delta) \; ,$$

with $\Sigma^U(z)$ the correlation part of the one-particle self energy

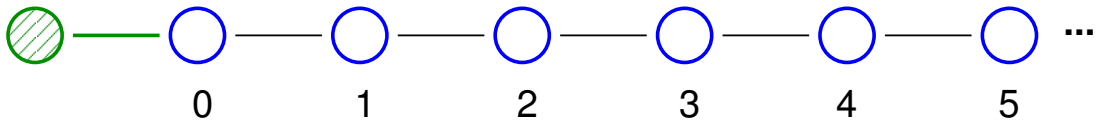
equations of motion give for the hybridization function:

$$\bar{\Delta}(z) = \sum_k V_k^2 \frac{1}{z - \varepsilon_k} \; .$$

imaginary part of $\bar{\Delta}(z)$

$$\Delta(\omega) = -\lim_{\delta \to 0} \mathrm{Im}\left[\bar{\Delta}(z = \omega + i\delta)\right] = \pi \sum_k V_k^2 \delta(\omega - \varepsilon_k) \; ,$$

another geometry: siAm defined for a semi-infinite chain



$$H_{\text{bath}} = \sum_{\sigma} \sum_{l=0}^{\infty} \varepsilon_l \, c_{l\sigma}^{\dagger} c_{l\sigma} + \sum_{\sigma} \sum_{l=0}^{\infty} t_l \left(c_{l\sigma}^{\dagger} c_{l+1\sigma} + c_{l+1\sigma}^{\dagger} c_{l\sigma} \right) \ ,$$

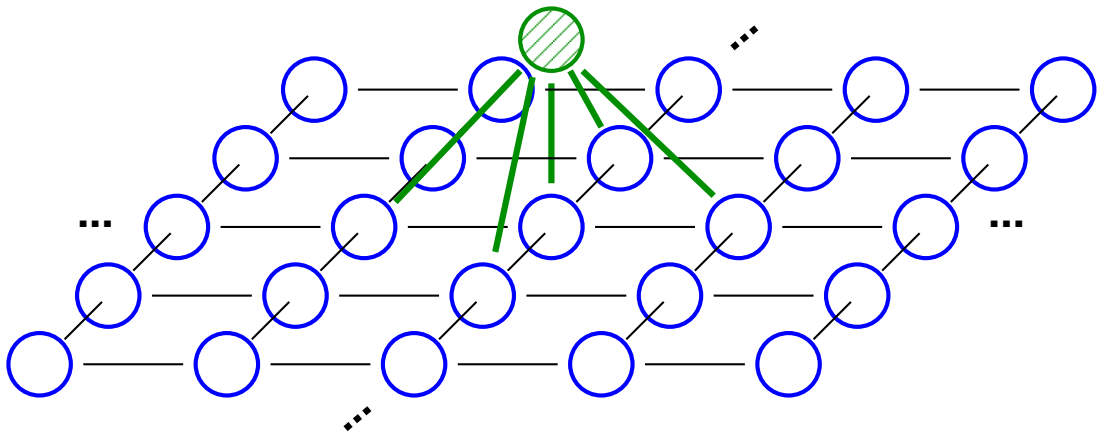
hybridization function can be written as a continued fraction

$$\bar{\Delta}(z) = \cfrac{V^2}{z - \varepsilon_0 - \cfrac{t_0^2}{z - \varepsilon_1 - \cfrac{t_1^2}{z - \varepsilon_2 - \cfrac{t_2^2}{z - \varepsilon_3 - \ldots}}}} \ .$$

generalize the impurity-bath coupling to

$$H_{\mathrm{imp-bath}} = \sum_{\sigma m} V_m \left(f_\sigma^\dagger c_{m\sigma} + c_{m\sigma}^\dagger f_\sigma \right) \ ,$$

example



in the k-representation

$$H_{\mathrm{imp-bath}} = \sum_{k\sigma} V_k \left(f_\sigma^\dagger b_{k\sigma} + b_{k\sigma}^\dagger f_\sigma \right) \ ,$$

with $V_k = \sum_m V_m a_{mk}$

integral representation of the siAm

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

hybridization function

$$
\Delta(\omega) = \pi h(g^{-1}(\omega))^2 \frac{\mathrm{d}}{\mathrm{d}\omega} g^{-1}(\omega) \ ,
$$

with $g^{-1}(\omega)$ the inverse function of $g(\varepsilon)$

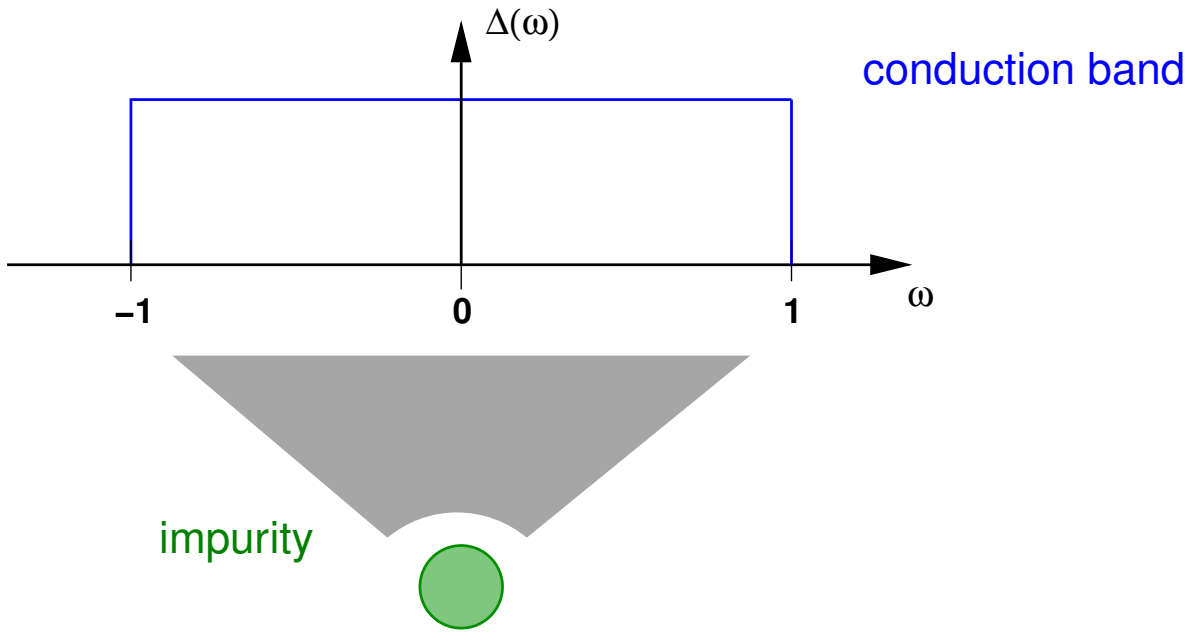
summary of Sec. 2

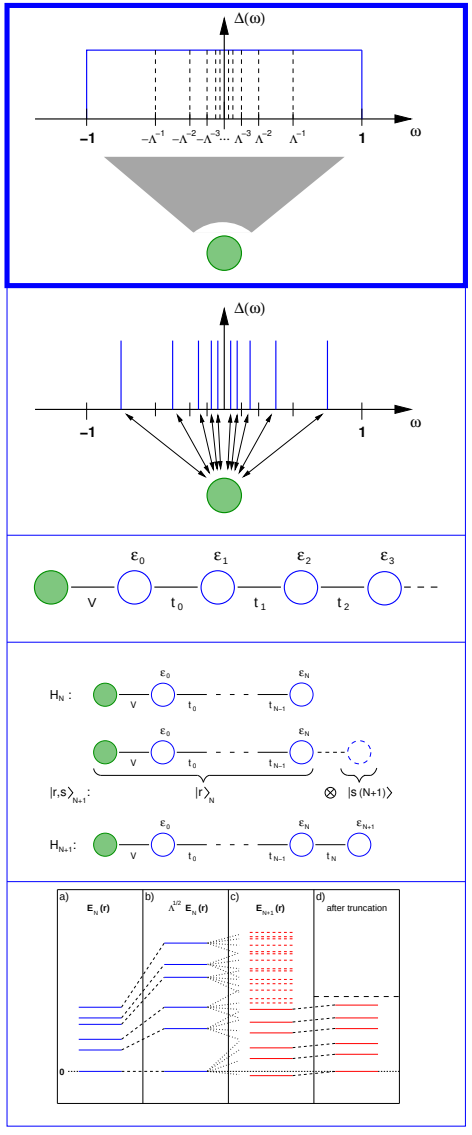
- the impurity-bath coupling and the structure of the bath are encoded in a single frequency-dependent quantity $\rightarrow$ the hybridization function $\Delta(\omega)$
- the dimensionality of the bath does not play a role
- the siAm defined on different geometries might give the same $\Delta(\omega)$; there is no unique mapping of the siAm with a given $\Delta(\omega)$ onto the site-representation
- for a given $\Delta(\omega)$, one can always write the siAm in a one-dimensional form

3. The numerical renormalization group

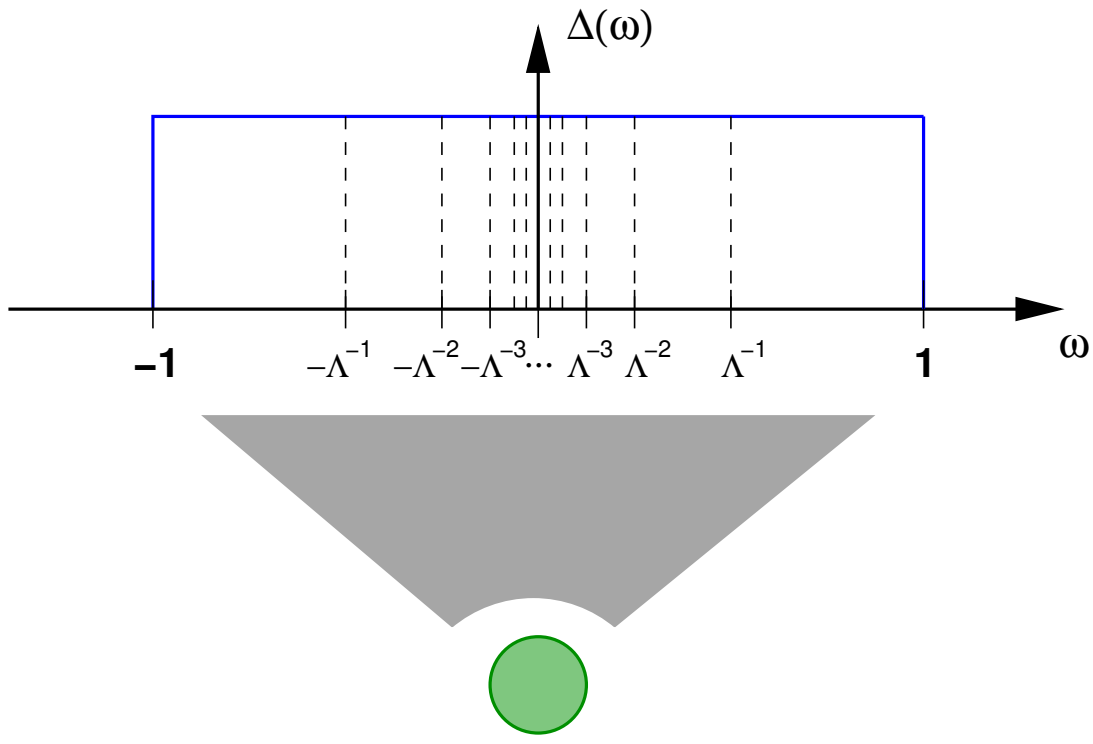
K.G. Wilson, Rev. Mod. Phys. **47**, 773 (1975) $\rightarrow$ Kondo problem

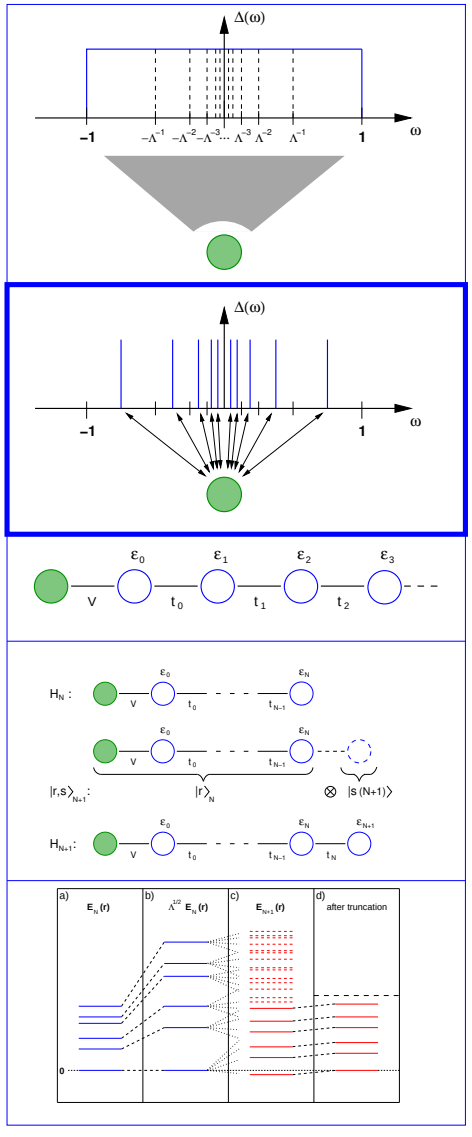
review: R. Bulla, T. Costi, and Th. Pruschke, Rev. Mod. Phys. **80**, 395 (2008)



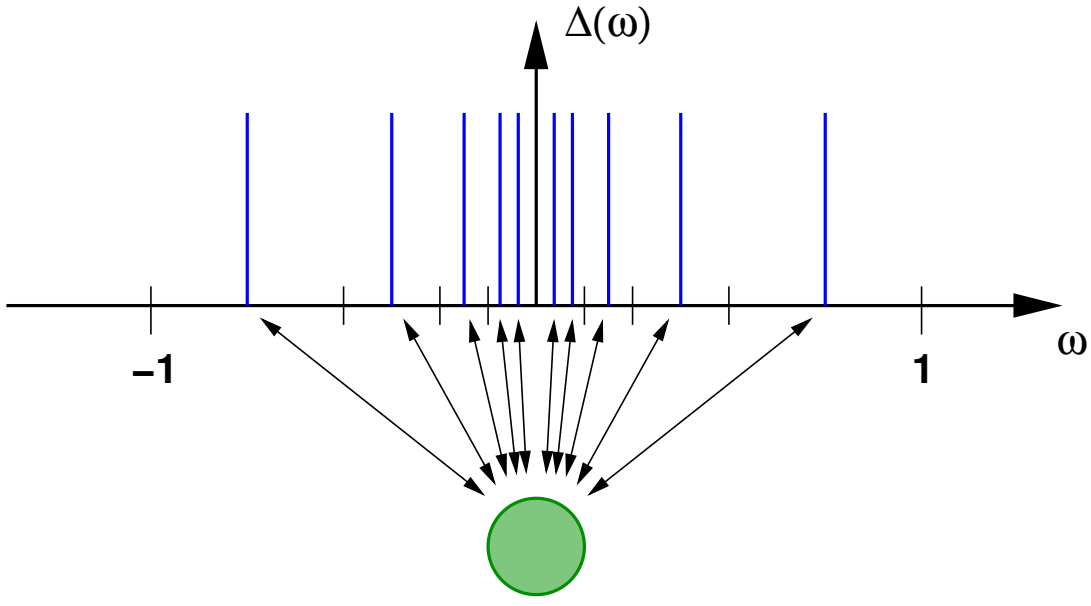


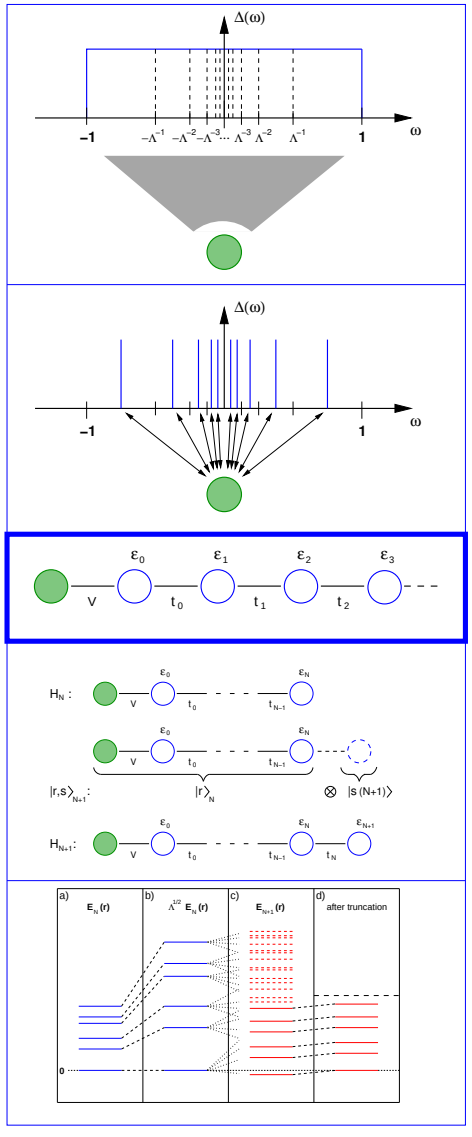
1. NRG-discretization parameter $\Lambda > 1$



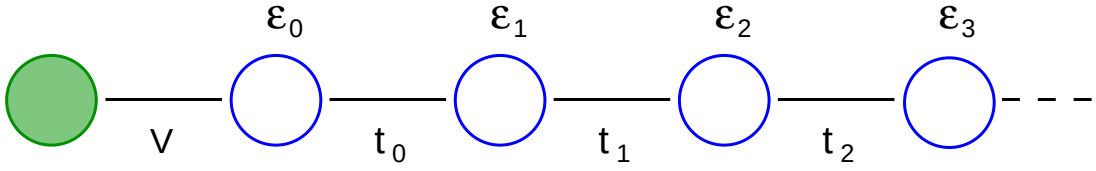


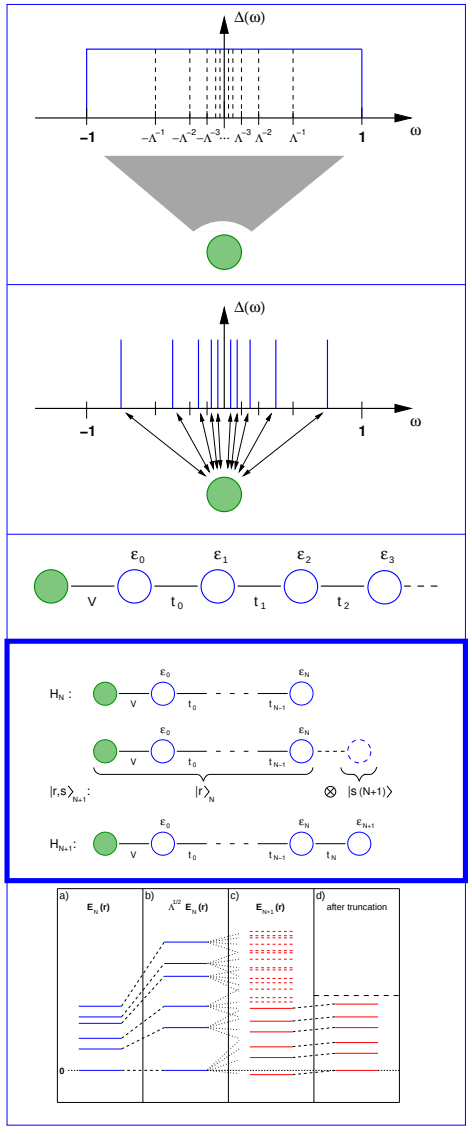
2. logarithmic discretization



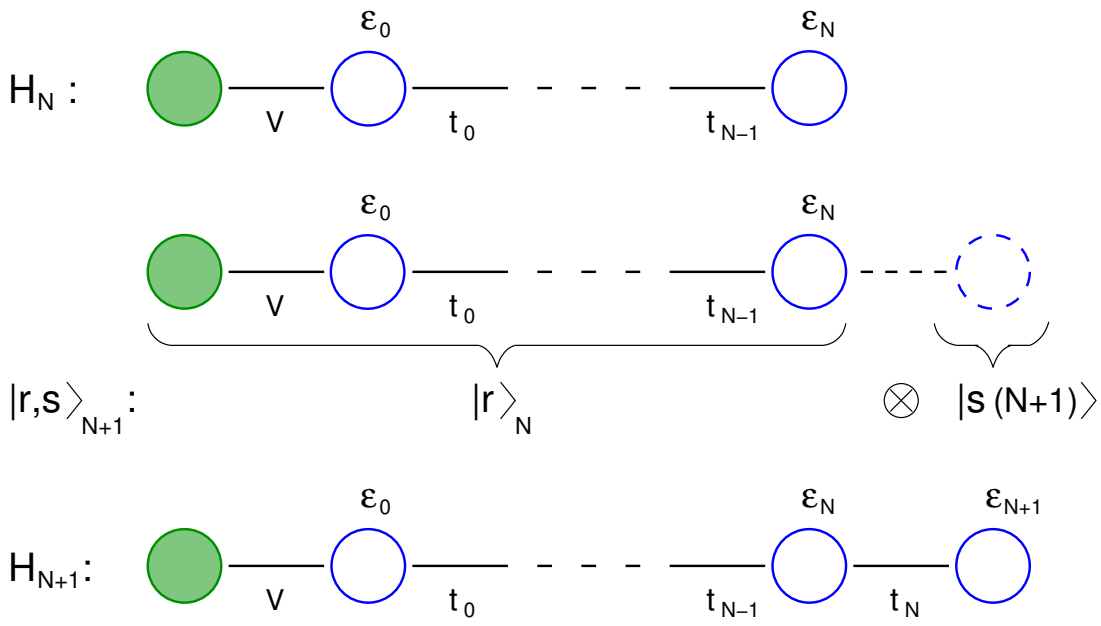


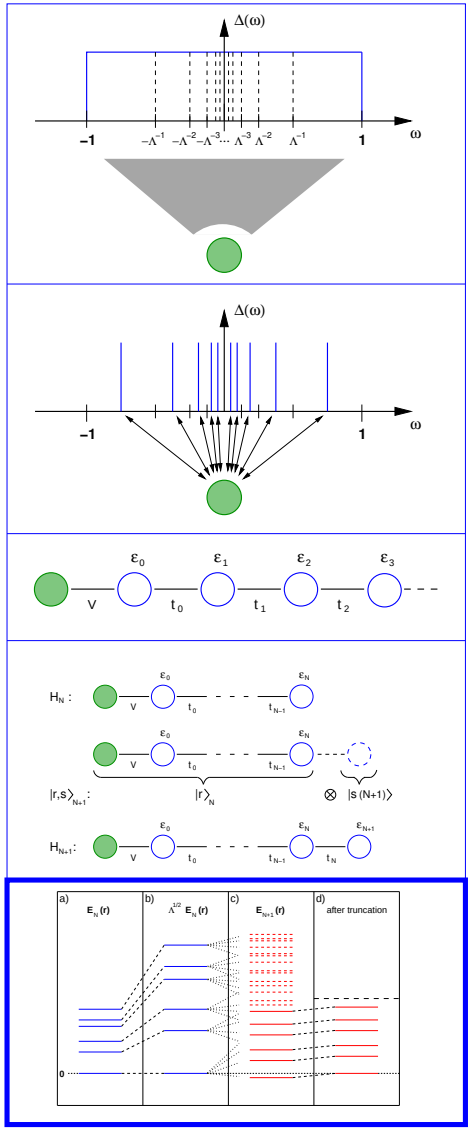
3. mapping on semi-infinite chain



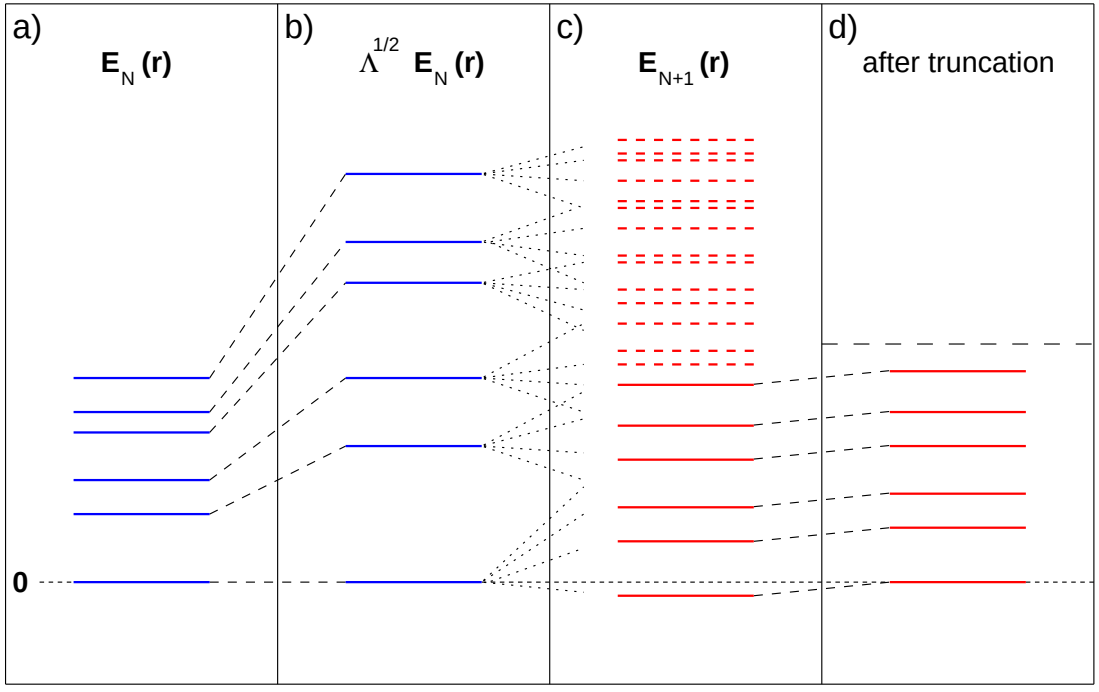


4. iterative diagonalization





5. truncation



3.1 Logarithmic discretization

starting point: siAm in the integral representation
$\Lambda > 1$ defines a set of intervals with discretization points

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

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

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

the inverse transformation

$$
\begin{aligned}
a_{np\sigma} &= \int_{-1}^{1} \mathrm{d}\varepsilon \left[\psi_{np}^{+}(\varepsilon)\right]^{*} a_{\varepsilon\sigma} \ , \\
b_{np\sigma} &= \int_{-1}^{1} \mathrm{d}\varepsilon \left[\psi_{np}^{-}(\varepsilon)\right]^{*} a_{\varepsilon\sigma} \ .
\end{aligned}
$$

transformed hybridization term

$$
\begin{aligned}
\int_{-1}^{1} \mathrm{d}\varepsilon \, h(\varepsilon) f_{\sigma}^{\dagger} a_{\varepsilon\sigma} = \quad & f_{\sigma}^{\dagger} \quad \sum_{np} \left[a_{np\sigma} \int^{+,n} \mathrm{d}\varepsilon \, h(\varepsilon) \psi_{np}^{+}(\varepsilon) \right. \\
& + \quad \left. b_{np\sigma} \int^{-,n} \mathrm{d}\varepsilon \, h(\varepsilon) \psi_{np}^{-}(\varepsilon) \right] ,
\end{aligned}
$$

with

$$
\int^{+,n} \mathrm{d}\varepsilon \equiv \int_{x_{n+1}}^{x_n} \mathrm{d}\varepsilon \ , \ \int^{-,n} \mathrm{d}\varepsilon \equiv \int_{-x_n}^{-x_{n+1}} \mathrm{d}\varepsilon \ .
$$

For a constant $h(\varepsilon) = h$

$$\int^{\pm,n} \mathrm{d}\varepsilon \, h\psi^{\pm}_{np}(\varepsilon) = \sqrt{d_n} h \delta_{p,0} \ .$$

$\Rightarrow$ the impurity couples only to the $p = 0$ components of the conduction band states!
For non-constant $h(\varepsilon)$, introduce a step function for $h(\varepsilon)$

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

with

$$h_n^{\pm 2} = \frac{1}{d_n} \int^{\pm,n} \mathrm{d}\varepsilon \, \frac{1}{\pi} \Delta(\varepsilon) \ .$$

the hybridization term then reads

$$\int_{-1}^{1} \mathrm{d}\varepsilon \, h(\varepsilon) f_\sigma^\dagger a_{\varepsilon\sigma} = \frac{1}{\sqrt{\pi}} f_\sigma^\dagger \sum_n \left[\gamma_n^+ a_{n0\sigma} + \gamma_n^- b_{n0\sigma} \right] \ ,$$

with $\gamma_n^{\pm 2} = \int^{\pm,n} \mathrm{d}\varepsilon \, \Delta(\varepsilon)$.

the conduction electron term transforms into

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

the discrete set of energies $\xi^{\pm}_{n}$ can be expressed as

$$\xi^{\pm}_{n} = \frac{\int^{\pm,n} \mathrm{d}\varepsilon \Delta(\varepsilon)\varepsilon}{\int^{\pm,n} \mathrm{d}\varepsilon \Delta(\varepsilon)} \quad \left[= \pm \frac{1}{2} \Lambda^{-n} (1+\Lambda^{-1}) \right] ,$$

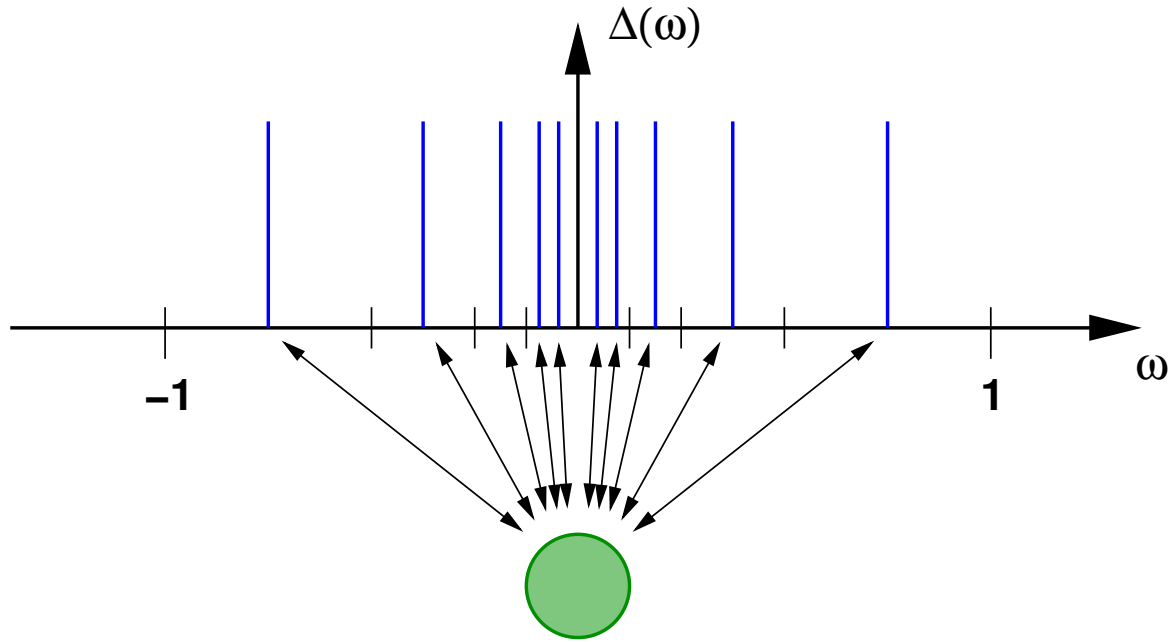
For a linear dispersion, $g(\varepsilon) = \varepsilon$, we have

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

The actual discretization of the Hamiltonian is now achieved by dropping the terms with $p \neq 0$ in the expression for the conduction band

Finally, after dropping the $p \neq 0$ terms and relabeling the operators $a_{n0\sigma} \equiv a_{n\sigma}$, etc., we arrive at the discretized Hamiltonian

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



3.2 Mapping on a semi-infinite chain

With

$$c_{0\sigma} = \frac{1}{\sqrt{\xi_0}} \sum_n \left[\gamma_n^+ a_{n\sigma} + \gamma_n^- b_{n\sigma} \right] ,$$

and

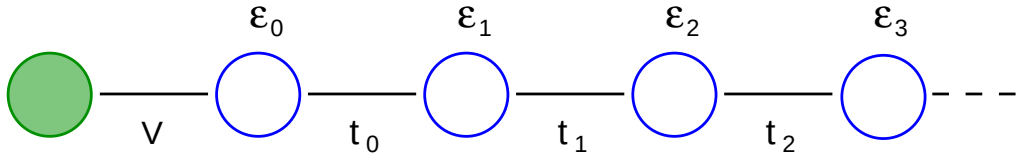
$$\xi_0 = \sum_n \left((\gamma_n^+)^2 + (\gamma_n^-)^2 \right) = \int_{-1}^{1} \mathrm{d}\varepsilon \Delta(\varepsilon) ,$$

the hybridization term can be written as

$$\frac{1}{\sqrt{\pi}} f_\sigma^\dagger \sum_n \left(\gamma_n^+ a_{n\sigma} + \gamma_n^- b_{n\sigma} \right) = \sqrt{\frac{\xi_0}{\pi}} f_\sigma^\dagger c_{0\sigma} ,$$

we aim at a Hamiltonian of the form

$$\begin{aligned} H &= H_{\mathrm{imp}} + \sqrt{\frac{\xi_0}{\pi}} \sum_\sigma \left[f_\sigma^\dagger c_{0\sigma} + c_{0\sigma}^\dagger f_\sigma \right] \\ &+ \sum_{\sigma n=0}^{\infty} \left[\varepsilon_n c_{n\sigma}^\dagger c_{n\sigma} + t_n \left(c_{n\sigma}^\dagger c_{n+1\sigma} + c_{n+1\sigma}^\dagger c_{n\sigma} \right) \right] , \end{aligned}$$



orthogonal transformation

$$a_{n\sigma} = \sum_{m=0}^{\infty} u_{mn} c_{m\sigma} \quad , \quad b_{n\sigma} = \sum_{m=0}^{\infty} v_{mn} c_{m\sigma} \; , c_{n\sigma} = \sum_{m=0}^{\infty} \left[u_{nm} a_{m\sigma} + v_{nm} b_{m\sigma} \right] \; .$$

For the coefficients u_{nm}, v_{nm}, as well as for the parameters ε_n, t_n, one can derive recursion relations (see lecture notes).

Analytical solutions for the recursion relations: 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

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

3.3 Iterative diagonalization

The chain Hamiltonian eq. (1) 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

$$H_0 = \Lambda^{-1/2}\Bigg[H_{\rm imp} + \sum_\sigma \varepsilon_0 c^\dagger_{0\sigma} c_{0\sigma}$$

$$+\sqrt{\frac{\xi_0}{\pi}}\sum_\sigma \left(f^\dagger_\sigma c_{0\sigma} + c^\dagger_{0\sigma} f_\sigma\right)\Bigg] \ .$$

renormalization group transformation

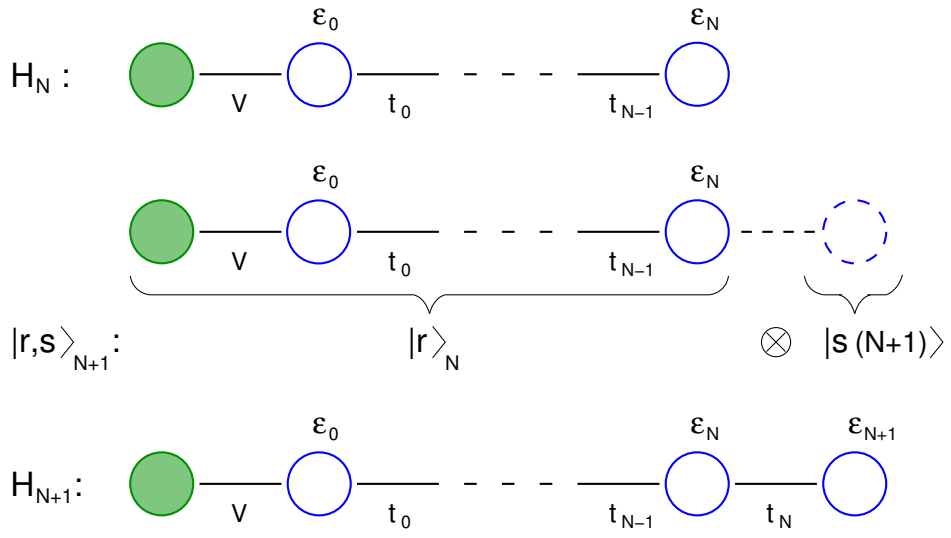
$$H_{N+1} = R\left(H_N\right) \ .$$

here, we characterize H_N, and thereby also the RG flow, directly by the many-particle energies $E_N(r)$

$$H_N|r\rangle_N = E_N(r)|r\rangle_N \ \ , \ \ r = 1, \ldots, N_{\rm s} \ ,$$

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

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



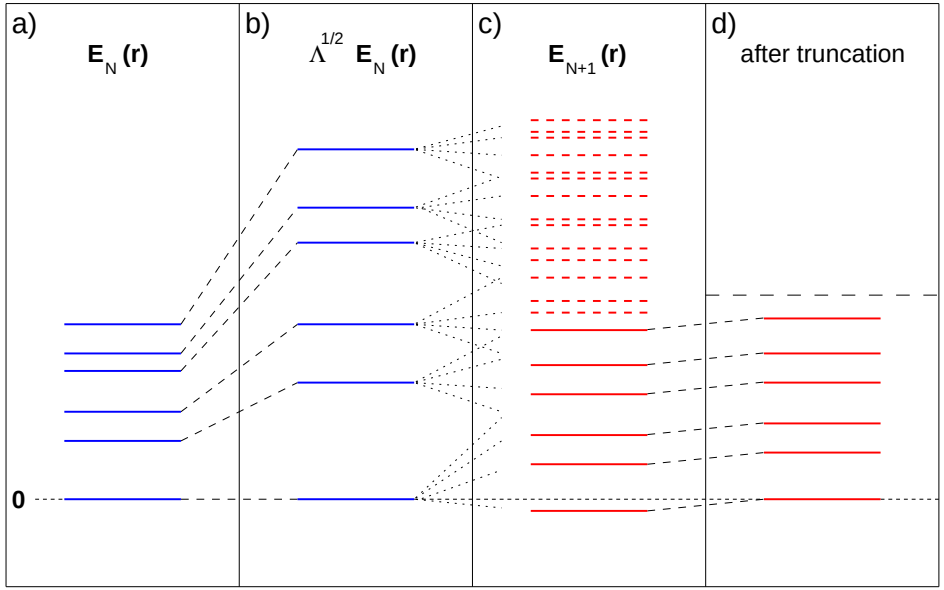
construct the Hamiltonian matrix for H_{N+1}:

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

Diagonalization gives the new eigenenergies $E_{N+1}(w)$ and eigenstates $|w\rangle_{N+1}$ which are related to the basis $|r; s\rangle_{N+1}$ via the unitary matrix U:

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

truncation

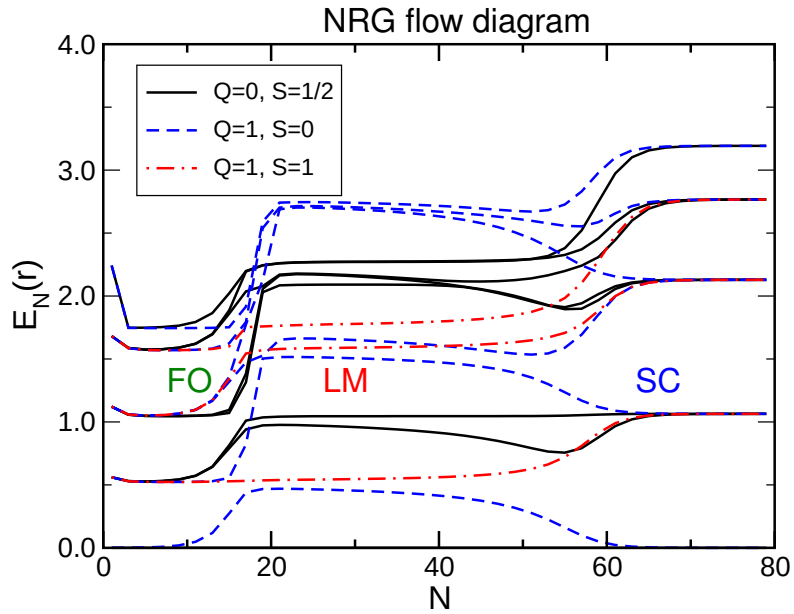


3.4 Renormalization group flow

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 $\Lambda = 2.5$

4. single-particle Green function

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

with the self-energy $\Sigma(z)$:

$$G(z) = \frac{1}{z - \varepsilon_\mathrm{f} - \Sigma(z)} \tag{2}$$

this self-energy consist of two parts:

$$\Sigma(z) = \Delta(z) + \Sigma^U(z) \quad , \tag{3}$$

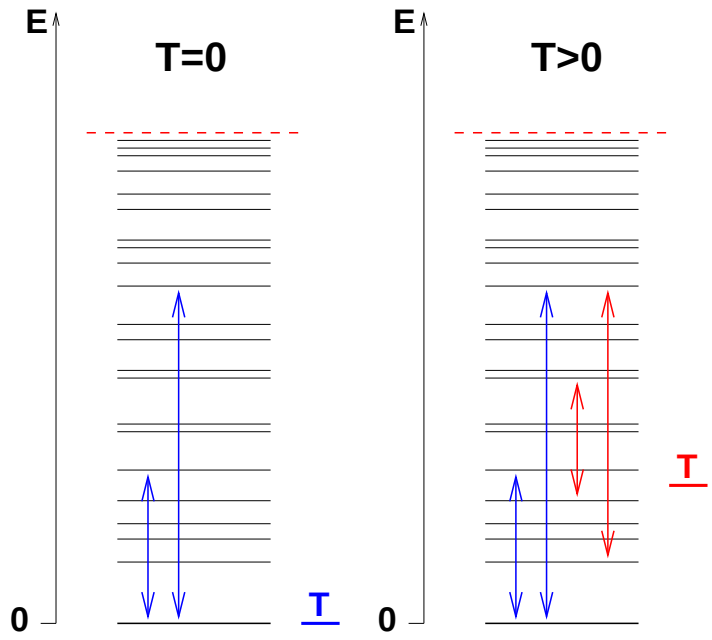
with $\Sigma^U(z)$ the contribution due to the U-term

spectral function:

$$A(\omega) = -\frac{1}{\pi} \mathrm{Im} \; G(\omega + i\delta^+) \; , \tag{4}$$

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

$$A_{\sigma N}(\omega) = \frac{1}{Z_N} \sum_{nm} \left| {}_N\left\langle n \left| f_\sigma^\dagger \right| m \right\rangle_N \right|^2 \delta\left(\omega - (E_n^N - E_m^N)\right) \left(e^{-\beta E_m^N} + e^{-\beta E_n^N}\right) \quad (5)$$

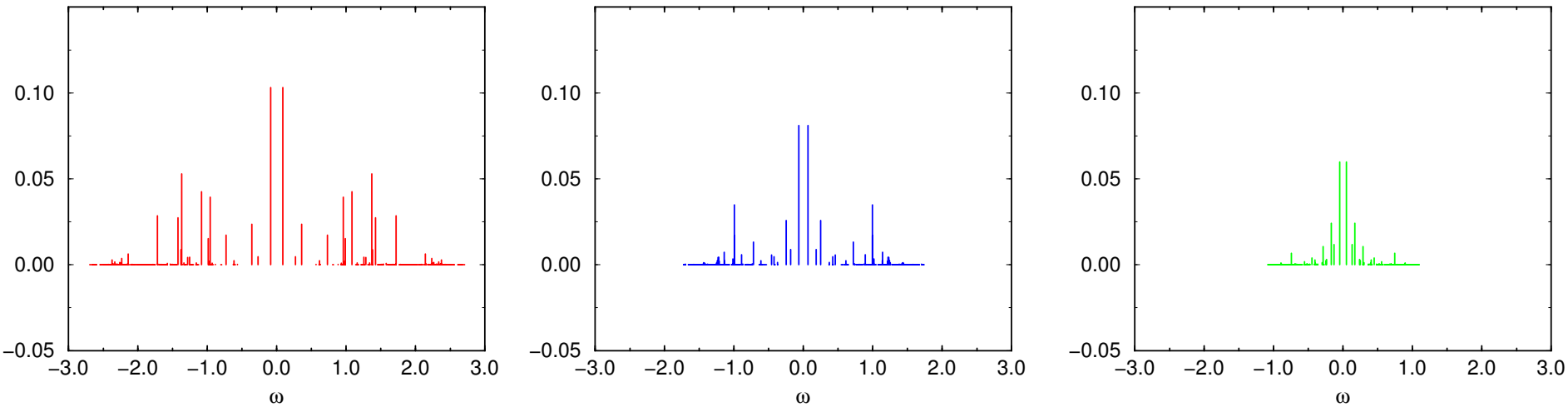


$T = 0$: transitions between ground state and all excited states

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

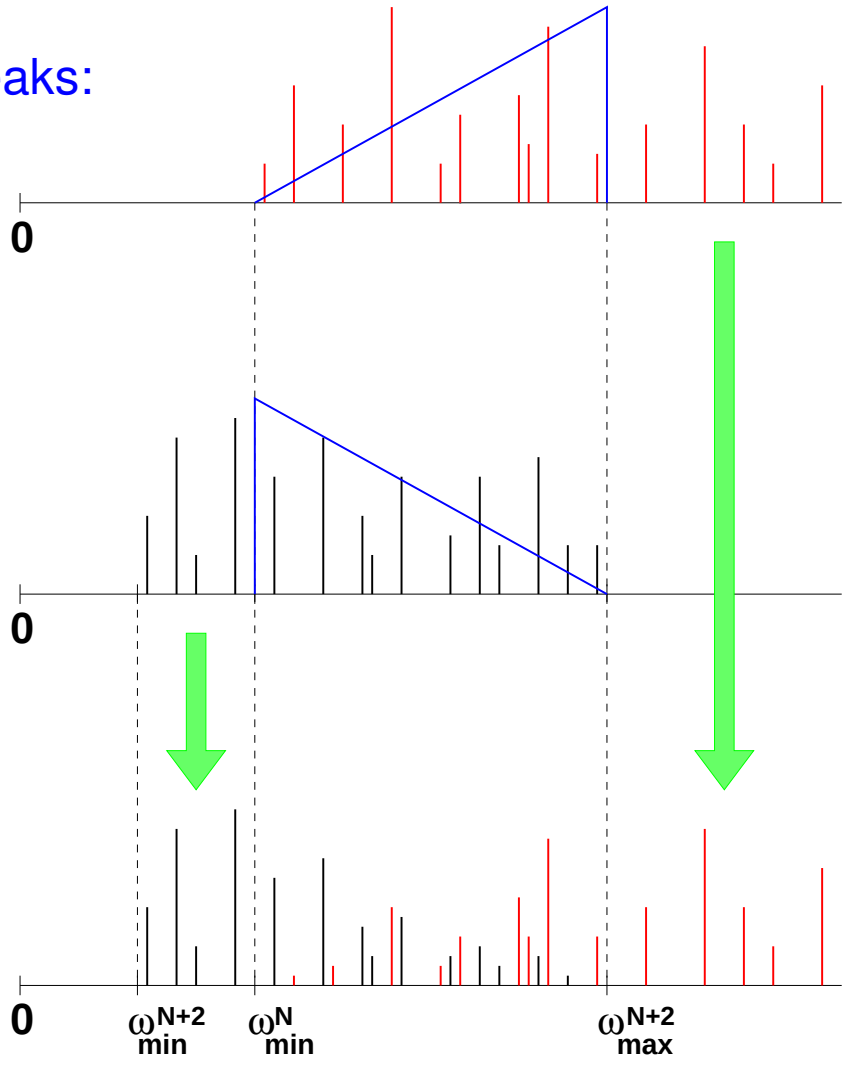
effect of the truncation on the spectral functions of each iteration:

$N = 14$ $N = 16$ $N = 18$



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

$$\delta(\omega - \omega_n) \to \frac{e^{-b^2/4}}{b\,\omega_n\sqrt{\pi}} \exp\left[-\frac{(\ln\omega - \ln\omega_n)^2}{b^2}\right] \tag{6}$$

results for the single-impurity Anderson model: