NRG IV: Dynamical correlators

NRG-IV.1

Goal: computing spectral functions via Lehmann representation using complete basis.

1. Completeness of Anders-Schiller basis [Anders2005], [Anders2006]

The combination of all sets of discarded states constructed in (NRG-III.5), $\{|\alpha,e\rangle_\ell^D \,|\, \ell = \ell_0,\dots,N\}$

forms a complete basis in full Hilbert space of length-N chain, known as 'Anders-Schiller (AS) basis':
(proof follows below)

$$\sum_{\vec{\sigma}_N} |\vec{\sigma}_N\rangle\langle\vec{\sigma}_N| \overset{\text{by definition}}{=} \mathbb{1}_{d^N\times d^N} \overset{\text{exact basis transformation}}{=} \sum_\ell \sum_{\alpha e_\ell} |\alpha,e\rangle_\ell^D\, {}_\ell^D\langle\alpha,e| \qquad (1)$$

These basis states are approximate eigenstates of Hamiltonian of length-N chain:

$$\hat{H}^N |\alpha,e\rangle_\ell \simeq \hat{H}^\ell |\alpha,e\rangle_\ell = E_\alpha^\ell |\alpha,e\rangle_\ell \qquad (2)$$

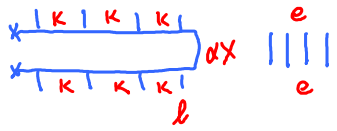
Here we made the 'NRG approximation': when acting on states from shell ℓ, approximate $\hat{H}^N$ by $\hat{H}^\ell$, i.e. neglect later-site parts of the Hamiltonian. Justification: they describe fine structure not relevant for capturing course structure of shell ℓ. The AS basis thus has following key properties:

- For small ℓ, energy resolution is bad, degeneracy high.
- As ℓ increases, energy resolution becomes finer, degeneracy decreases.

Projectors:

Projector onto sector X of shell ℓ:

$$\hat{P}_\ell^X = \sum_{\alpha e} |\alpha e\rangle_{\ell\,\ell}^{X\,X}\langle\alpha e| = \sum_\alpha |\alpha X\rangle\langle\alpha X| \otimes \sum_e |e\rangle\langle e| \qquad (13)$$



K and D sectors partition shell into two disjoint sets of orthonormal states, hence

$$P_\ell^{X'} P_\ell^X = \delta^{X'X} P_\ell^X \qquad (14)$$

Refinement of K sector of shell ℓ:

$$\hat{P}_\ell^K = \hat{P}_{\ell+1}^D + \hat{P}_{\ell+1}^K \qquad (15)$$

Iterate until end of chain:

$$= \hat{P}_{\ell+1}^D + \hat{P}_{\ell+2}^D + \hat{P}_{\ell+2}^K = \dots \qquad (16)$$

Hence: (for any $\ell'' > \ell$)

$$P_\ell^K = \sum_X P_{\ell+1}^X = \sum_{\ell'=\ell}^{\ell''} P_{\ell'}^D + P_{\ell''}^K = \sum_{\ell'=\ell}^{N} P_{\ell'}^D \qquad (17)$$

For $\ell = \ell_0$:

$$\mathbb{1}_{d^N\times d^N} = P_{\ell_0}^D + P_{\ell_0}^K = \sum_{\ell=\ell_0}^{N} P_\ell^D \equiv \sum_\ell \qquad (18)$$

Unit operator can be expressed as sum over D-projectors of all shells, hence AS basis is complete!

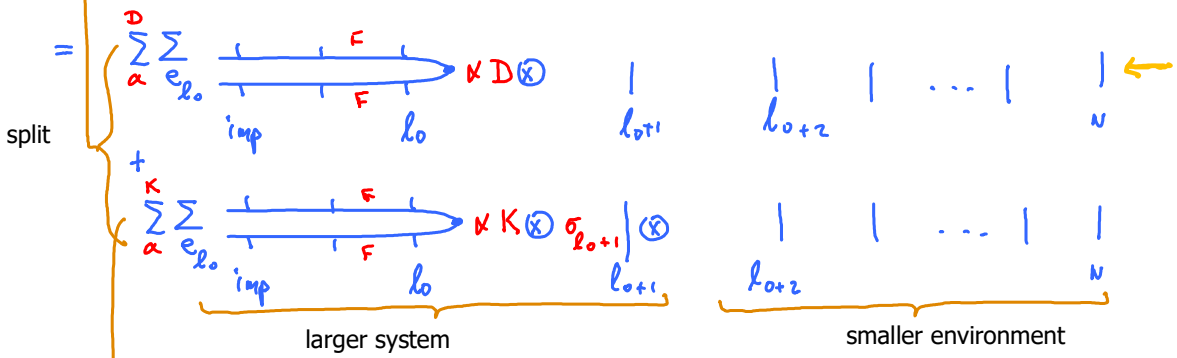
General projector products:

$$P_{\ell'}^{X'} P_\ell^X \overset{(14,17)}{=} \begin{cases} \delta^{KX'} P_\ell^X & \text{if } \ell' < \ell \\ \delta^{X'X} P_\ell^X & \text{if } \ell' = \ell \\ P_{\ell'}^{X'} \delta^{XK} & \text{if } \ell' > \ell \end{cases} \qquad (19)$$

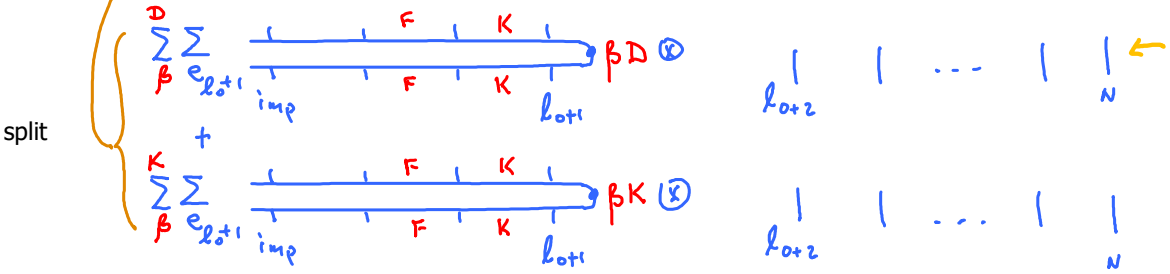
Graphical depiction of completeness of AS basis

Transform to basis which diagonalizes sites imp to l_0, retaining full (F) spectrum at each step):

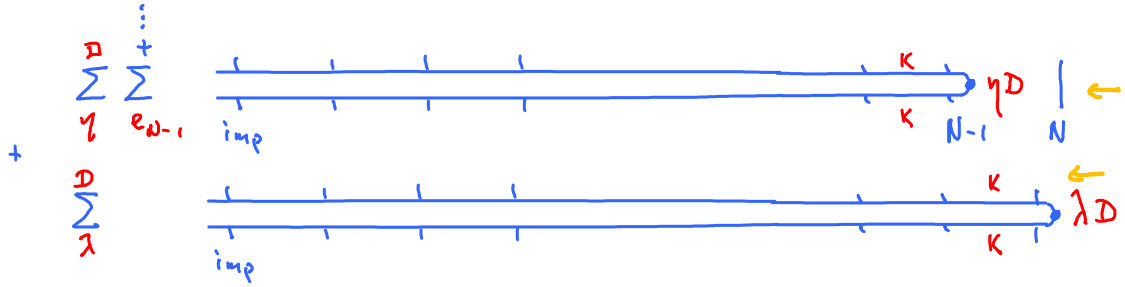
Split into discarded and kept states. In latter sector, move one site from environment into system:



Now diagonalize, split again, and iterate:



Iterate until the entire chain is diagonal, and declare all states of last iteration as 'discarded':



The collection of all terms marked ← is the resolution of identity in AS basis:

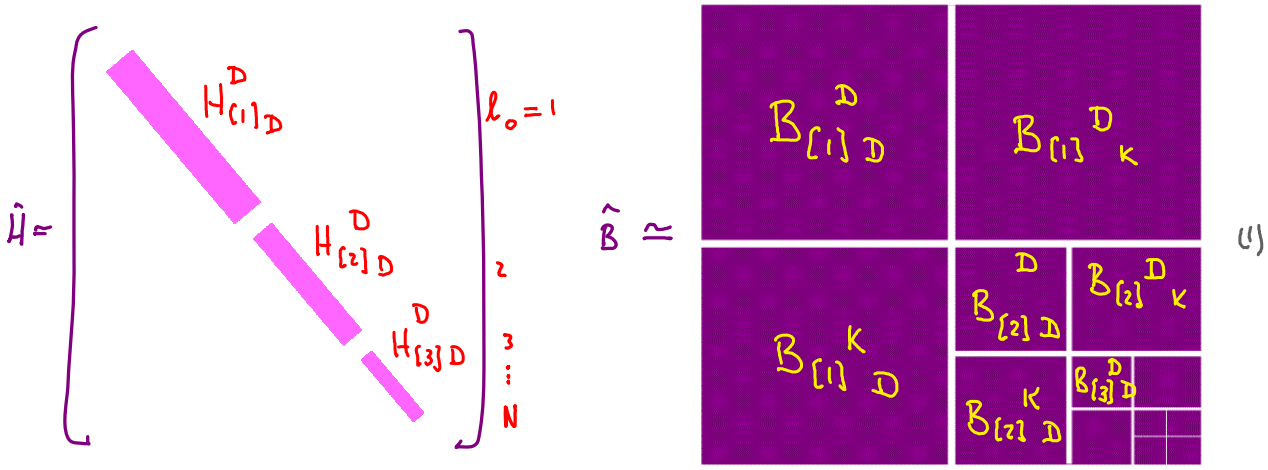
$$= \sum_{\ell \geq \ell_0}^{N} \sum_{\alpha}^{D} \sum_{e_\ell}$$

2. Operator expansions

[Weichselbaum2007], [Peters2006]

non-trivial only on sites $-1, \dots, n_0$

Below we will show that the Hamiltonian and 'local' operators have following structure in AS basis:



(1)

Hamiltonian is diagonal:

$$\hat{H}^N \overset{(I.2)}{\simeq} \sum_\ell \sum_\alpha E^\ell_\alpha \, |\alpha e\rangle^D_\ell \, {}^D_\ell\langle \alpha e| \,, \qquad (2)$$

General operator: exclude KK to avoid overcounting!

$$\hat{B} \simeq \sum_\ell \sum_{x'x}^{\neq KK} \sum_e |\alpha' e\rangle^{x'}_\ell \, [B_{[\ell]x}]^{\alpha'}_{\alpha} \, {}^x_\ell\langle \alpha e| \qquad (2)$$

Operators are diagonal in 'environment' states! Hence environment can easily be traced out!

The expression for $\hat{H}^N$ follows from (IV.1.2). That for a local operator $\hat{B}$ can be found as follows:

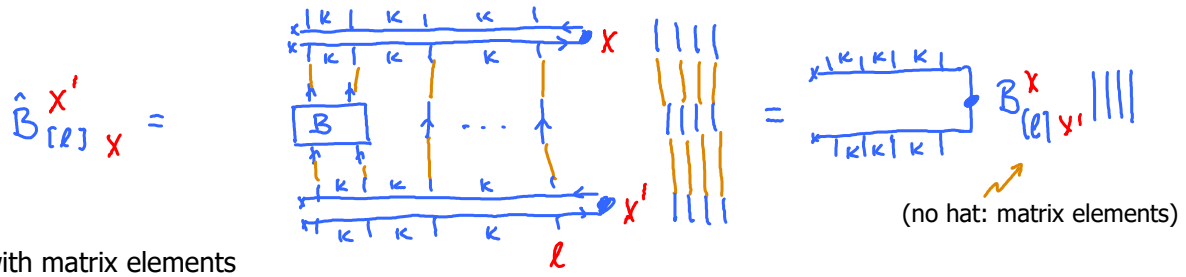
Suppose $\hat{B}$ is a 'local operator', living on sites $\leq \ell_0$, e.g. on sites imp and 0 :

(3)

Start from the local operator's exactly known representation on length-ℓ_0 chain,

$$\hat{B} = \sum_{xx' \in \{K,D\}} |\alpha' e\rangle^{x'}_{\ell_0} \, [B_{[\ell_0]x}]^{\alpha'}_{\alpha} \, {}^x_{\ell_0}\langle \alpha e| \equiv \sum_{x'x} \hat{B}^{x'}_{[\ell_0]x} \qquad (4)$$

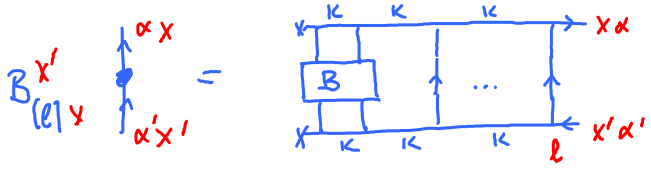
Define operator projections to X'X sector of shell : $\hat{B}^{x'}_{[\ell]x} = \hat{P}^{x'}_\ell \hat{B} \hat{P}^x_\ell$ (5)



(6)

(no hat: matrix elements)

with matrix elements



(7)

can be computed iteratively during forward sweep, starting from $\ell = \ell_0$

$$= B^{K}_{[\ell-1]K} \quad \text{(diagram: } K \to Y,\ \sigma_\ell,\ K \to X'\text{)} \quad = \left[A^{\dagger}_{[\ell]}{}^{X'}_{K}\right]^{\alpha'}_{\sigma_\ell\beta} \left[B^{K}_{[\ell-1]K}\right]^{\beta'}_{\beta} \left[A^{K}_{[\ell]X}\right]^{\beta\sigma_\ell}_{\alpha} \tag{8}$$

only KK enters here!

Refine KK sector iteratively, using $P^{K}_{\ell} \overset{(1.14)}{=} \sum_{X} P^{X}_{\ell+1}$:

$$\hat{B}^{K}_{[\ell_0]K} = \hat{P}^{K}_{\ell_0} \hat{B} \hat{P}^{K}_{\ell_0} = \sum_{X'X}^{\neq KK} \hat{P}^{X'}_{\ell_0+1} \hat{B} \hat{P}^{X}_{\ell_0+1} + \hat{P}^{K}_{\ell_0+1} \hat{B} \hat{P}^{K}_{\ell_0+1} \tag{9}$$

Iterate to end of chain: $$= \sum_{\ell>\ell_0}^{N} \sum_{X'X}^{\neq KK} \hat{P}^{X'}_{\ell} \hat{B} \hat{P}^{X}_{\ell} = \sum_{\ell>\ell_0}^{N} \sum_{X'X}^{\neq KK} \hat{B}^{X'}_{[\ell]X} \tag{10}$$

Full operator: $$\hat{B} = \sum_{X} \hat{B}^{X}_{[\ell_0]X} \overset{(10)}{=} \sum_{\ell\geq\ell_0}^{N} \sum_{X'X}^{\neq KK} \hat{B}^{X'}_{[\ell]X} = \sum_{\ell} \sum_{X'X}^{\neq KK}$$ (diagram: $Y \to X'$, ℓ) $$\tag{11}$$

Note: matrix elements are always 'shell-diagonal' (computed using same-length chains).

Time-dependent operators

$$\hat{B}(t) = e^{i\hat{H}^N t} \hat{B} e^{-i\hat{H}^N t} = \sum_{\ell} \sum_{X'X}^{\neq KK} \hat{B}^{X'}_{[\ell]X}(t) \tag{12}$$

with time-dependent matrix elements, evaluated using NRG approximation (1.2):

$$\left[B^{X'}_{[\ell]X}(t)\right]^{\alpha'}_{\alpha} \simeq {}^{X'}_{\ell}\langle\alpha'| e^{i\hat{H}^{\ell}t} \hat{B} e^{-i\hat{H}^{\ell}t} |\alpha\rangle^{X}_{\ell} = \left[B^{X'}_{[\ell]X}\right]^{\alpha'}_{\alpha} e^{i(E^{\ell}_{\alpha'} - E^{\ell}_{\alpha})t} \tag{13}$$

Important: since we iteratively refined only KK sector, the time-dependent factor is 'shell-diagonal': factors with $e^{i(E^{\ell'}_{\alpha'} - E^{\ell}_{\alpha})t}$, $\ell' \neq \ell$ do not occur. Using different shells to compute $E_{\alpha'}$ and E_{α} would yield them with different accuracies, which would be inconsistent.

Fourier transform: $$\hat{B}(\omega) = \int \frac{dt}{2\pi} e^{i\omega t} \hat{B}(t) \overset{(12,13)}{=} \sum_{\ell} \sum_{X'X}^{\neq KK} \hat{B}^{X'}_{[\ell]X}(\omega) \tag{15}$$

$$\left[B^{X'}_{[\ell]X}(\omega)\right]^{\alpha'}_{\alpha} = \left[B^{X'}_{[\ell]X}\right]^{\alpha'}_{\alpha} \delta(\omega - (E^{\ell}_{\alpha} - E^{\ell}_{\alpha'})) \tag{16}$$

Operator product expansions: $\hat{B}\hat{C}$ Proceed iteratively, refining only KK-KK sector:

$$\hat{B}^{K}_{[\ell]K} \hat{C}^{K}_{[\ell]K} = \hat{P}^{K}_{\ell} \hat{B} \hat{P}^{K}_{\ell} \hat{C} \hat{P}^{K}_{\ell} \overset{(1.14)}{=} \sum_{X''X'X} \hat{P}^{X''}_{\ell+1} \hat{B} \hat{P}^{X'}_{\ell+1} \hat{C} \hat{P}^{X}_{\ell+1} = \sum_{X'XX''} \hat{B}^{X''}_{[\ell+1]X'} \hat{C}^{X'}_{[\ell+1]X} \tag{17}$$

Start from $\ell = \ell_0$ and iterate: (18)

$$\hat{B}\hat{C} = \sum_{X''X'X} \hat{B}^{X''}_{[\ell_0]X'} \hat{C}^{X'}_{[\ell_0]X} = \sum_{\ell} \sum_{X''X'X}^{\neq KKK} \hat{B}^{X''}_{[\ell]X'} \hat{C}^{X'}_{[\ell]X} = \sum_{\ell} \sum_{X''X'X}^{\neq KKK}$$ (diagram: C, B, X, X', X'') $$\Big|\Big|\Big|$$

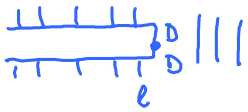
3. Full density matrix

[Weichselbaum2007]

NRG-IV.3

NRG approximation

$$\hat\rho \equiv e^{-\beta \hat H^N} \simeq \sum_\ell \sum_{\alpha\sigma} |\alpha,\sigma\rangle_\ell^D \underbrace{\frac{e^{-\beta E_\alpha^\ell}}{Z}}_{\rho_\ell^{DD}} {}_\ell^D\langle \alpha,\sigma| = \sum_\ell$$



(1)

$$= \sum_{\ell=n_0}^{N} \hat\rho_{[\ell]D}^D \quad , \quad [\rho_{[\ell]D}^D] = \delta^\alpha_{\alpha'} \frac{e^{-\beta E_\alpha^\ell}}{Z} \qquad (2)$$

Sector projections of $\hat\rho$ for shell ℓ, defined as $\hat\rho_{[\ell]x}^{x'} = \hat P_\ell^{x'} \hat\rho \hat P_\ell^x$, are given by:

$$\hat\rho_{[\ell]D}^D \quad , \quad \hat\rho_{[\ell]K}^K \overset{(1.19)}{=} \sum_{\ell'>\ell}^{N} \hat\rho_{[\ell']D}^D \quad , \quad \hat\rho_{[\ell]K}^D = \hat\rho_{[\ell]D}^K = 0 \qquad (3)$$

provides refinement for rest of chain

density matrix is sector-diagonal

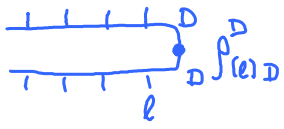
Reduced density matrix for length-ℓ chain is obtained by tracing out environment of all later sites:

$$\bar\rho_{[\ell]x}^{x'} = \operatorname*{Tr}_{\text{sites}>\ell} [\hat\rho_{[\ell]x}^{x'}] \qquad (\bar\rho_{[\ell]D}^K = \bar\rho_{[\ell]K}^D \overset{(3)}{=} 0) \qquad (4)$$

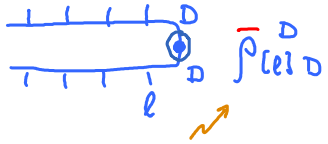
$d^{N-\ell}$ degeneracy of environment for shell ℓ

DD-sector:

$$\bar\rho_{[\ell]D}^D =$$



$$\bar\rho_{[\ell]D}^D \qquad (5)$$



indicates sum over local basis due to trace

(no hat: matrix elements)

with matrix elements

$$[\bar\rho_{[\ell]D}^D]_\alpha^{\alpha'} = [\rho_{[\ell]D}^D]_\alpha^{\alpha'} d^{N-\ell} \overset{(2)}{=} \delta^{\alpha'}_\alpha \underbrace{\frac{e^{-\beta E_\alpha^\ell}}{Z_\ell^D}}_{\text{density matrix of D-sector of shell } \ell \text{ (without environment)}} \underbrace{\frac{Z_{[\ell]}^D}{Z} d^{N-\ell}}_{w_\ell} \qquad (6)$$

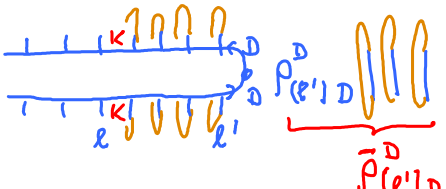
relative weight of D-sector of shell ℓ to total partition function, with $\sum_\ell w_\ell = 1$

where $Z_\ell^D = \sum_\alpha^D e^{-\beta E_\alpha^\ell}$ (7)

is partition function for D-sector of shell ℓ (without environment)

KK-sector:

$$\bar\rho_{[\ell]K}^K =$$

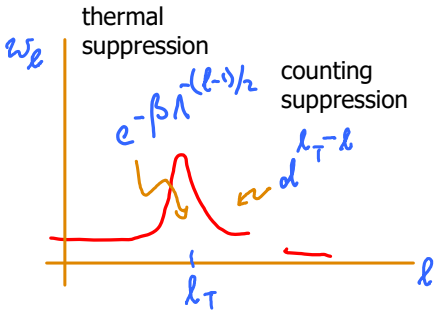


$$\bar\rho_{[\ell]K}^K \qquad (7)$$

(8)

Starting at $\ell = N$, the KK matrix elements can be computed iteratively via a backward sweep.

The weights w_ℓ, viewed as a function of ℓ, are peaked near ℓ_T, with a width of five to ten shells (depending on Λ, d and D_{kept})



Reason: the Boltzmann factors $e^{-\beta E_s^\ell}$ in partition functions yield $\simeq 0$ for $E_s^\ell \gg T$ or $\simeq 1$ for $E_s^\ell \ll T$. Hence

$$w_\ell \overset{(2)}{=} \frac{d^{N-\ell} Z_\ell^D}{Z} \overset{(3)}{=} \frac{d^{N-\ell} \sum_\alpha e^{-\beta E_\alpha^\ell}}{\sum_{\ell'} \sum_{\alpha' e'} e^{-\beta E_{\alpha'}^{\ell'}}} \propto \frac{d^{N-\ell}\, e^{-\beta\Lambda^{-(\ell-1)/2}}}{\underbrace{\sum_{\ell'>\ell_T} \sum_{e'}}_{\simeq d^{N-\ell_T}}} \simeq d^{\ell_T-\ell}\, e^{-\beta\Lambda^{-(\ell-1)/2}} \qquad (9)$$

sum over environment of shell ℓ_T yields

Thus, the weight functions ensure in a natural manner that shells whose characteristic energy lies close to temperature have dominant weight, while avoiding the brutal single-shell approximation $w_\ell = \delta_{\ell,\ell_T}$.

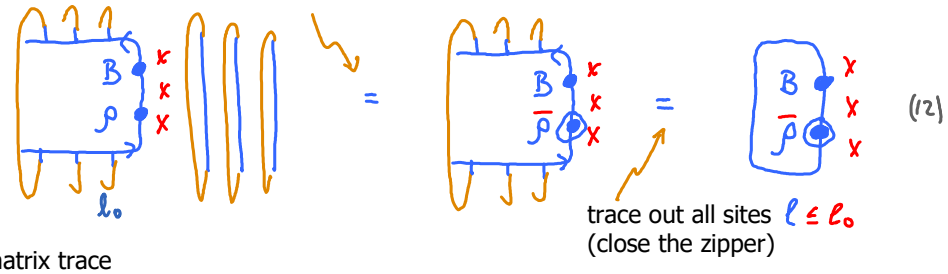
Thermal expectation value:

$$\langle \hat{B} \rangle_T \underset{\text{definition}}{=} Tr\left[\hat{\rho}\,\hat{B}\right] \overset{(2.18)}{\underset{\text{shell-}\ell_0\text{ representation}}{=}} \sum_{x''x'x} \underbrace{\delta^{x''}_{x}}_{\text{due to trace}} Tr\Big[\hat{\rho}_{[\ell_0]}{}^{x''}_{x'}\, \hat{B}_{[\ell_0]}{}^{x'}_{x}\Big] \qquad (10)$$

$$= \sum_x \underbrace{Tr}_{\text{all sites}} \Big[\hat{\rho}_{[\ell_0]}{}^{x}_{x}\, \hat{B}_{[\ell_0]}{}^{x}_{x}\Big] = \sum_x \underbrace{Tr}_{\text{sites} \le \ell_0} \Big[\hat{\bar{\rho}}_{[\ell_0]}{}^{x}_{x}\, \hat{B}_{[\ell_0]}{}^{x}_{x}\Big] \qquad (11)$$

operator trace

trace out all sites $\ell > \ell_0$



(12)

trace out all sites $\ell \le \ell_0$ (close the zipper)

$$= \sum_x \underbrace{tr}_{\text{shell } \ell_0} \Big[\bar{\rho}_{[\ell_0]}{}^{x}_{x}\, B_{[\ell_0]}{}^{x}_{x}\Big] = \sum_x \sum_{\alpha'\alpha} \Big[\bar{\rho}_{[\ell_0]}{}^{x}_{x}\Big]^{\alpha'}_{\alpha} \Big[B_{[\ell_0]}{}^{x}_{x}\Big]^{\alpha}_{\alpha'} \qquad (13)$$

matrix trace

can be computed using solely shell-ℓ_0 matrix elements
(but reduced density matrix requires backward sweep along entire chain)

Note: traces of shell-diagonal operator products simplify to traces of matrix products, with full density matrix replaced by reduced density matrix.

4. Spectral functions: full-density-matrix (fdm) NRG

[Weichselbaum2007]

AS basis, being complete set of (approximate) energy eigenststate, is suitable for use in Lehmann representation of spectral function, with the identification $\{|\alpha\rangle\} = \{|se\rangle^D_n,\ n = n_0 .., N\}$

$$A^{BC}(\omega) = \int \frac{dt}{2\pi} e^{i\omega t}\ \mathrm{Tr}\left[\hat\rho\ \hat B(t)\ \hat C\right] = \mathrm{Tr}\left[\hat B(\omega)\ \hat C\ \hat\rho\right] \quad (1)$$

(NRG-II.1)

trace is cyclic

Insert representation of these three operators in complete AS basis:

$$\mathrm{Tr}\Big[\sum_{\ell}\sum_{\bar\ell}\sum_{\tilde\ell} |\tilde\alpha',\tilde e\rangle^{\tilde x'}_{\tilde\ell}\Big[B_{[\tilde\ell]}(\omega)\Big]^{\tilde x'}_{\tilde x}\Big]^{\tilde\alpha'}_{\tilde\alpha}\langle\tilde\alpha,\tilde e| \underset{\tilde x\,\tilde x'\neq KK}{|\bar\alpha',\bar e\rangle^{\bar x'}_{\ell}}\Big[C_{[\bar\ell]}{}^{\bar x'}_{\bar x}\Big]^{\bar\alpha'}_{\bar\alpha}\underset{\bar x'\bar x\neq KK}{\langle\bar\alpha,\bar e|}|\alpha,e\rangle^{D}_{\ell}\Big[\rho_{[\ell]}{}^{D}_{D}\Big]^{\alpha}_{\alpha}\langle\alpha,e|\Big] \quad (2)$$

Looks intimidating, but can be simplified by systematically using (NRG-III.5.12) for overlaps.

Simpler approach (leading to same result) uses operator expansion (2.18):

$$A^{BC}(\omega) = \mathrm{Tr}\left[\hat B(\omega)(\hat C\hat\rho)\right] = \sum_{\ell}\sum_{x''x'x}^{\neq KKK}\mathrm{Tr}\Big[\hat B_{[\ell](\omega)}{}^{x''}_{x'}\ \underbrace{(\hat C\hat\rho)_{[\ell]}{}^{x'}_{x}}_{\text{trace is cyclic}\ \delta^{x''}_{x}}\Big] \quad (3)$$

Perform trace in same way as for thermal expectation value, (3.10): trace over sites $\ell' > \ell$ yields reduced density matrix, trace over sites $\ell' \le \ell$ yields matrix trace over shell ℓ :

$$A^{BC}(\omega) = \sum_{\ell}\sum_{x'x}^{\neq KK}\ \underset{\text{shell }\ell}{\mathrm{tr}}\Big[B_{[\ell](\omega)}{}^{x}_{x'}\ (C\bar\rho)_{[\ell]}{}^{x'}_{x}\Big] \quad (4)$$

$$= \sum_{\ell}\sum_{x'x}^{\neq KK}\ \sum_{\alpha\alpha'}\Big[B_{[\ell]}{}^{x}_{x'}\Big]^{\alpha}_{\alpha'}\,\delta\big(\omega-(E^{\ell}_{\alpha'}-E^{\ell}_{\alpha})\big)\Big[C_{[\ell]}{}^{x'}_{x}\,\bar\rho_{[\ell]x}{}^{x}\Big]^{\alpha'}_{\alpha} \quad (5)$$

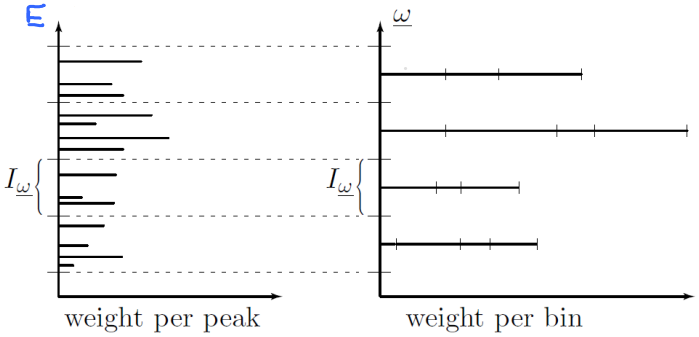
resolves frequency at scale $\omega \sim \Lambda^{-\ell/2}$

Each term involves a trace over <u>matrix</u> products involving only a single shell.

Easy to evaluate numerically.

To deal with delta functions, use 'binning': partition frequency axis into discrete bins, and replace $\delta(\omega - E)$ by bin function:

$$\underline{\delta}(\underline{\omega} - E) = \begin{cases} 1 & \text{if } E \in \underline{I}_{\underline{\omega}} \\ 0 & \text{otherwise} \end{cases}$$



Thus assigns energy $\underline{\omega}$ to all peaks lying in the same bin.

Finally, broaden using log-Gaussian broadening kernel, (NRG-III.3.4).

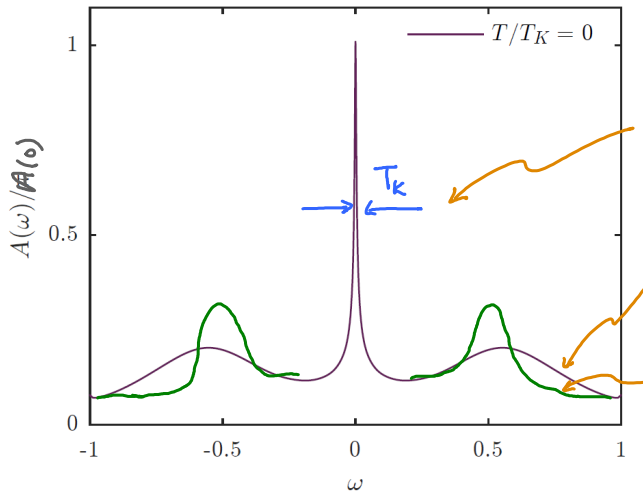
Spectral function of Anderson impurity model (at particle-hole symmetry, $\varepsilon_d = -U/2$ and zero magnetic field, $h = 0$)

$$A_s(\omega) \equiv A^{d_s^\dagger d_s}(-\omega) + A^{d_s d_s^\dagger}(\omega)$$

Can be computed using fdm-NRG. Technical issues:

- Include Z-factors to take care of fermionic signs.
- Broaden final result using log-Gaussian broadening kernel (NRG-III.3.4).

Result: for $\Gamma/U \ll 1$ (e.g. = 0.1) and $T \ll T_K$ (e.g. = 0), one obtains



NRG correctly captures width of central peak around $\omega = 0$, the 'Kondo resonance'.

NRG overbroadens the side peaks, which lie at high energies.

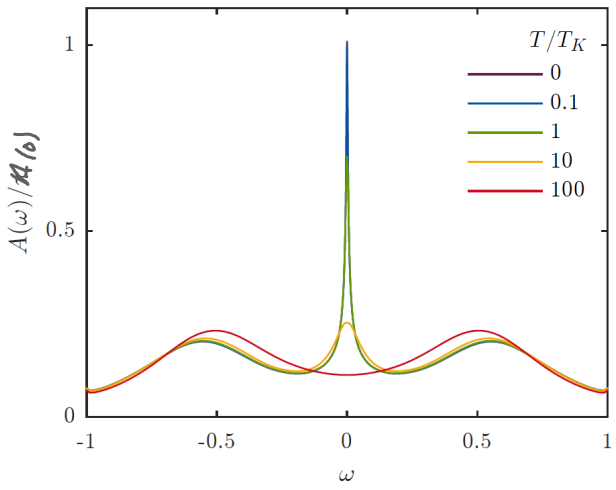
The true form of side peaks is narrower.

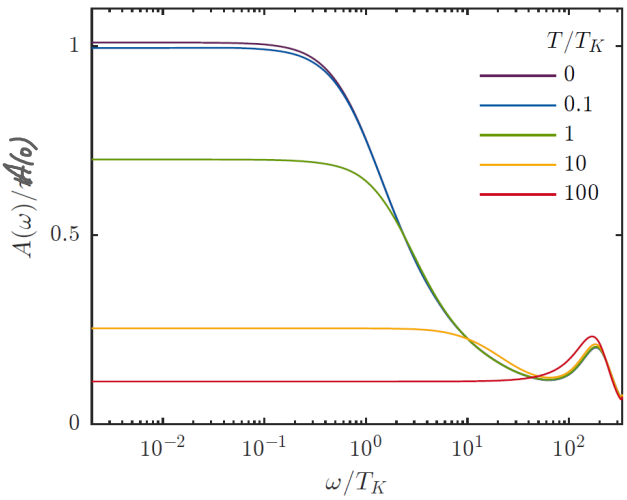
Over-broadening at large frequencies can be reduced using 'adaptive broadening' technique [Lee2016].

Exact result for peak height at T=0: $\pi\Gamma A_s(\omega = 0) = 1$

NRG reproduces this with an error of < 0.1 % if D_{kept} is large enough.

With increasing temperature, Kondo resonance broadens and weakens as T approaches and passes T_K.





Sum rule: we expect (for any temperature):

$$\int d\omega\, A_s(\omega) = \langle d_s^\dagger d_s \rangle_T + \langle d_s d_s^\dagger \rangle_T = \langle \{d_s, d_s^\dagger\} \rangle_T = 1 \quad (\{\cdots\} = 1)$$

Due to use of complete basis, fdmNRG fulfills this sum rules to machine precision, with error $< 10^{-15}$