NRG IV: Dynamical correlators

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), $\{ |\alpha,e\rangle^D_\ell \,|\, \ell = \ell_0,\dots,\mathcal{L} \}$

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

$$\sum_{\vec\sigma_{\mathcal L}} |\vec\sigma_{\mathcal L}\rangle\langle\vec\sigma_{\mathcal L}| \overset{\text{by definition}}{=} \mathbb{1}_{d^{\mathcal L}\times d^{\mathcal L}} \overset{\substack{\text{exact basis}\\ \text{transformation}}}{=} \sum_\ell \sum_{\alpha e_\ell} |\alpha,e\rangle^D_\ell \, {}^D_\ell\langle\alpha,e| \qquad (1)$$

These basis states are approximate eigenstates of Hamiltonian of length- $\mathcal L$ chain:

$$\hat H^{\mathcal L} |\alpha,e\rangle_\ell \simeq \hat H^\ell |\alpha,e\rangle_\ell = E^\ell_\alpha |\alpha,e\rangle_\ell \qquad (2)$$

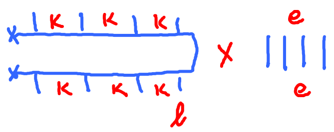
Here we made the 'NRG approximation': when acting on states from shell ℓ , approximate $\hat H^{\mathcal L}$ by $\hat H^\ell$, i.e. neglect later-site parts of the Hamiltonian. Justification: they describe fine structure not relevant for capturing course structure of shell ℓ. The AS basis thus has following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

$$\hat P^X_\ell = \sum_{\alpha e} |\alpha e\rangle^X_\ell \, {}^X_\ell\langle\alpha e| = \qquad (13)$$

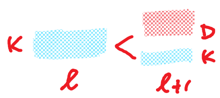


K and D sectors partition shell into two disjoint sets of orthonormal states, hence

$$P^{X'}_\ell P^X_\ell = \delta^{X'X} P^X_\ell \qquad (14)$$

Refinement of K sector of shell ℓ:

$$\hat P^K_\ell = \hat P^D_{\ell+1} + \underbrace{\hat P^K_{\ell+1}} \qquad (15)$$



Iterate until end of chain:

$$= \hat P^D_{\ell+1} + \hat P^D_{\ell+2} + \hat P^K_{\ell+2} = \dots \qquad (16)$$

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

$$P^K_\ell = \sum_X P^X_{\ell+1} = \sum_{\ell'>\ell}^{\ell''} P^D_{\ell'} + P^K_{\ell''} = \sum_{\ell'>\ell}^{N} P^D_{\ell'} \qquad (17)$$

For $\ell = \ell_0$:

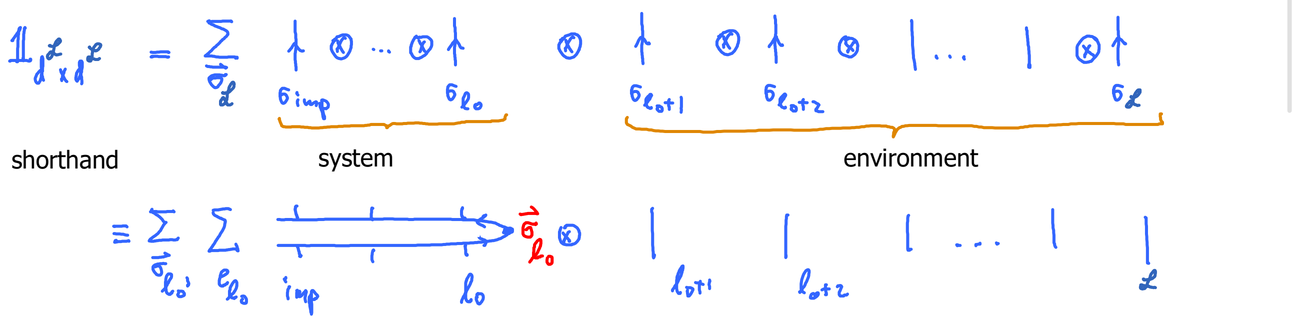
$$\mathbb{1}_{d^{\mathcal L}\times d^{\mathcal L}} = P^D_{\ell_0} + P^K_{\ell_0} = \underbrace{\sum_{\ell=\ell_0}^{\mathcal L}}_{\equiv \sum_\ell} P^D_\ell \qquad (18)$$

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

General projector products:

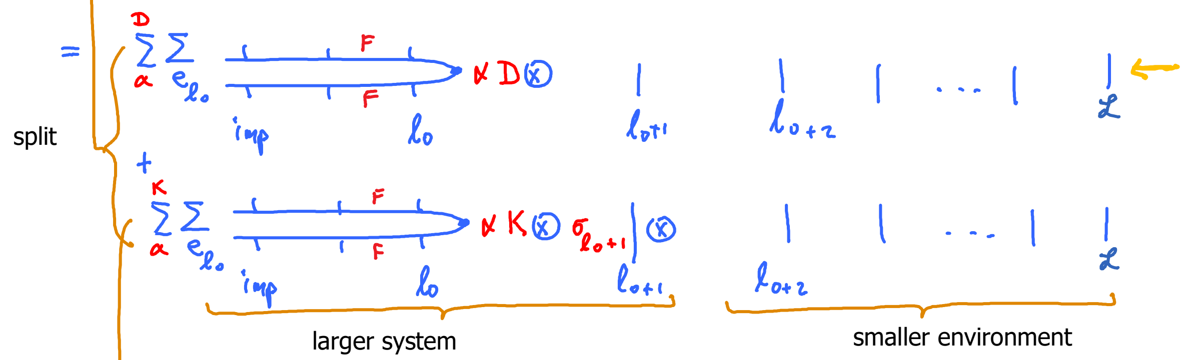
$$P^{X'}_{\ell'} P^X_\ell \overset{(14,17)}{=} \begin{cases} \delta^{KX'} P^X_\ell & \text{if } \ell' < \ell \\ \delta^{X'X} P^X_\ell & \text{if } \ell' = \ell \\ P^{X'}_{\ell'} \delta^{XK} & \text{if } \ell' > \ell \end{cases} \qquad (19)$$

Graphical depiction of completeness of AS basis

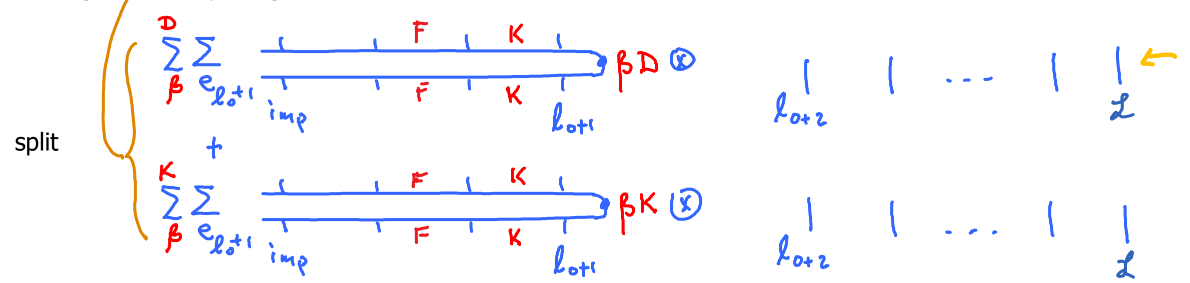


Transform to basis which diagonalizes sites imp to ℓ_0, keeping (K) the full spectrum at each step):

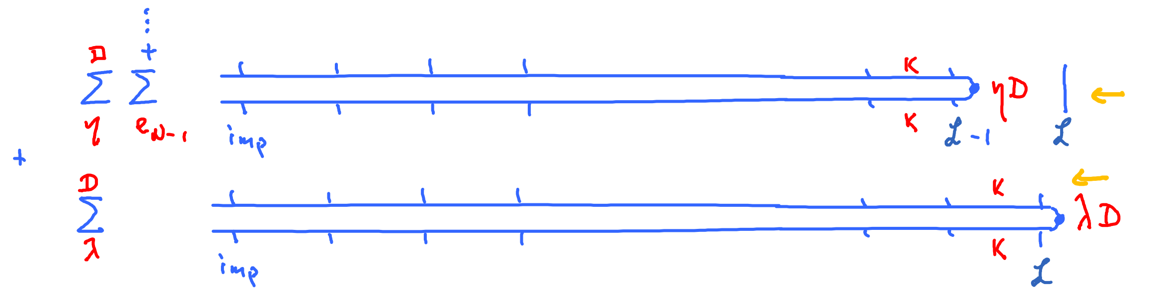
Split into discarded and kept states. In latter sector, move one site from environment into system:



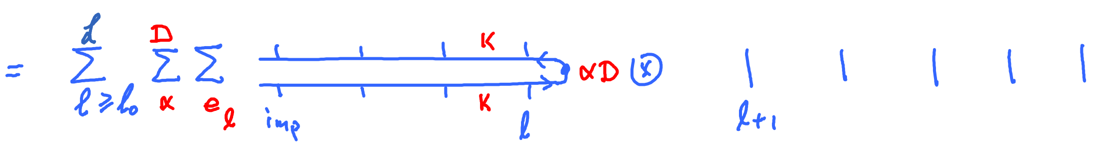
Now diagonalize, split again, and iterate:



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:



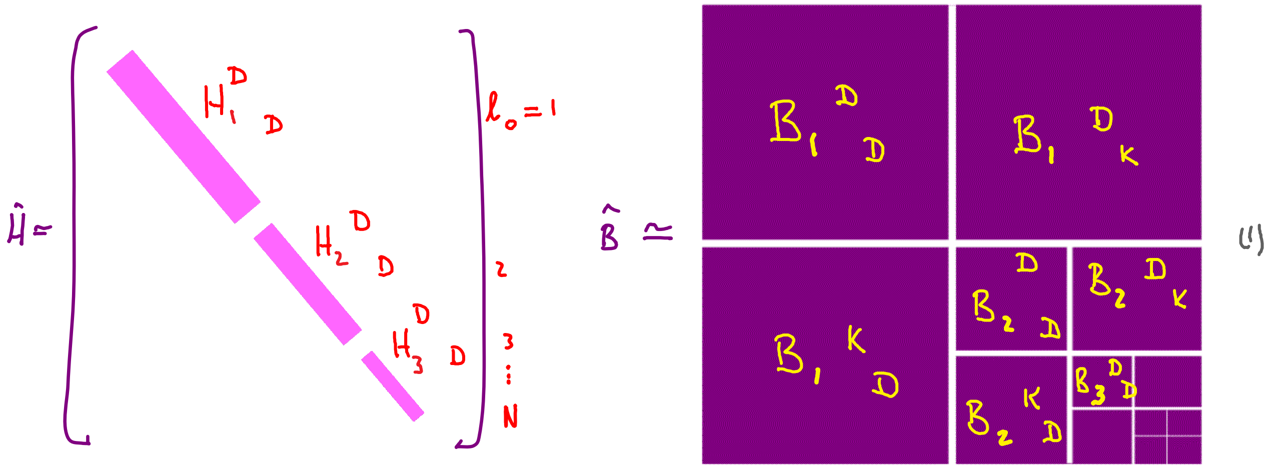
2. Operator expansions

[Weichselbaum2007], [Peters2006]

NRG-IV.2

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:

General operator: exclude KK to avoid overcounting!

$$\hat{H}^{\mathcal{L}} \overset{(1.2)}{\simeq} \sum_{\ell} \sum_{\alpha e} E^{\ell}_{\alpha} \, |\alpha, e\rangle^D_\ell \; {}^D_\ell\langle \alpha, e| , \qquad \hat{B} \simeq \sum_{\ell} \sum_{X'X}^{\neq KK} \sum_{\alpha} \sum_{e} |\alpha', e\rangle^{X'}_\ell \left[B_{[\ell]}{}^{X'}{}_X\right] {}^X_\ell\langle \alpha, e| \qquad (2)$$

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

The expression for $\hat{H}^{\mathcal{L}}$ 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 :

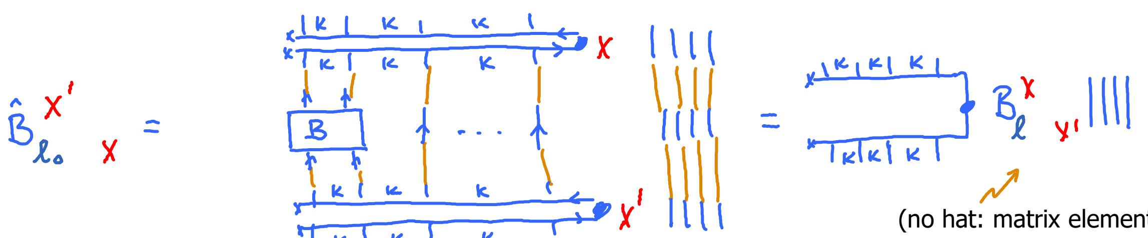
$$\hat{B} = \qquad (3)$$

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

$$\hat{B} = \sum_{XX' \in \{K,D\}} |\alpha' e\rangle^{X'}_{\ell_0} \left[B_{\ell_0}{}^{X'}{}_X\right]^{\alpha'}{}_{\alpha} \; {}^X_{\ell_0}\langle \alpha e| =: \sum_{X'X} \hat{B}_{\ell_0}{}^{X'}{}_X \qquad (4)$$

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

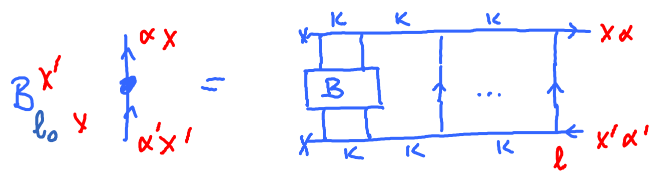
$$\hat{B}_{\ell_0}{}^{X'}{}_X = \qquad (6)$$



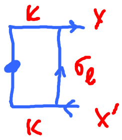
(no hat: matrix elements)

with matrix elements

$$B_{\ell_0}{}^{X'}{}_X = \qquad (7)$$



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

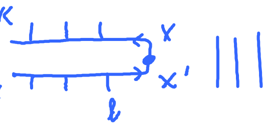
$$= \mathcal{B}^K_{\ell-1\;K}$$  $$= \left[A^{\dagger\,X'}_{\ell\;\;K}\right]^{\alpha'}_{\sigma_\ell\beta} \left[B_{\ell-1}{}^{K}{}_{K}\right]^{\beta'}{}_{\beta} \left[A_\ell{}^{K}{}_{X}\right]^{\beta\sigma_\ell}{}_{\alpha} \qquad (8)$$

only KK enters here!

Refine KK sector iteratively, using $P^K_\ell \overset{(1.14)}{=} \sum_X P^X_{\ell+1}$:

$$\hat{B}^K_{\ell_0\;K} = \hat{P}^K_{\ell_0}\,\hat{B}\,\hat{P}^K_{\ell_0} = \sum^{\neq KK}_{X'X} \hat{P}^{X'}_{\ell_0+1}\,\hat{B}\,\hat{P}^X_{\ell_0+1} + \hat{P}^K_{\ell_0+1}\,\hat{B}\,\hat{P}^K_{\ell_0+1} \qquad (9)$$

Iterate to end of chain: $$= \sum^{\mathcal{L}}_{\ell>\ell_0} \sum^{\neq KK}_{X'X} \hat{P}^{X'}_\ell\,\hat{B}\,\hat{P}^X_\ell = \sum^{N}_{\ell>\ell_0} \sum^{\neq KK}_{X'X} \hat{B}^{X'}_{\ell\;X} \qquad (10)$$

Full operator: $$\hat{B} = \sum_X \hat{B}^X_{\ell_0\;X} \overset{(10)}{=} \sum^{\mathcal{L}}_{\ell\geq\ell_0} \sum^{\neq KK}_{X'X} \hat{B}^{X'}_{\ell\;X} = \sum_\ell \sum^{\neq KK}_{X'X}$$  $$(11)$$

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

<u>Time-dependent operators</u>

$$\hat{B}(t) = e^{i\hat{H}^{\mathcal{L}}t}\,\hat{B}\,e^{-i\hat{H}^{\mathcal{L}}t} =: \sum_\ell \sum^{\neq KK}_{X'X} \hat{B}^{X'}_{\ell\;X}(t) \qquad (12)$$

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

$$\left[B_\ell{}^{X'}{}_X(t)\right]^{\alpha'}{}_\alpha \doteq {}^{X'}_{\ell}\langle\alpha'|\,e^{i\hat{H}^\ell t}\,\hat{B}\,e^{-i\hat{H}^\ell t}\,|\alpha\rangle^X_\ell = \left[B_\ell{}^{X'}{}_X\right]^{\alpha'}{}_\alpha\, e^{i(E^\ell_{\alpha'} - E^\ell_\alpha)t} \qquad (13)$$

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.

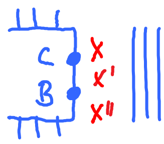
Fourier transform: $$\hat{B}(\omega) = \int\frac{dt}{2\pi}\, e^{i\omega t}\,\hat{B}(t) \overset{(12,13)}{=} \sum_\ell \sum^{\neq KK}_{X'X} \hat{B}_\ell{}^{X'}{}_X(\omega) \qquad (15)$$

$$\left[B_\ell{}^{X'}{}_X(\omega)\right]^{\alpha'}{}_\alpha = \left[B_\ell{}^{X'}{}_X\right]^{\alpha'}{}_\alpha\; \delta\!\left(\omega - (E^\ell_\alpha - E^\ell_{\alpha'})\right) \qquad (16)$$

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

$$\hat{B}_\ell{}^K{}_K\,\hat{C}_\ell{}^K{}_K = \hat{P}^K_\ell\,\hat{B}\,\hat{P}^K_\ell\,\hat{C}\,\hat{P}^K_\ell \overset{(1.14)}{=} \sum_{X''X'X} \hat{P}^{X''}_{\ell+1}\,\hat{B}\,\hat{P}^{X'}_{\ell+1}\,\hat{C}\,\hat{P}^X_{\ell+1} = \sum_{X'XX''} \hat{B}_{\ell+1}{}^{X''}{}_{X'}\,\hat{C}_{\ell+1}{}^{X'}{}_X \qquad (17)$$

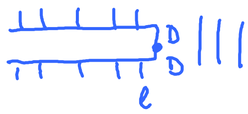
Start from $\ell = \ell_0$ and iterate: (18)

$$\hat{B}\,\hat{C} = \sum_{X''X'X} \hat{B}_{\ell_0}{}^{X''}{}_{X'}\,\hat{C}_{\ell_0}{}^{X'}{}_{X'} = \sum_\ell \sum^{\neq KKK}_{X''X'X} \hat{B}_\ell{}^{X''}{}_{X'}\,\hat{C}_\ell{}^{X'}{}_X = \sum_\ell \sum^{\neq KKK}_{X''X'X}$$ 

3. Full density matrix

[Weichselbaum2007]

NRG approximation

$$\hat\rho \equiv e^{-\beta \hat H^{\mathcal{L}}} \overset{\text{NRG approximation}}{\simeq} \sum_\ell \underbrace{\sum_{\alpha e} |\alpha, e\rangle_\ell^D \frac{e^{-\beta E_\alpha^\ell}}{Z} {}_\ell^D\langle \alpha, e|}_{\hat\rho_{[\ell]D}^{D}} = \sum_\ell$$  (1)

$$= \sum_{\ell=n_0}^{\mathcal{L}} \hat\rho_\ell^{D}{}_{D} \; , \qquad [\rho_\ell^D{}_D] = \delta^{\alpha}{}_{\alpha'} \frac{e^{-\beta E_\alpha^\ell}}{Z} \qquad (2)$$

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:

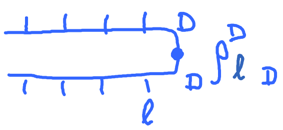
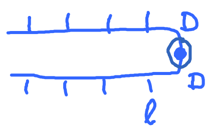
$$\hat\rho_\ell^{D}{}_{D} \; , \quad \hat\rho_\ell^{K}{}_{K} \overset{(1.19)}{=} \sum_{\ell'>\ell}^{\mathcal{L}} \hat\rho_{[\ell']D}^{D} \; , \qquad \hat\rho_\ell^{D}{}_{K} = \hat\rho_\ell^{K}{}_{D} = 0 \qquad (3)$$

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:

$$\hat{\bar\rho}_\ell{}^{X'}{}_{X} = \mathrm{Tr}_{\text{sites} > \ell} \left[\hat\rho_\ell^{X'}{}_{X} \right] \qquad \left(\bar\rho_\ell{}^{K}{}_{D} = \bar\rho_\ell{}^{D}{}_{K} \overset{(3)}{=} 0 \right) \qquad (4)$$

DD-sector:

$$\hat{\bar\rho}_\ell{}^{D}{}_{D} =$$  $$d^{N-\ell}$$ degeneracy of environment for shell ℓ $$=$$  $$\bar\rho_\ell{}^{D}{}_{D} \qquad (5)$$

indicates sum over local basis due to trace

(no hat: matrix elements)

with matrix elements

$$[\bar\rho_\ell{}^{D}{}_{D}]^{\alpha'}{}_{\alpha} = [\rho_\ell^D{}_D]^{\alpha'}{}_{\alpha} \, d^{\mathcal{L}-\ell} \overset{(2)}{=} \underbrace{\delta^{\alpha'}{}_{\alpha} \frac{e^{-\beta E_\alpha^\ell}}{Z_\ell^D}} \; \underbrace{\frac{Z_\ell^D \, d^{\mathcal{L}-\ell}}{Z}}_{w_\ell} \qquad (6)$$

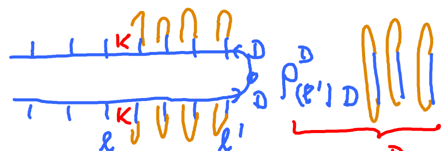
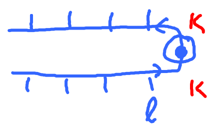
where $Z_\ell^D = \sum_\alpha^D e^{-\beta E_\alpha^\ell}$ (7)

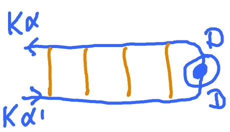
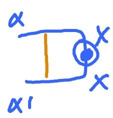
is partition function for D-sector of shell ℓ (without environment)

density matrix of D-sector of shell ℓ (without environment)

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

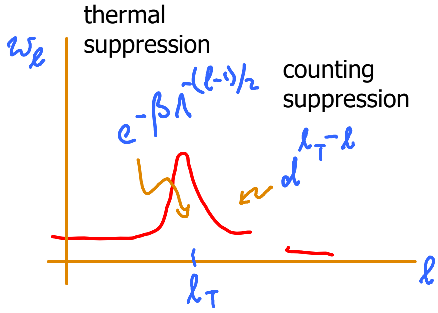
KK-sector:

$$\hat{\bar\rho}_\ell{}^{K}{}_{K} = \sum_{\ell'>\ell}$$  $$\underbrace{\qquad}_{\bar\rho_{[\ell']D}^{D}} =$$  $$\bar\rho_\ell{}^{K}{}_{K} \qquad (7)$$

$$[\bar\rho_\ell{}^{K}{}_{K}]^{\alpha'}{}_{\alpha}$$  $$= \sum_{\ell'>\ell}$$  $$\bar\rho_{\ell'}{}^{D}{}_{D} = \sum_X$$  $$\bar\rho_{\ell+1}{}^{X}{}_{X} \qquad (8)$$

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 $e^{-\beta E^\ell_s}$ in partition functions yield $\simeq 0$ for $E^\ell_s \gg T$ or $\simeq 1$ for $E^\ell_s \ll T$. Hence

$$w_\ell \overset{(2)}{=} \frac{d^{\mathcal{L}-\ell} Z^D_\ell}{Z} \overset{(3)}{=} \frac{d^{\mathcal{L}-\ell} \sum_\alpha e^{-\beta E^\ell_\alpha}}{\sum_{\ell'} \sum_{\alpha' e'} e^{-\beta E^{\ell'}_{\alpha'}}} \propto \frac{d^{\mathcal{L}-\ell}\, e^{-\beta \Lambda^{-(\ell-1)/2}}}{\underbrace{\sum_{\ell'>\ell_T} \sum_{e'}}} \simeq d^{\ell_T-\ell} e^{-\beta\Lambda^{-(\ell-1)/2}} \qquad (9)$$

sum over environment of shell ℓ_T yields $\simeq d^{\mathcal{L}-\ell_T}$

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 $w_\ell = \delta_{\ell,\ell_T}$.

<u>Thermal expectation value:</u>

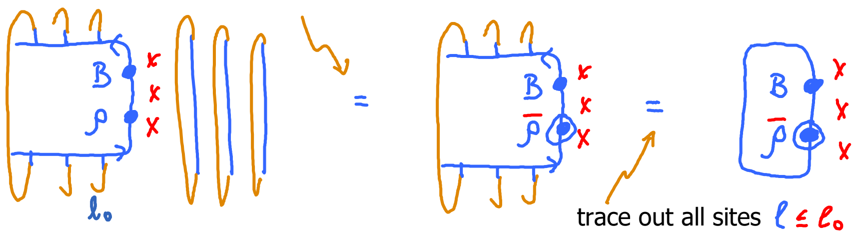
$$\langle \hat B \rangle_T \underset{\text{definition}}{=} \mathrm{Tr}[\hat\rho \hat B] \overset{(2.18)}{\underset{\substack{\text{shell-}\ell_0\\ \text{representation}}}{=}} \sum_{x''x'x} \mathrm{Tr}\Big[\underbrace{\hat\rho_{\ell_0}{}^{x''}{}_{x'}}_{(3)\ \delta^{x''}_{x'}}\, \hat B_{\ell_0}{}^{x'}{}_{x}\Big] \qquad (10)$$

$\delta^{x''}_{x}$ due to trace

operator trace

$$= \sum_x \underset{\text{all sites}}{\mathrm{Tr}} \left[\hat\rho_{\ell_0}{}^x{}_x\, \hat B_{\ell_0}{}^x{}_x\right] = \sum_x \underset{\text{sites} \le \ell_0}{\mathrm{Tr}} \left[\hat{\bar\rho}_{\ell_0}{}^x{}_x\, \hat B_{\ell_0}{}^x{}_x\right] \qquad (11)$$

trace out all sites $\ell > \ell_0$



(12)

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

matrix trace

$$= \sum_x \underset{\text{shell } \ell_0}{\mathrm{tr}} \left[\bar\rho_{\ell_0}{}^x{}_x\, B_{\ell_0}{}^x{}_x\right] = \sum_x \sum_{\alpha'\alpha} \left[\bar\rho_{\ell_0}{}^x{}_x\right]^{\alpha'}{}_{\alpha} \left[B_{\ell_0}{}^x{}_x\right]^{\alpha}{}_{\alpha'} \qquad (13)$$

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

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

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

[Weichselbaum2007] [Lee2021]

AS basis, being complete set of (approximate) energy eigenstate, is suitable for use in Lehmann representation of spectral function, with the identification $\{|\alpha\rangle\} = \{|\alpha e\rangle^D_\ell,\ \ell = \ell_0, \dots, \mathcal{L}\}$

$$\mathcal{A}^{BC}(\omega) \overset{\text{(NRG-II.1)}}{=} \int \frac{dt}{2\pi}\, e^{i\omega t}\ \mathrm{Tr}\left[\hat\rho\ \hat B(t)\ \hat C\right] \underset{\text{trace is cyclic}}{=} \mathrm{Tr}\left[\hat B(\omega)\ \hat C\ \hat\rho\right] \tag{1}$$

Insert representation of these three operators in complete AS basis:

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

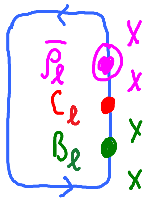
Looks intimidating, but can be simplified by systematically using (NRG-III.5.12) for overlaps.

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

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

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

$$\mathcal{A}^{BC}(\omega) = \sum_\ell \sum_{X'X}^{\neq KK} \mathrm{tr}_{\text{shell } \ell}\left[B_\ell(\omega)^{X}{}_{X'}\ (C\bar\rho)_\ell{}^{X'}{}_{X}\right] \tag{4}$$

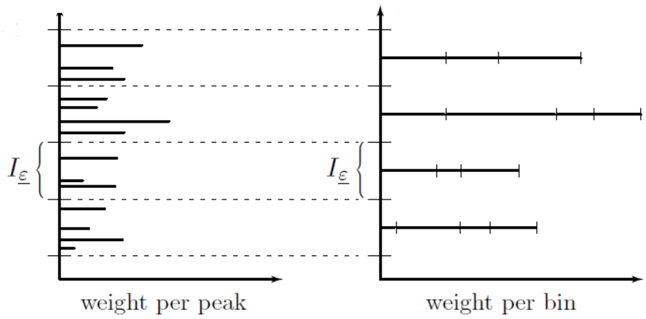


$$= \sum_\ell \sum_{X'X}^{\neq KK} \sum_{\alpha\alpha'} \left[B_\ell{}^{X}{}_{X'}\right]^{\alpha}{}_{\alpha'}\ \delta\big(\omega - (E^\ell_{\alpha'} - E^\ell_{\alpha})\big)\ \left[C_\ell{}^{X'}{}_{X}\ \bar\rho^{X}{}_{X}\right]^{\alpha'}{}_{\alpha} \tag{5}$$

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.

$E = E^\ell_{\alpha'} - E^\ell_{\alpha}$



To deal with delta functions, use 'binning':
partition frequency axis into discrete bins, I_ε ,
centered on set of discrete energies, $\{\varepsilon\}$, and replace

$\delta(\omega - E)$ by $\delta(\omega - \varepsilon) =$ if $E \in I_\varepsilon$

This assigns energy ε to all peaks lying in same bin.

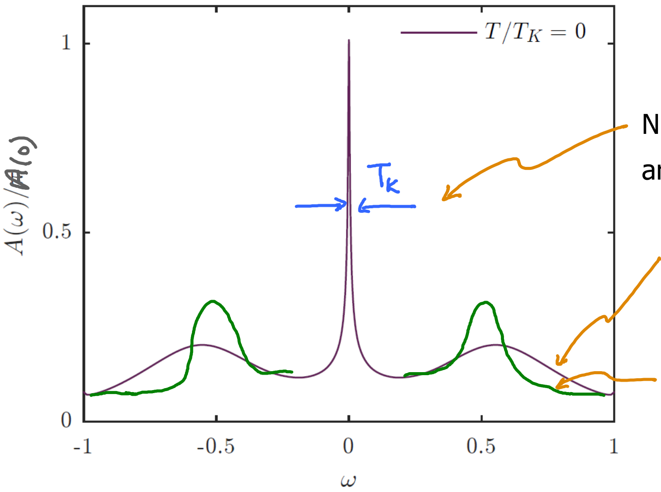
Finally, broaden using log-Gaussian broadening kernel, (NRG-III.3.4).

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

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

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.

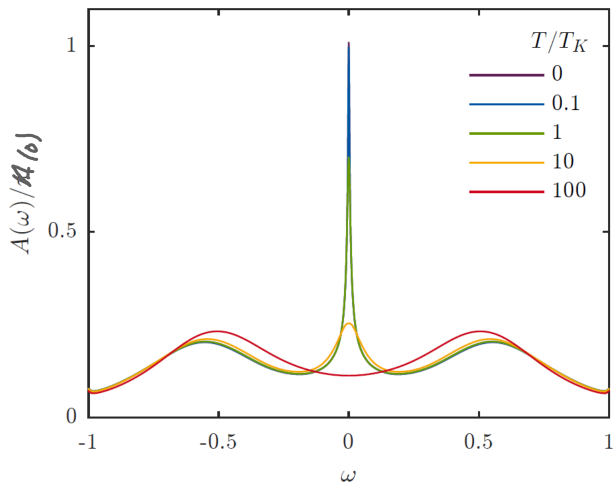
The true form of side peaks is narrower.

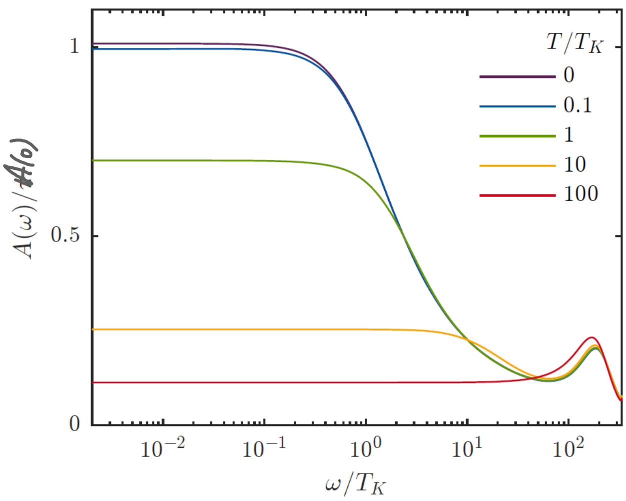
Over-broadening at large frequencies can be reduced using 'adaptive broadening' technique [Lee2016].

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 <u>any</u> temperature):

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

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