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), $\{ |\alpha, e\rangle^D_\ell \,|\, \ell = \ell_0, \ldots, N \}$

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

(proof follows below)

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

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

$$\hat{H}^N |\alpha, e\rangle_\ell \simeq \hat{H}^\ell |\alpha, e\rangle_\ell = E^\ell_\alpha |\alpha, e\rangle_\ell \tag{2}$$

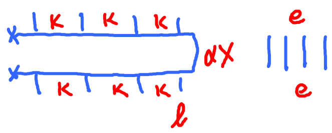
Here we made the 'NRG approximation': when acting on states from shell ℓ, approximate $\hat{H}^N$ by $\hat{H}^\ell$, i.e. neglect later-site parts of the Hamiltonian. Justification: they describe fine structure not relevant for capturing course structure of shell ℓ. The AS basis thus has following key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

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

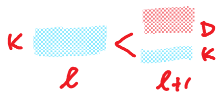


K and D sectors partition shell into two disjoint sets of orthonormal states, hence

$$P^{X'}_\ell P^X_\ell = \delta^{X'X} P^X_\ell \tag{14}$$

Refinement of K sector of shell ℓ:

$$\hat{P}^K_\ell = \hat{P}^D_{\ell+1} + \hat{P}^K_{\ell+1} \tag{15}$$



Iterate until end of chain:

$$= \hat{P}^D_{\ell+1} + \underbrace{\hat{P}^D_{\ell+2} + \hat{P}^K_{\ell+2}} = \ldots \tag{16}$$

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

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

For $\ell = \ell_0$:

$$\mathbb{1}_{d^N \times d^N} = P^D_{\ell_0} + P^K_{\ell_0} = \sum_{\ell = \ell_0}^{N} P^D_\ell \tag{18}$$

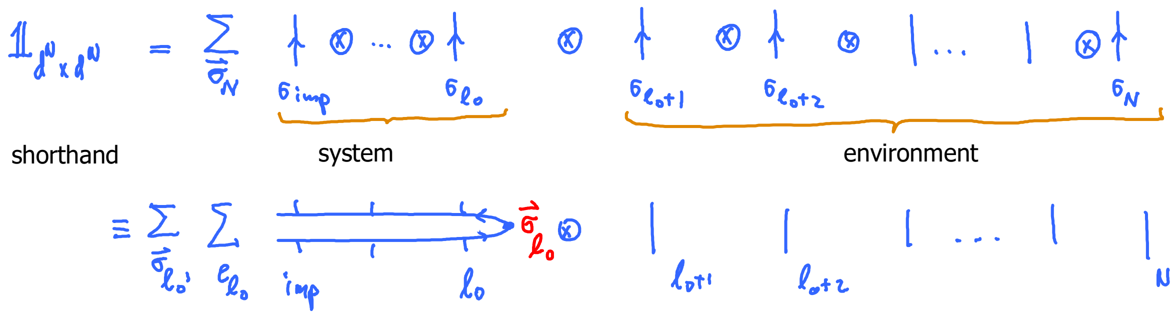
$$\underbrace{\sum_{\ell=\ell_0}^{N}} \equiv \sum_\ell$$

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

General projector products:

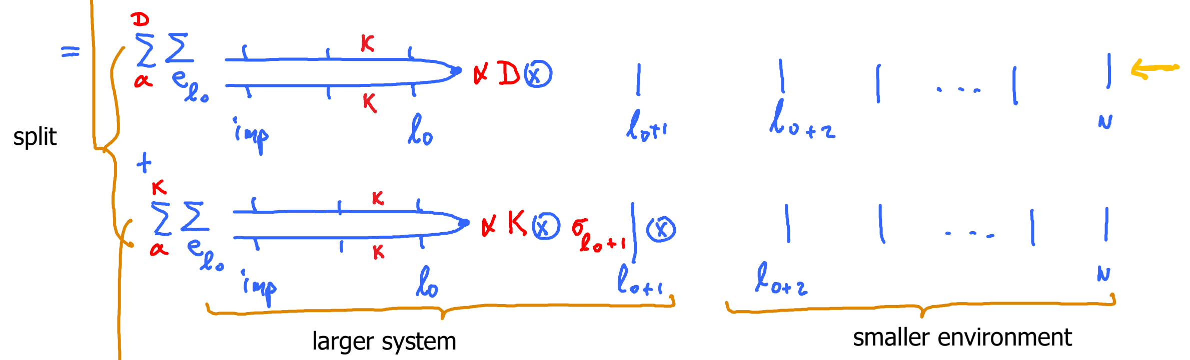
$$P^{X'}_{\ell'} P^X_\ell \overset{(14,17)}{=} \begin{cases} \delta^{KX'} P^X_\ell & \text{if } \ell' < \ell \\ \delta^{X'X} P^X_\ell & \text{if } \ell' = \ell \\ P^{X'}_{\ell'} \delta^{XK} & \text{if } \ell' > \ell \end{cases} \tag{19}$$

Graphical depiction of completeness of AS basis

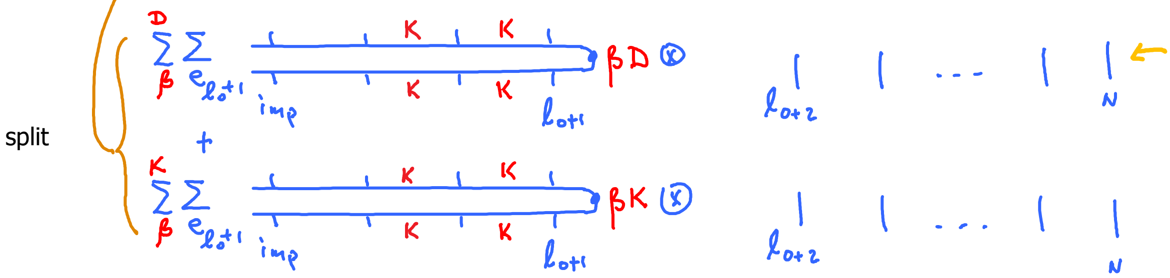


Transform to basis which diagonalizes sites imp to ℓ_0, keeping (K) the full spectrum at each step):

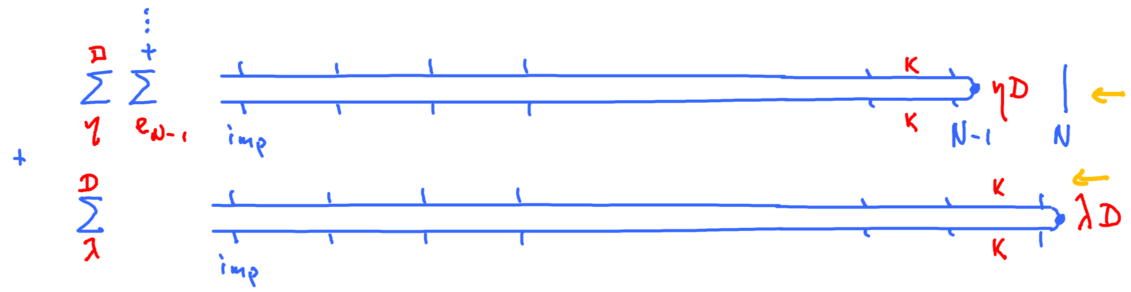
Split into discarded and kept states. In latter sector, move one site from environment into system:



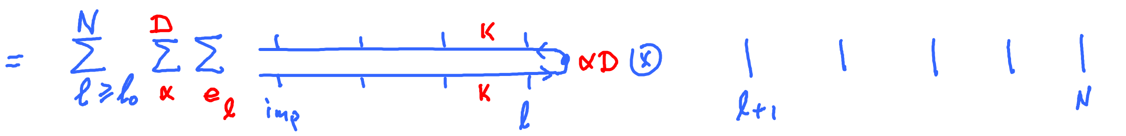
Now diagonalize, split again, and iterate:



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

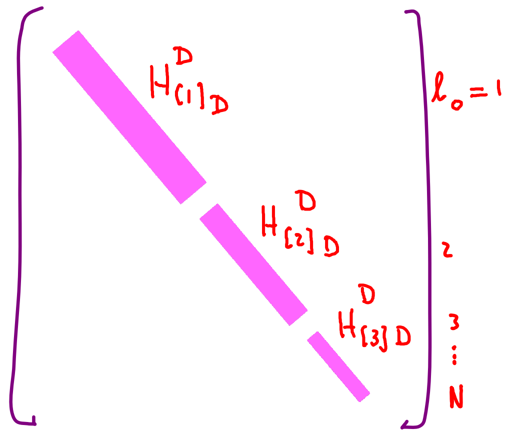


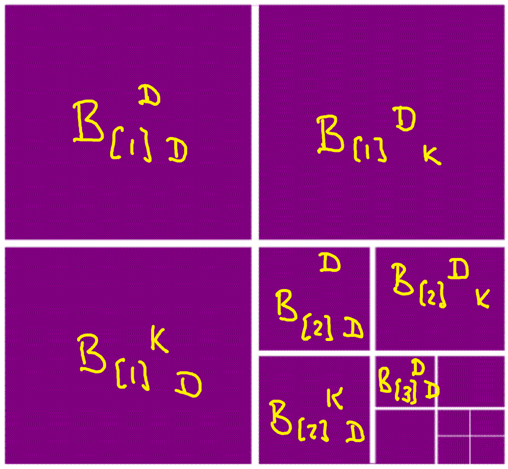
The collection of all terms marked ← is the resolution of identity in AS basis:



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:

$\hat{H} \simeq$ 

$\hat{B} \simeq$  (1)

Hamiltonian is diagonal: General operator: exclude KK to avoid overcounting!

$$\hat{H}^N \overset{(1.2)}{\simeq} \sum_\ell \sum_{\alpha e} E_\alpha^\ell \, |\alpha e\rangle_\ell^D \, {}_\ell^D\langle \alpha, e| \, , \qquad \hat{B} \simeq \sum_\ell \sum_{X'X}^{\neq KK} \sum_\alpha \sum_e |\alpha' e\rangle_\ell^{X'} \left[B_{[\ell]X}^{X'}\right] {}_\ell^X\langle \alpha, e| \tag{2}$$

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:

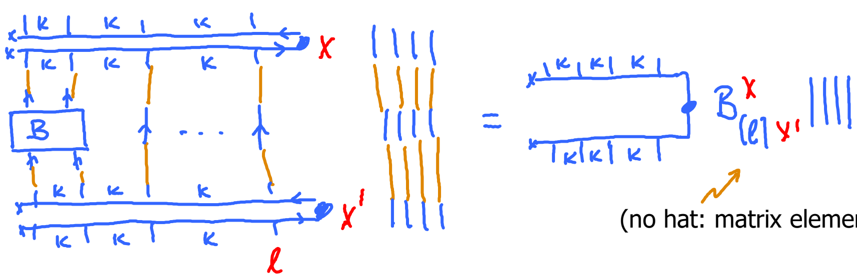
Suppose $\hat{B}$ is a 'local operator', living on sites $\leq \ell_0$, e.g. on sites imp and 0 :

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

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

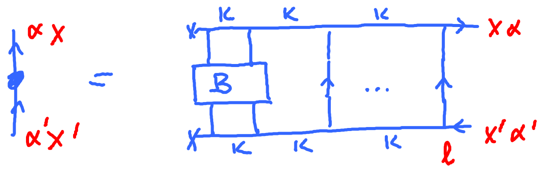
$$\hat{B} = \sum_{XX' \in \{K,D\}} |\alpha' e\rangle_{\ell_0}^{X'} \left[B_{[\ell_0]}{}^{X'}{}_X\right]^{\alpha'}{}_\alpha \, {}_{\ell_0}^{X}\langle \alpha e| \equiv \sum_{X'X} \hat{B}_{[\ell_0]X}^{X'} \tag{4}$$

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

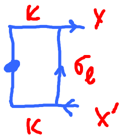
$\hat{B}_{[\ell]X}^{X'} =$  (6)

(no hat: matrix elements)

with matrix elements

$B_{[\ell]X}^{X'}$  (7)

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

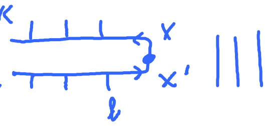
$$= \mathcal{B}^{K}_{[\ell-1]K} \quad$$  $$= \left[A^{\dagger\, X'}_{[\ell]\;K}\right]^{\alpha'}_{\sigma_\ell \beta'} \left[\mathcal{B}^{K}_{[\ell-1]K}\right]^{\beta'}_{\beta} \left[A^{K}_{[\ell]\,X}\right]^{\beta\sigma_\ell}_{\alpha} \qquad (8)$$

only KK enters here!

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

$$\hat{\mathcal{B}}^{K}_{[\ell_0]K} = \hat{P}^{K}_{\ell_0}\,\hat{\mathcal{B}}\,\hat{P}^{K}_{\ell_0} = \sum_{X'X}^{\neq KK} \hat{P}^{X'}_{\ell_0+1}\,\hat{\mathcal{B}}\,\hat{P}^{X}_{\ell_0+1} + \hat{P}^{K}_{\ell_0+1}\,\hat{\mathcal{B}}\,\hat{P}^{K}_{\ell_0+1} \qquad (9)$$

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

Full operator: $$\hat{\mathcal{B}} = \sum_{X} \hat{\mathcal{B}}^{X}_{[\ell_0]X} \overset{(10)}{=} \sum_{\ell\geq\ell_0}^{N} \sum_{X'X}^{\neq KK} \hat{\mathcal{B}}^{X'}_{[\ell]X} = \sum_{\ell} \sum_{X'X}^{\neq KK}$$  $$\qquad (11)$$

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

<u>Time-dependent operators</u>

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

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

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

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.

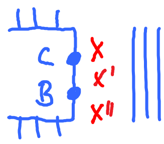
Fourier transform: $$\hat{\mathcal{B}}(\omega) = \int \frac{dt}{2\pi}\, e^{i\omega t}\,\hat{\mathcal{B}}(t) \overset{(12,13)}{=} \sum_{\ell} \sum_{X'X}^{\neq KK} \hat{\mathcal{B}}^{X'}_{[\ell]X}(\omega) \qquad (15)$$

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

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

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

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

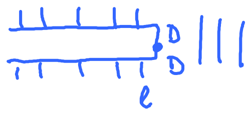
$$\hat{\mathcal{B}}\,\hat{\mathcal{C}} = \sum_{X''X'X} \hat{\mathcal{B}}^{X''}_{[\ell_0]X'}\,\hat{\mathcal{C}}^{X'}_{[\ell_0]X'} = \sum_{\ell} \sum_{X''X'X}^{\neq KKK} \hat{\mathcal{B}}^{X''}_{[\ell]X'}\hat{\mathcal{C}}^{X'}_{[\ell]X} = \sum_{\ell} \sum_{X''X'X}^{\neq KKK}$$ 

3. Full density matrix

[Weichselbaum2007]

NRG approximation

$$\hat\rho \equiv e^{-\beta \hat H^N} \simeq \sum_\ell \underbrace{\sum_{\alpha e} |\alpha,e\rangle_\ell^D \, \frac{e^{-\beta E_\alpha^\ell}}{Z} \, {}_\ell^D\langle \alpha, e|}_{\hat\rho^D_{[\ell]D}} = \sum_\ell \qquad (1)$$



$$= \sum_{\ell=n_0}^{N} \hat\rho^D_{[\ell]D} , \qquad [\rho^D_{[\ell]D}] = \delta^{\alpha}_{\alpha'} \, \frac{e^{-\beta E^\ell_\alpha}}{Z} \qquad (2)$$

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

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

provides refinement for rest of chain

density matrix is sector-diagonal

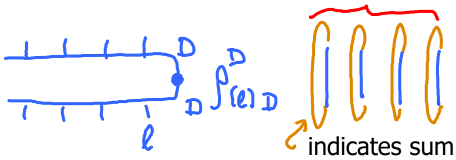
<u>Reduced density matrix</u> for length-ℓ chain is obtained by tracing out environment of all later sites:

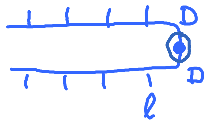
$$\hat{\bar\rho}^{X'}_{[\ell]X} = \mathrm{Tr}_{\text{sites} > \ell} \{ \hat\rho^{X'}_{[\ell]X} \} \qquad \left(\bar\rho^K_{[\ell]D} = \bar\rho^D_{[\ell]K} \overset{(3)}{=} 0 \right) \qquad (4)$$

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

DD-sector:

$$\hat{\bar\rho}^D_{[\ell]D} = \qquad\qquad = \qquad \bar\rho^D_{[\ell]D} \qquad (5)$$





indicates sum over local basis due to trace

(no hat: matrix elements)

with matrix elements

$$[\bar\rho^D_{[\ell]D}]^{\alpha'}_{\alpha} = [\rho^D_{[\ell]D}]^{\alpha'}_{\alpha} \, d^{N-\ell} \overset{(2)}{=} \underbrace{\delta^{\alpha'}_{\alpha} \, \frac{e^{-\beta E^\ell_\alpha}}{Z^D_\ell}} \; \underbrace{\frac{Z^D_{[\ell]}}{Z} \, d^{N-\ell}}_{w_\ell} \qquad (6)$$

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

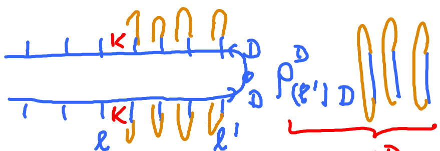
relative weight of D-sector of shell ℓ to total partition function, with $\sum_\ell w_\ell = 1$

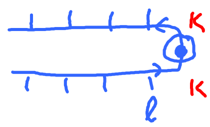
where $Z^D_\ell = \sum_\alpha^D e^{-\beta E^\ell_\alpha}$ (7)

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

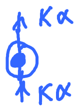
KK-sector:

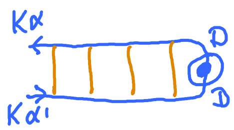
$$\hat{\bar\rho}^K_{[\ell]K} = \sum_{\ell'>\ell} \qquad \underbrace{\hat\rho^D_{[\ell']D}}_{\bar\rho^D_{[\ell']D}} \qquad = \qquad \bar\rho^K_{[\ell]K} \qquad (7)$$

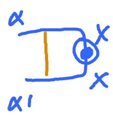




$$[\bar\rho^K_{[\ell]K}]^{\alpha'}_{\alpha} \qquad = \sum_{\ell'>\ell} \qquad \bar\rho^D_{[\ell']D} \qquad = \sum_X \qquad \bar\rho^X_{[\ell+1]X} \qquad (8)$$

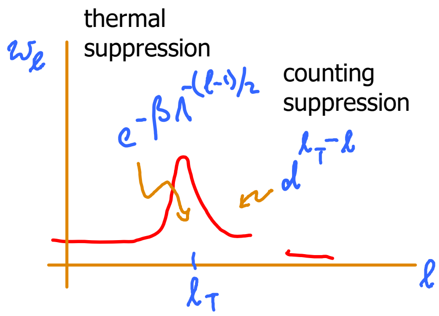






Starting at $\ell = N$, the KK matrix elements can be computed iteratively via a backward sweep.

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

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

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

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

Thermal expectation value:

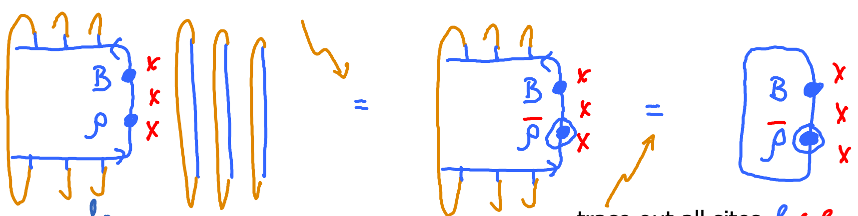
$\delta^{X''}_{X}$ due to trace

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

operator trace

$$= \sum_X \mathrm{Tr}_{\text{all sites}}\left[\hat\rho[\ell_0]^X_X\, \hat B[\ell_0]^X_X\right] = \sum_X \mathrm{Tr}_{\text{sites} \le \ell_0}\left[\hat{\bar\rho}[\ell_0]^X_X\, \hat B[\ell_0]^X_X\right] \qquad (11)$$

trace out all sites $\ell > \ell_0$



(12)

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

matrix trace

$$= \sum_X \mathrm{tr}_{\text{shell } \ell_0}\left[\bar\rho[\ell_0]^X_X\, B[\ell_0]^X_X\right] = \sum_X \sum_{\alpha'\alpha} \left[\bar\rho[\ell_0]^X_X\right]^{\alpha'}_{\alpha} \left[B[\ell_0]^X_X\right]^{\alpha}_{\alpha'} \qquad (13)$$

can be computed using solely shell-ℓ_0 matrix elements
(but reduced density matrix requires backward sweep along 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] [Lee2021]

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

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

Insert representation of these three operators in complete AS basis:

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

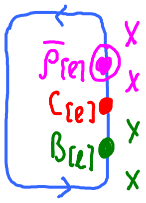
Looks intimidating, but can be simplified by systematically using (NRG-III.5.12) for overlaps.

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

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

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 :

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



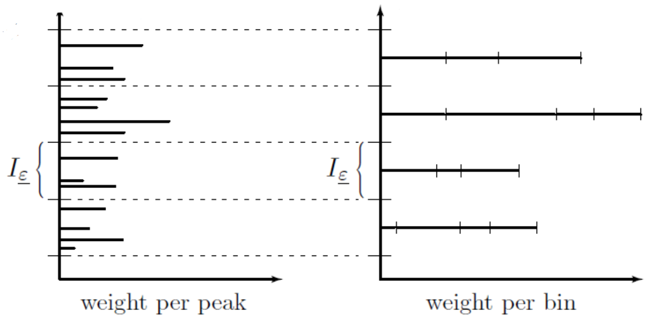
$$= \sum_{\ell}\sum_{X'X}^{\neq KK} \sum_{\alpha\alpha'} \left[B_{[\ell]}{}^{X}{}_{X'}\right]^{\alpha}{}_{\alpha'}\, \delta\big(\omega - (E^{\ell}_{\alpha'} - E^{\ell}_{\alpha})\big) \left[C_{[\ell]}{}^{X'}{}_{X}\, \bar\rho_{[\ell]}{}^{X}{}_{X}\right]^{\alpha'}{}_{\alpha} \qquad (5)$$

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

Each term involves a trace over matrix 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).

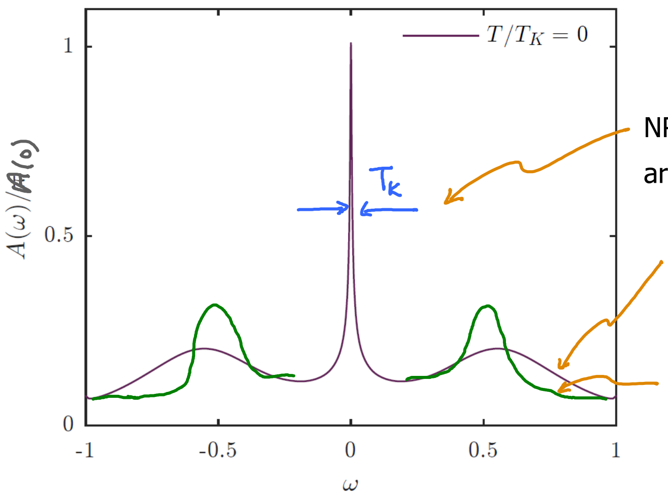
Spectral function of Anderson impurity model (at particle-hole symmetry, $\varepsilon_d = -U/2$ and zero magnetic field, $h = 0$)

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

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.

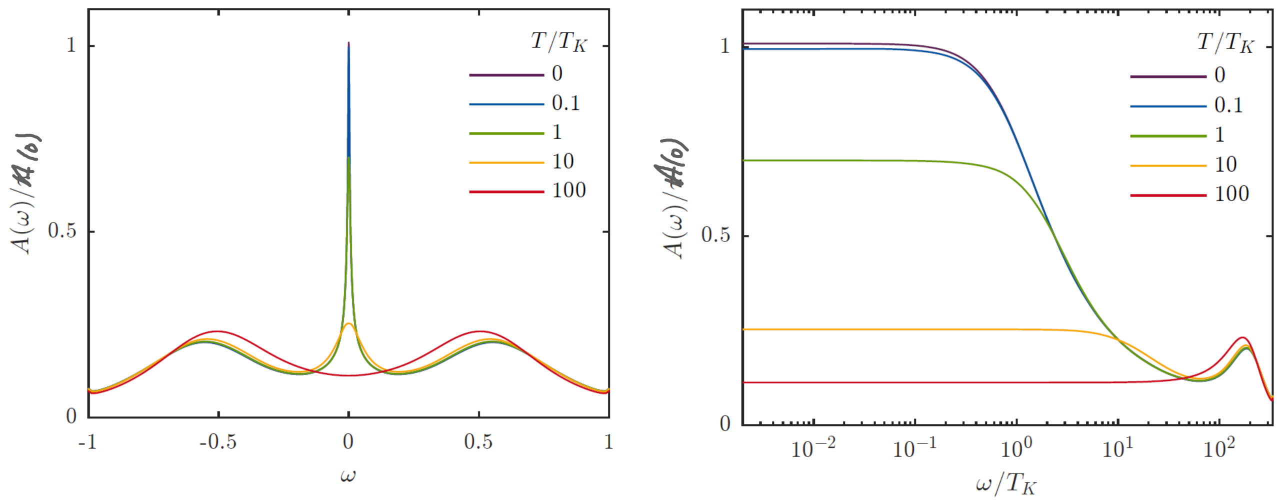
The true form of side peaks is narrower.

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 <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 $< 10^{-15}$