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

forms a complete basis in full Hilbert space of length-$\mathcal{L}$ chain, known as 'Anders-Schiller (AS) basis':
(proof follows below)

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

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

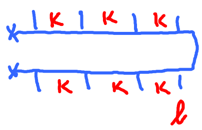
$$\hat{H}^\mathcal{L} |\alpha, e\rangle_\ell \simeq \hat{H}^\ell |\alpha, e\rangle_\ell = E_\alpha^\ell |\alpha, e\rangle_\ell \qquad (2)$$

Here we made the 'NRG approximation': when acting on states from shell ℓ, approximate $\hat{H}^\mathcal{L}$ 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:

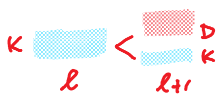
$$\hat{P}_\ell^X = \sum_{\alpha e} |\alpha e\rangle_\ell^X \, {}_\ell^X\langle\alpha e| = $$  $$\times \; \mathbb{1}_e \qquad (13)$$

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 $\ell = \ell_0$:

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

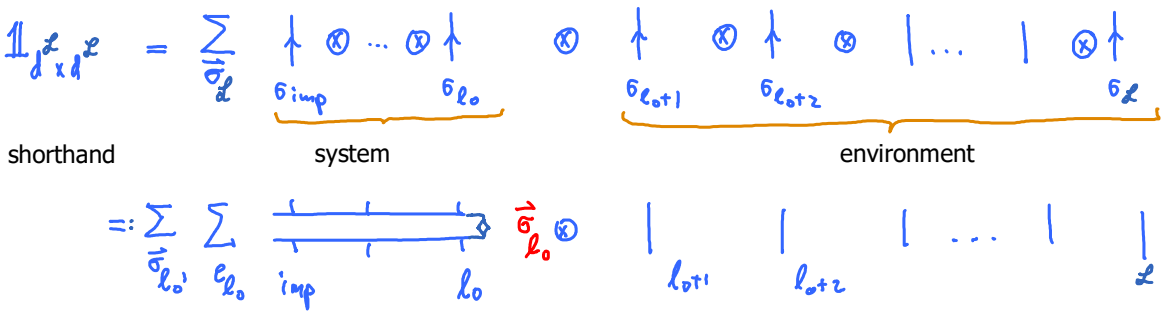
$$\sum_{\ell=\ell_0}^{\mathcal{L}} \equiv \sum_\ell$$

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

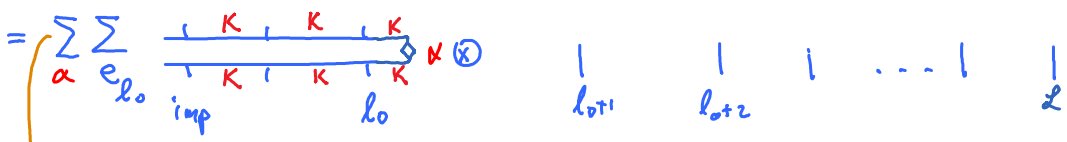
General projector products:

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

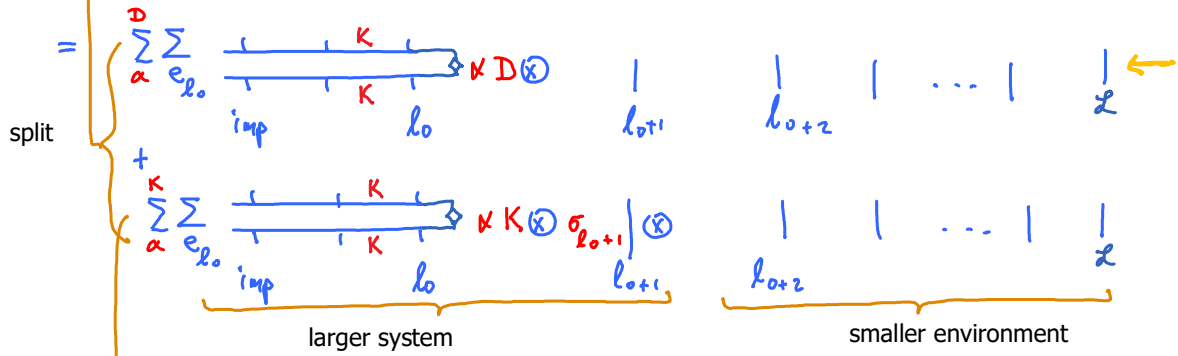
Graphical depiction of completeness of AS basis



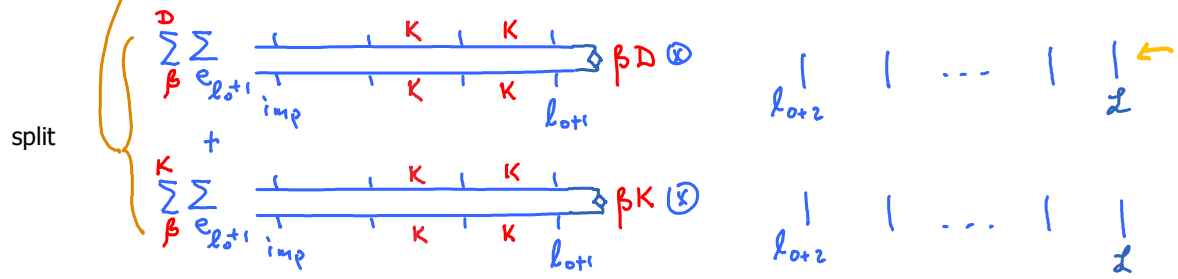
Transform to basis which diagonalizes sites imp to l_0, keeping (K) the full spectrum at each step):



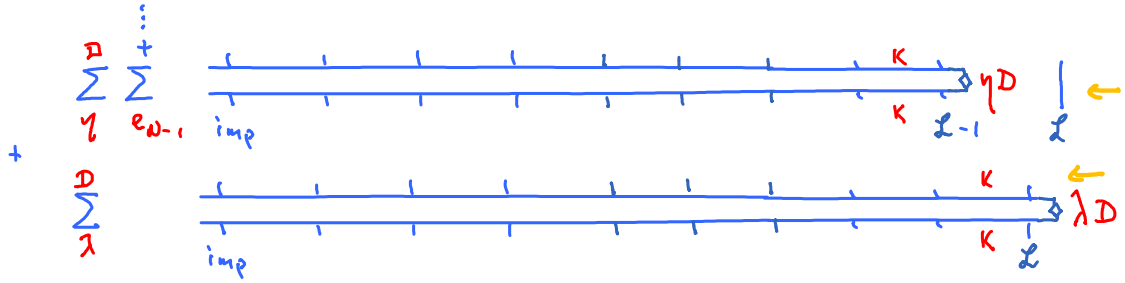
Split into discarded and kept states. In latter sector, move one site from environment into system:



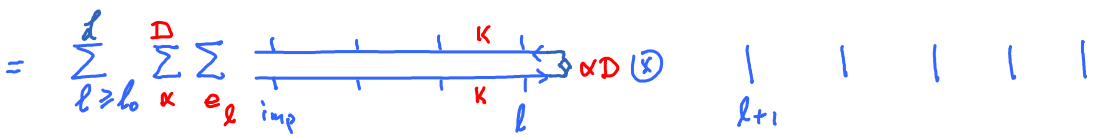
Now diagonalize, split again, and iterate:



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:

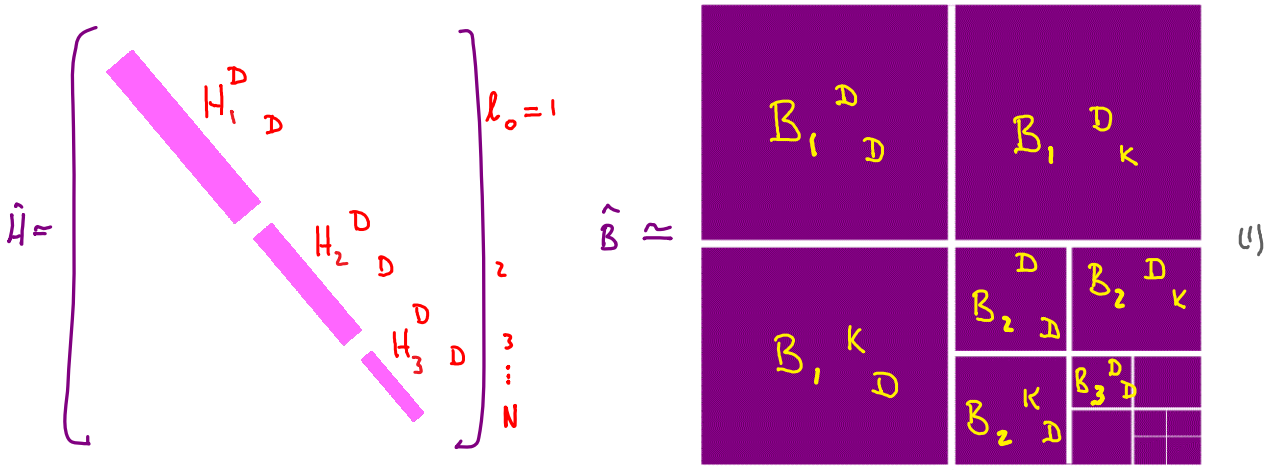


2. Operator expansions

[Weichselbaum2007], [Peters2006]

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

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



(1)

Hamiltonian is diagonal:

$$\hat{H}^{\ell} \overset{(I.2)}{\simeq} \sum_{\ell} \sum_{\alpha e} E_{\alpha}^{\ell} \, |\alpha e\rangle_{\ell}^{D\,D} \langle \alpha e|_{\ell} ,$$

General operator: exclude KK to avoid overcounting!

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

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

The expression for $\hat{H}^{\ell}$ 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 :

$$\hat{B} =$$

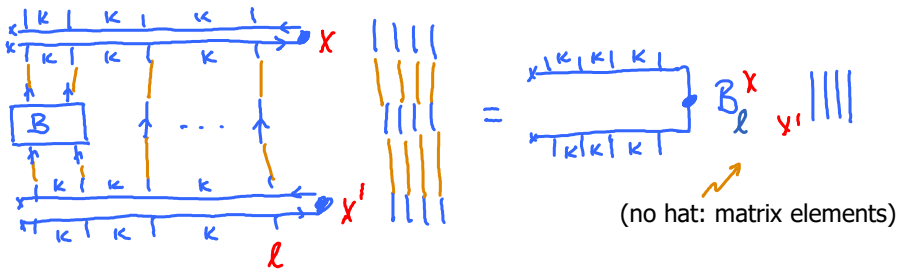
(3)

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

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

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

$\hat{B}_{\ell_0}{}^{x'}{}_{x} =$

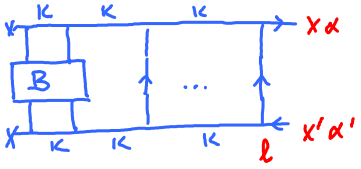


(6)

(no hat: matrix elements)

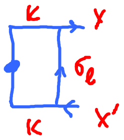
with matrix elements

$B_{\ell_0}{}^{x'}{}_{y}$ =



(7)

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

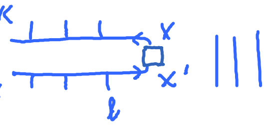
$$= \mathcal{B}^{K}_{\ell-1\;K}$$  $$= \left[A^{\dagger\,X'}_{\ell\;K}\right]^{\alpha'}_{\sigma_\ell\beta'} \left[\mathcal{B}^{K}_{\ell-1\;K}\right]^{\beta'}_{\beta} \left[A^{K}_{\ell\;X}\right]^{\beta\sigma_\ell}_{\alpha} \qquad (8)$$

only KK enters here!

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

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

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

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

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

Time-dependent operators

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

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

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

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.

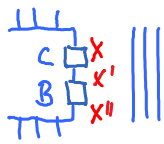
Fourier transform: $$\hat{\mathcal{B}}(\omega) = \int \frac{dt}{2\pi}\, e^{i\omega t}\,\hat{\mathcal{B}}(t) \overset{(12,13)}{=} \sum_{\ell} \sum_{X'X}^{\neq KK} \hat{\mathcal{B}}^{X'}_{\ell\;X}(\omega) \qquad (15)$$

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

Operator product expansions: $\hat{\mathcal{B}}\,\hat{\mathcal{C}}$ 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)

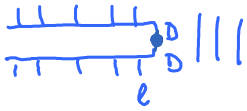
$$\hat{\mathcal{B}}\,\hat{\mathcal{C}} = \sum_{X''X'X} \hat{\mathcal{B}}^{X''}_{\ell_0\;X'}\,\hat{\mathcal{C}}^{X'}_{\ell_0\;X} = \sum_{\ell} \sum_{X''X'X}^{\neq KKK} \hat{\mathcal{B}}^{X''}_{\ell\;X'}\hat{\mathcal{C}}^{X'}_{\ell\;X} = \sum_{\ell} \sum_{X''X'X}^{\neq KKK}$$ 

3. Full density matrix

[Weichselbaum2007]

NRG approximation

$$\hat\rho \equiv e^{-\beta \hat H^{\mathcal{L}}} \overset{\eta}{\simeq} \sum_\ell \sum_{\alpha e} |\alpha,e\rangle^D_\ell \frac{e^{-\beta E^\ell_\alpha}}{Z} {}^D_\ell\langle \alpha,e| = \sum_\ell \hat\rho^D_{[\ell]D} \qquad (1)$$



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

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:

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

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:

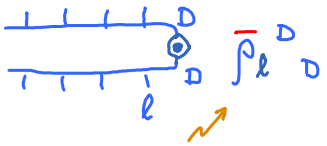
$$\bar\rho^{X'}_{\ell\,X} = \operatorname*{Tr}_{\text{sites}>\ell} [\hat\rho^{X'}_{\ell\,X}] \qquad (\bar\rho^K_{\ell\,D} = \bar\rho^D_{\ell\,K} \overset{(3)}{=} 0) \qquad (4)$$

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

DD-sector:

$$\bar\rho^D_{\ell\,D} =$$

$$= \bar\rho^D_{\ell\,D} \qquad (5)$$



indicates sum over local basis due to trace

(no hat: matrix elements)

with matrix elements

$$[\bar\rho^D_{\ell\,D}]^{\alpha'}_{\alpha} = [\rho^D_{\ell\,D}]^{\alpha'}_{\alpha} d^{\mathcal{L}-\ell} \overset{(2)}{=} \delta^{\alpha'}_{\alpha} \underbrace{\frac{e^{-\beta E^\ell_\alpha}}{Z^D_\ell}}_{\text{density matrix of D-sector of shell } \ell \text{ (without environment)}} \underbrace{\frac{Z^D_\ell}{Z} d^{\mathcal{L}-\ell}}_{w_\ell} \qquad (6)$$

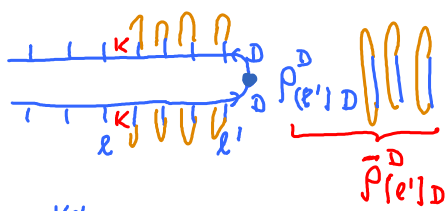
where $Z^D_\ell = \sum_\alpha{}^D e^{-\beta E^\ell_\alpha}$ (7)

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

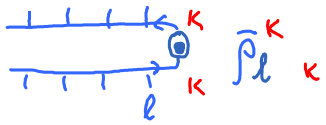
relative weight of D-sector of shell ℓ to total partition function, with $\sum_\ell w_\ell = 1$

KK-sector:

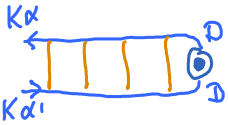
$$\bar\rho^K_{\ell\,K} = \sum_{\ell'>\ell}$$



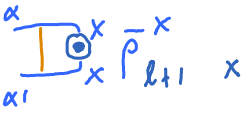
$$= \bar\rho^K_{\ell\,K} \qquad (7)$$



$$[\bar\rho^K_{\ell\,K}]^{\alpha'}_{\alpha} = \sum_{\ell'>\ell}$$



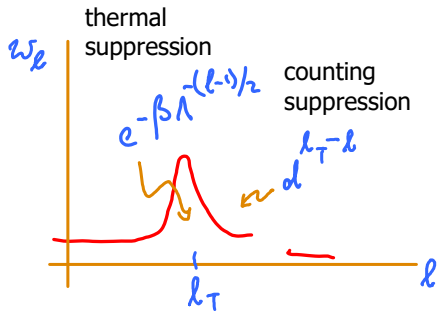
$$= \sum_{x}$$



$$(8)$$

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

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

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

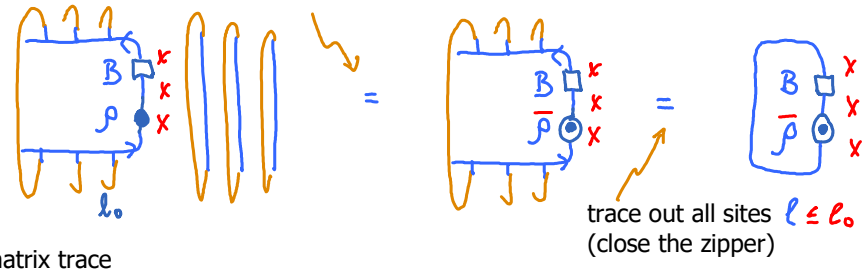
Thermal expectation value:

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

$\delta^{x''}_{x}$ due to trace; (3) $\delta^{x''}_{x'}$

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

operator trace; trace out all sites $\ell > \ell_0$



(12)

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

matrix trace

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

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

NRG-IV.4

[Weichselbaum2007] [Lee2021]

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

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

Insert representation of these three operators in complete AS basis:

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

$\tilde x \tilde x' \neq KK$; $\bar x' \bar x \neq KK$

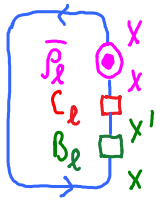
Looks intimidating, but can be simplified by systematically using (NRG-III.5.12) for overlaps.

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

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

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 :

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



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

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.

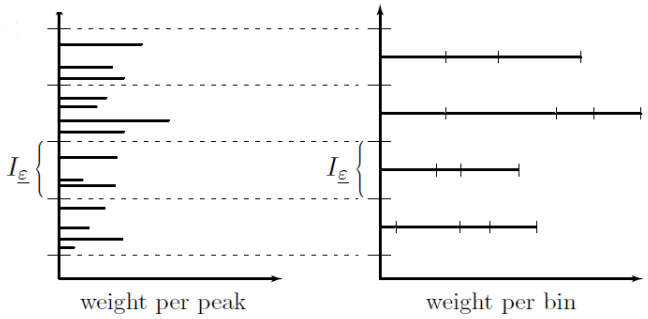
To deal with delta functions, use 'binning':

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 $E \in I_\varepsilon$

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



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

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

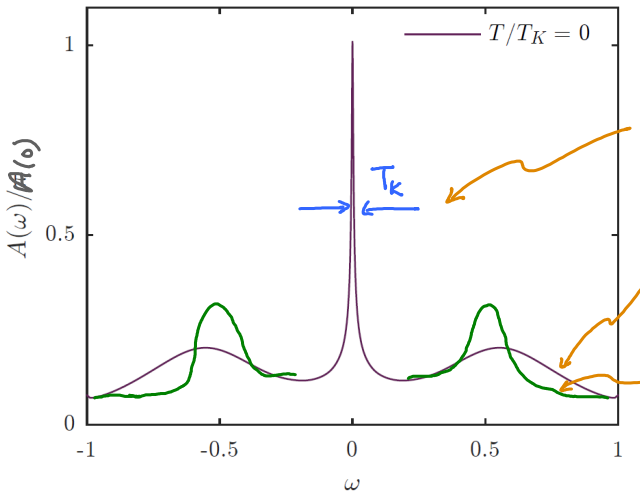
Spectral function of Anderson impurity model (at particle-hole symmetry, $\varepsilon_d = -U/2$ and zero magnetic field, $h = 0$)

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

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.

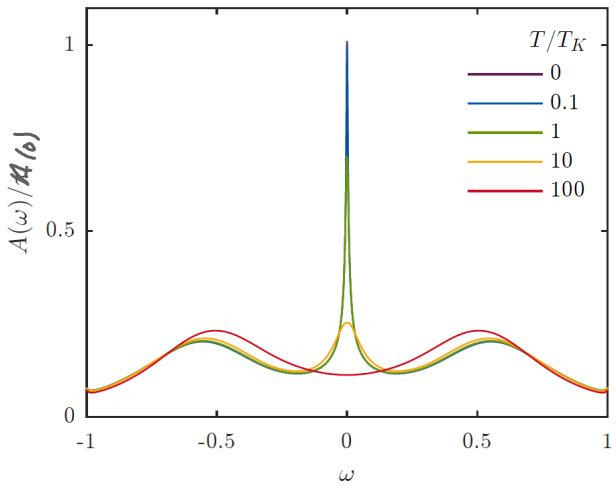
The true form of side peaks is narrower.

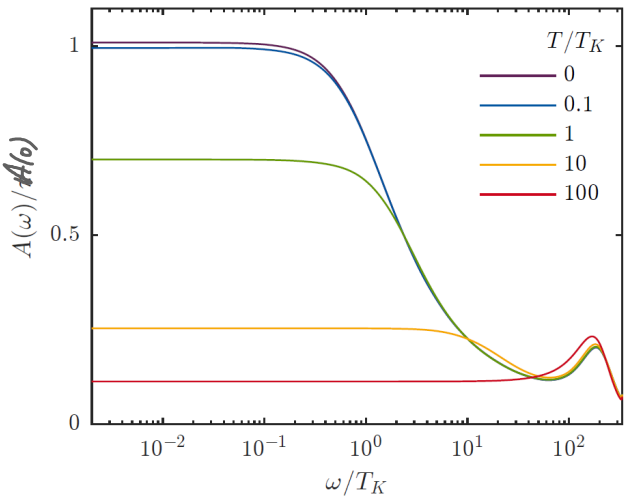
Over-broadening at large frequencies can be reduced using 'adaptive broadening' technique [Lee2016].

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 any temperature):

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

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