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), $\{ |\alpha, e\rangle_\ell^D \mid \ell = l_0, \dots, N \}$

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

$$\sum_{\vec{\sigma}_N} |\vec{\sigma}_N\rangle\langle\vec{\sigma}_N| \overset{\text{by definition}}{=} \mathbb{1}_{d^N \times d^N} \overset{\text{exact basis transformation}}{=} \sum_{\ell=l_0}^{N} \sum_{\alpha e} |\alpha, e\rangle_\ell^D \, {}_\ell^D\langle \alpha, e| \qquad (1)$$

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

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

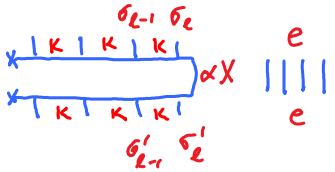
Here we made the 'NRG approximation': when acting on states from shell ℓ, approximate $\hat{H}^N$ by $\hat{H}^\ell$, i.e. neglect later-site parts of the Hamiltonian. Justification: they describe fine structure not relevant for capturing course structure of shell ℓ. The AS basis thus has following key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

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



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

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

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 $\ell = l_0$:

$$\mathbb{1}_{d^N \times d^N} = P_{l_0}^D + P_{l_0}^K = \sum_{\ell=l_0}^{N} P_\ell^D = \sum_\ell \qquad (18)$$

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

General projector products:

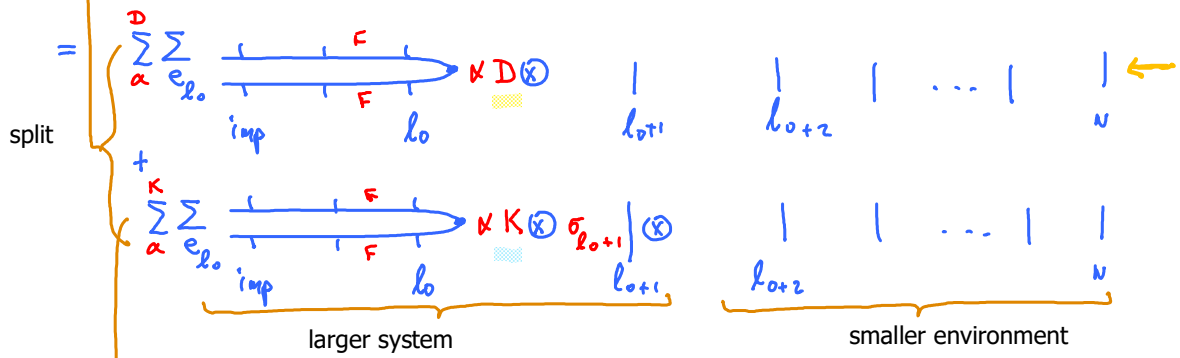
$$P_{\ell'}^{X'} P_\ell^X \overset{(14,17)}{=} \begin{cases} \delta^{KX'} P_\ell^X & \text{if } \ell' < \ell \\ \delta^{XX'} P_\ell^X & \text{if } \ell' = \ell \\ P_{\ell'}^{X'} \delta^{KK} & \text{if } \ell' > \ell \end{cases} \qquad (19)$$

$\rho^{x'}_{l'}$ δ^{KK} if $l' > l$

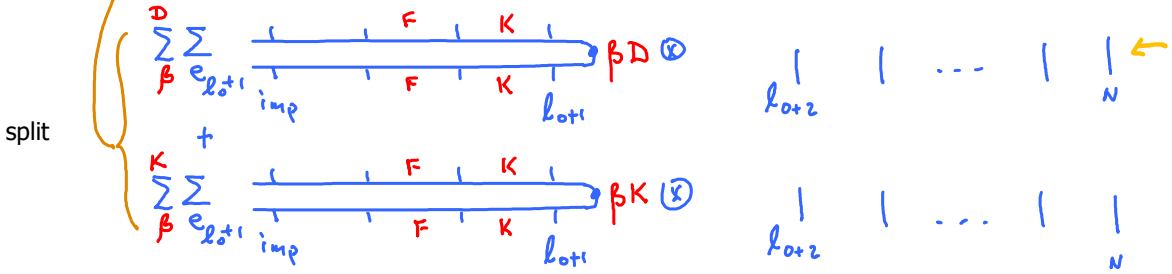
Graphical depiction of completeness of AS basis

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

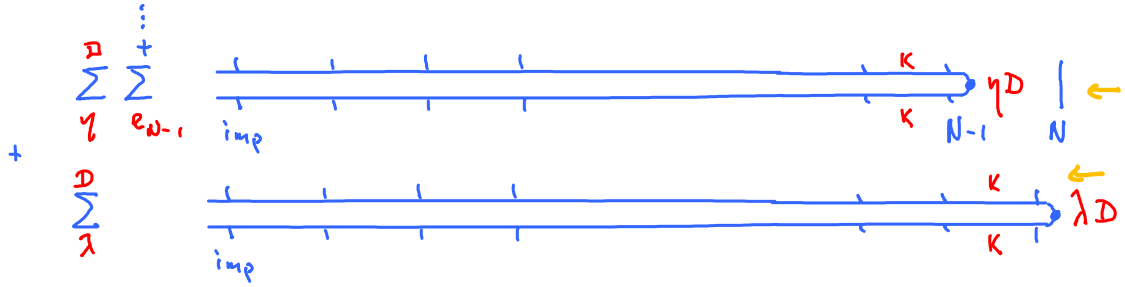
Split into discarded and kept states. In latter sector, move one site from environment into system:



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:

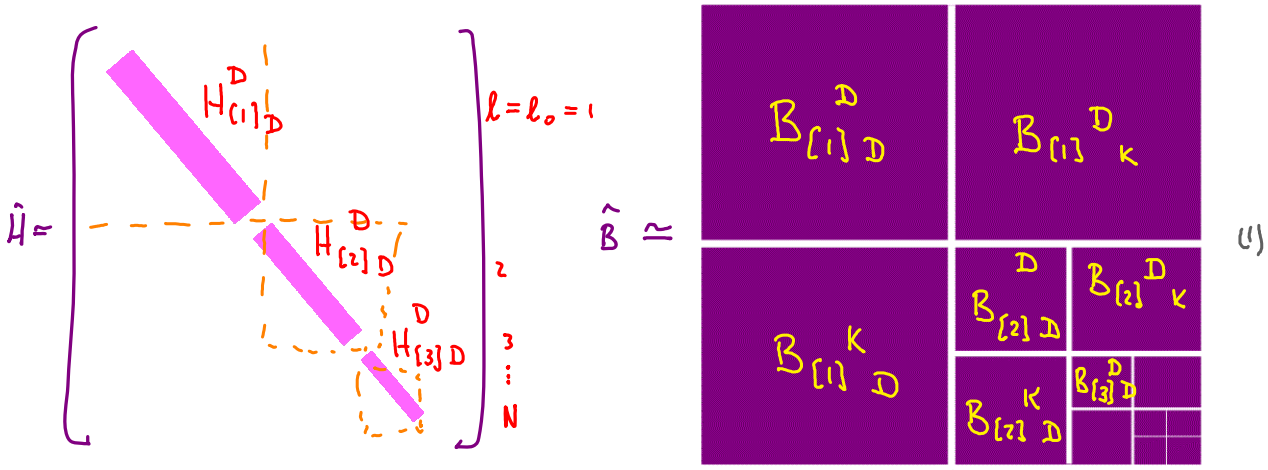
$$= \sum_{\ell \geq \ell_0}^{N} \sum_{\alpha}^{D} \sum_{e_\ell}$$

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:

$$\hat{H}^N \overset{(I.2)}{\simeq} \sum_l \sum_\alpha E^l_\alpha \, |\alpha e\rangle^D_l \, {}^D_l\langle \alpha e| \,,$$

General operator: exclude KK to avoid overcounting!

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

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 $\hat{B}$ operator can be found as follows:

Suppose $\hat{B}$ is a 'local operator', living on sites $\leq l_0$, (e.g. on sites imp and 0) :

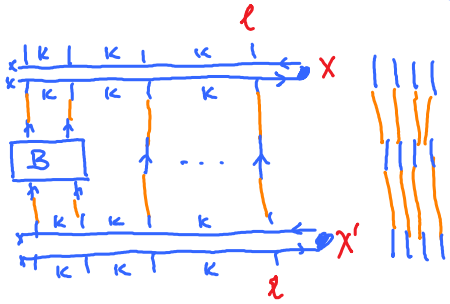
$$\hat{B} = \quad B^{\sigma_{imp}\,\sigma_0}_{\sigma'_{imp}\,\sigma'_0} \otimes |_{\sigma_2} \otimes \dots \otimes |_{\sigma_{l_0}} \otimes |_{\sigma_{l_0+1}} \otimes |_{\sigma_{l_0+2}} \otimes \dots \otimes |_{\sigma_N} \qquad (3)$$

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

$$\hat{B} = \sum_{x x' \in \{K,0\}} \sum_{\alpha' \alpha e} |\alpha' e\rangle^{x'}_{l_0} \, [B_{[l_0]x}]^{\alpha'}_{\alpha} \, {}^x_{l_0}\langle \alpha e| \equiv \sum_{x'x} \hat{B}^{x'}_{[l_0]x} \qquad (4)$$

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

$\hat{B}^{x'}_{[l]x} =$



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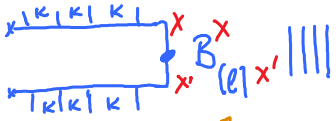
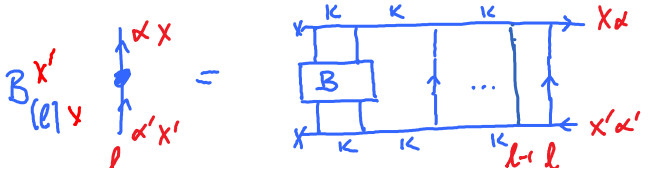


(6)

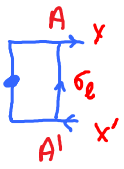
(no hat: matrix elements)

with matrix elements



(7)

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



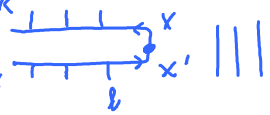
$$= B_{[\ell-1]} \quad = \left[A^{\dagger}_{[\ell]}\right]^{\alpha'}_{\sigma_\ell \beta} \left[B_{[\ell-1]}\right]^{\beta'}_{\beta} \left[A_{[\ell]}\right]^{\beta \sigma_\ell}_{\alpha} \qquad (8)$$

only KK enters here!

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

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

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

Full operator: $\hat{B} = \sum_x \hat{B}^x_{[\ell_0]x} = \sum_{\ell \geq \ell_0}^{N} \sum_{x'x}^{\neq KK} \hat{B}^{x'}_{[\ell]x} = \sum_\ell \sum_{x'x}^{\neq KK}$  (11)

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

Time-dependent operators

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

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

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

resolution $\sim \Lambda^{-\ell/2}$

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.

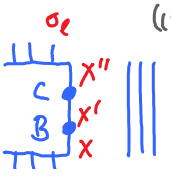
Fourier transform: $\hat{B}(\omega) = \int \frac{dt}{2\pi} e^{i\omega t} \hat{B}(t) \overset{(12,13)}{=} \sum_\ell \sum_{x'x}^{\neq KK} \hat{B}^{x'}_{[\ell]x}(\omega)$ (15)

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

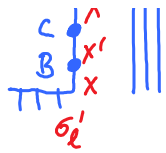
Operator product expansions: $\hat{B}\hat{C}$ Proceed iteratively, refining only KK-KK sector:

$$\hat{B}^K_{[\ell]K} \hat{C}^K_{[\ell]K} = \hat{P}^K_\ell \hat{B} \hat{P}^K_\ell \hat{C} \hat{P}^K_\ell \overset{(1.14)}{=} \sum_{xx'x''} \hat{P}^x_{\ell+1} \hat{B} \hat{P}^{x'}_{\ell+1} \hat{C} \hat{P}^{x''}_{\ell+1} = \sum_{x'xx''} \hat{B}^x_{[\ell+1]x'} \hat{C}^{x'}_{[\ell+1]x''} \qquad (17)$$

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

$$\hat{B}\hat{C} = \sum_{xx'x''} \hat{B}^x_{[\ell_0]x'} \hat{C}^{x'}_{[\ell_0]x''} = \sum_{\ell \geq \ell_0}^{N} \sum_{xx'x''}^{\neq KKK} \hat{B}^x_{[\ell]x'} \hat{C}^{x'}_{[\ell]x''} = \sum_\ell \sum_{xx'x''}^{\neq KKK}$$ 

$$\hat{B}\,\hat{C} = \sum_{xx'x''} \hat{B}^{\,x}_{[\ell_0]\,x'}\,\hat{C}^{\,x'}_{[\ell_0]\,x''} = \sum_{\ell \geq \ell_0}^{N} \sum_{xx'x''}^{\neq xxx} \hat{B}^{\,x}_{[\ell]\,x'}\,\hat{C}^{\,x'}_{[\ell]\,x''} = \sum_{\ell} \sum_{xx'x''}^{\neq xxx}$$

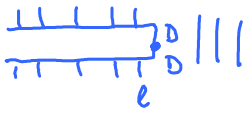


3. Full density matrix

[Weichselbaum2007]

NRG-IV.3

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



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

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:

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

provides refinement for rest of chain

density matrix is sector-diagonal

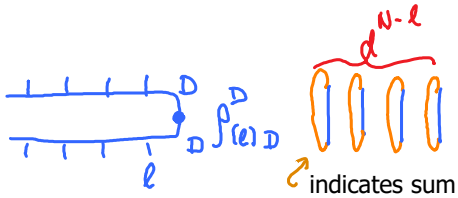
Reduced density matrix for length-ℓ chain is obtained by tracing out environment of all later sites:

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

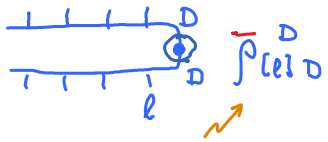
degeneracy of environment for shell ℓ

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

$$\big[\bar\rho_{[\ell]D}^D\big]_\alpha^{\alpha'} = \big[\rho_{[\ell]D}^D\big]_\alpha^{\alpha'} d^{N-\ell} \overset{(2)}{=} \delta^{\alpha'}_{\ \alpha} \frac{e^{-\beta E_\alpha^\ell}}{Z_\ell^D} \frac{Z_\ell^D}{Z} d^{N-\ell} \qquad (6)$$

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

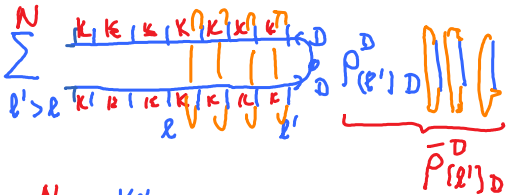
relative weight of D-sector of shell ℓ to total partition function, with $\sum_\ell w_\ell = 1$

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

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

KK-sector:

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



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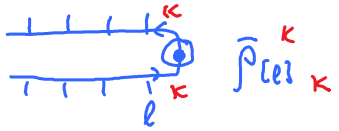
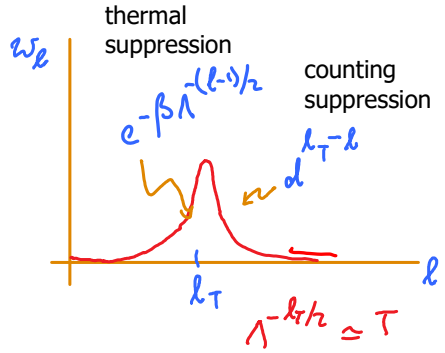


$$\bar\rho_{[\ell]K}^K \qquad (7)$$

$$= \sum_x \bar\rho_{[\ell+1]x}^x \qquad (8)$$

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

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

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

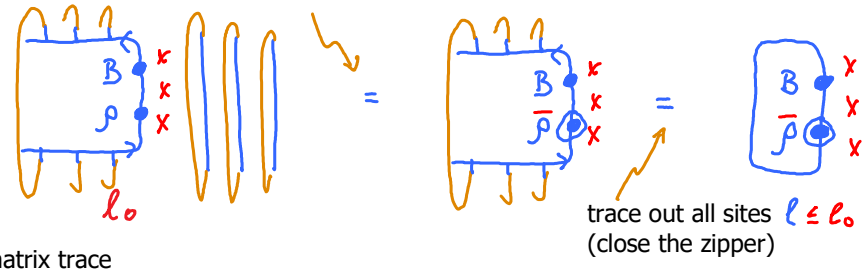
Thermal expectation value:

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

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

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

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



(12)

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

(matrix trace)

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

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

[Weichselbaum2007]

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

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

trace is cyclic

Insert representation of these three operators in complete AS basis:

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

$\tilde x \tilde x' \neq kk$ $\qquad$ $\bar x' \bar x \neq kk$

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

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

$$A^{BC}(\omega) = \mathrm{Tr}\left[\hat B(\omega)(\hat C\hat\rho)\right] = \sum_{\ell \geq \ell_0}^{N} \sum_{kk'x''}^{\neq kkk} \mathrm{Tr}\Big[\hat B_{[\ell]}(\omega)^x{}_{x'}\ \underbrace{(\hat C\hat\rho)_{[\ell]}^{x'}{}_{x''}}_{\text{trace is cyclic}}\Big] \qquad (3)$$

$\delta^x{}_{x''}$

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 :

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

$$= \sum_\ell \sum_{xx'}^{\neq kk} \sum_{\alpha\alpha'} \big[B_{[\ell]}{}^x{}_{x'}\big]^\alpha_{\alpha'}\ \delta\big(\omega - (E^\ell_{\alpha'} - E^\ell_\alpha)\big)\ \big[C_{[\ell]}{}^{x'}{}_x\ \rho_{[\ell]}{}^x{}_x\big]^{\alpha'}_\alpha \qquad (5)$$

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

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

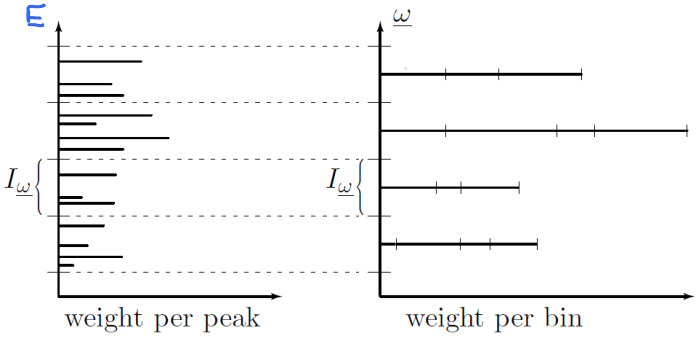
Easy to evaluate numerically.

To deal with delta functions, use 'binning':

partition frequency axis into discrete bins,

and replace $\delta(\omega - E)$ by bin function:

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



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

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

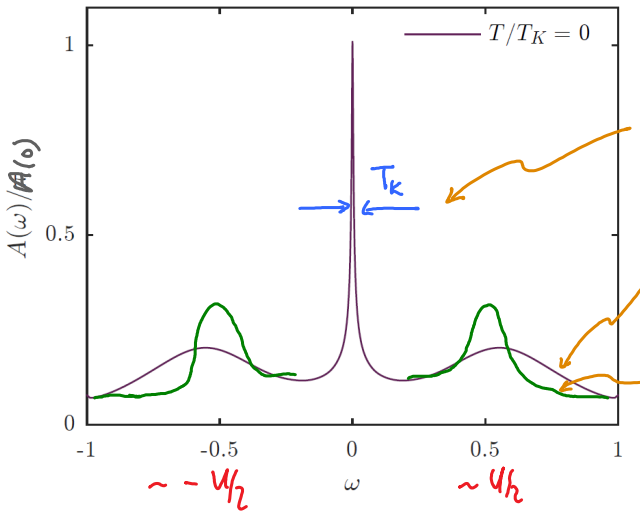
Spectral function of Anderson impurity model (at particle-hole symmetry, $\varepsilon_d = -U/2$ and zero magnetic field, $h = 0$)

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

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'.

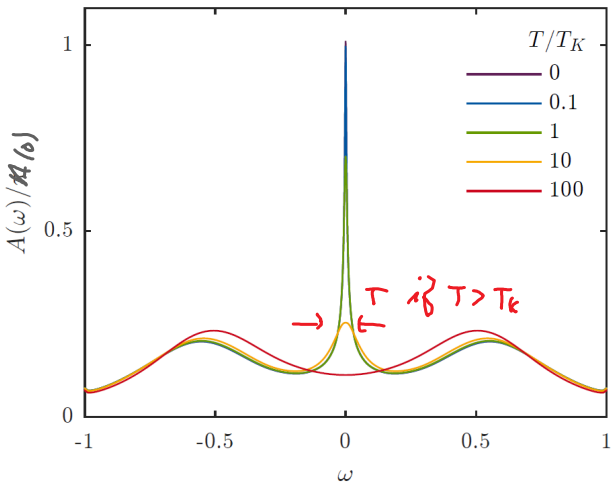
NRG overbroadens the side peaks, which lie at high energies.

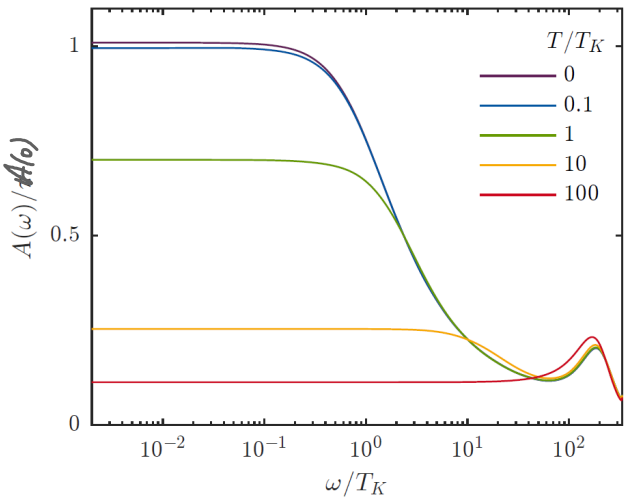
The true form of side peaks is narrower.
Over-broadening at large frequencies can be reduced using 'adaptive broadening' technique [Lee2016].

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 $< 10^{-15}$