tNRG III: Thermal and Dynamical Quantities

NRG-III.1

1. Thermodynamic observables

[Wilson1975, Sec. IX], [Krishna-murthy1980a, Sec. I.E]

Thermal expectation values:

$$\langle \hat{O} \rangle_T = \mathrm{Tr}[\hat{\rho}\,\hat{O}] = \frac{\mathrm{Tr}[e^{-\beta \hat{H}} \hat{O}]}{\mathrm{Tr}[e^{-\beta \hat{H}}]} = \frac{\sum_\alpha e^{-\beta E_\alpha} \langle \alpha | \hat{O} | \alpha \rangle}{\sum_\alpha e^{-\beta E_\alpha}} \qquad (1)$$

Trace is over a complete set of many-body states, $\{|\alpha\rangle\}$. A complete set was not available in Wilson's formulation of NRG (it was found only in 2005 by Anders & Schiller in 2005, to be discussed later). However, Wilson argued that dominant contribution comes from states with $E_\alpha \simeq T$. Reason: (2)

For $E_\alpha \gg T$, we have $e^{-\beta E_\alpha} \ll 1$ ('thermal suppression') (3)

(will be shown explicitly later)

For $E_\alpha \ll T$, we have $e^{-\beta E_\alpha} \simeq 1$, but there are much fewer such states than (4)
states with $E_\alpha \simeq T$, hence their weight in the trace is negligibly small ('counting suppression')

Wilson's iteration scheme yields, for each chain length ℓ, a 'shell' of eigenstates of $\hat{H}^\ell$:

$$\hat{H}^\ell |\alpha\rangle_\ell = E^\ell_\alpha |\alpha\rangle_\ell , \quad \alpha = 1, \dots, D_{\mathrm{kept}} \qquad (5)$$

He thus proposed to compute the expectation value using only a single shell (single-shell approximation), namely the one, say shell ℓ_T, whose characteristic energy matches the temperature:

$$\Lambda^{-(\ell_T - 1)/2} \simeq T , \qquad \text{hence} \quad \ell_T \simeq 2 \ln(1/T)/\ln\Lambda + 1 \qquad (6)$$

$$\langle \hat{O} \rangle_T \simeq \frac{\sum_{\alpha \in \text{shell } \ell_T} e^{-\beta(E^{\ell_T}_\alpha - E^{\ell_T}_g)} {}_{\ell_T}\langle \alpha | \hat{O} | \alpha \rangle_{\ell_T}}{\sum_{\alpha \in \text{shell } \ell_T} e^{-\beta(E^{\ell_T}_\alpha - E^{\ell_T}_g)}} \qquad (7)$$

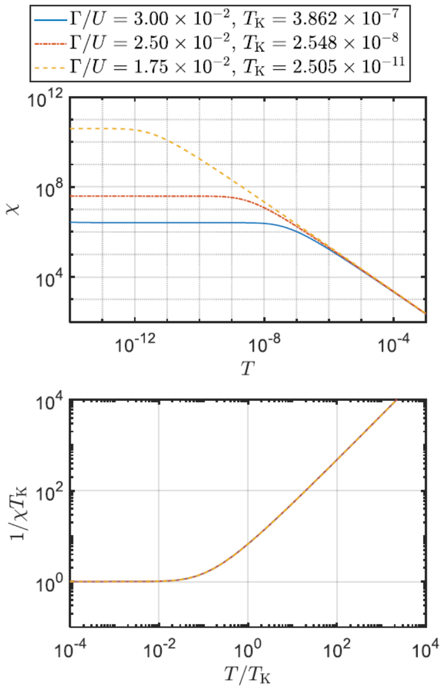
To compute (7) explicitly, express it in terms of rescaled energies and temperature:

Wilson's choice; often the -1 is ommitted

$$\tilde{E}^\ell_\alpha \overset{\text{(NRG-II.4.4)}}{=} \Lambda^{(\ell-1)/2} (E^\ell_\alpha - E^\ell_g) , \qquad \tilde{\beta}_\ell \equiv \Lambda^{-(\ell-1)/2} \beta \qquad (8)$$

$$\boxed{\langle \hat{O} \rangle_T \simeq \frac{\sum_{\alpha \in \text{shell } \ell_T} e^{-\tilde{\beta}_{\ell_T} \tilde{E}^{\ell_T}_\alpha} {}_{\ell_T}\langle \alpha | \hat{O} | \alpha \rangle_{\ell_T}}{\sum_{\alpha \in \text{shell } \ell_T} e^{-\tilde{\beta}_{\ell_T} \tilde{E}^{\ell_T}_\alpha}} \equiv \langle \hat{O} \rangle_{\ell_T}} \qquad (9)$$

Thermodynamic observables of physical interest [Krishna-murthy1980a]



Spin susceptibility: (10)

$$\chi = \frac{d}{dh}\langle S_z(h)\rangle_T \Big|_{h=0}$$

$$= \frac{d}{dh}\frac{\mathrm{Tr}\left[e^{-\beta(H-hS_z)}S_z\right]}{\mathrm{Tr}\left[e^{-\beta(H-hS_z)}\right]} \qquad (11)$$

$$= \beta\,\frac{\mathrm{Tr}\left[e^{-\beta H}S_z^2\right]}{\mathrm{Tr}\left[e^{-\beta H}\right]} - \beta\left[\frac{\mathrm{Tr}\left[e^{-\beta H}S_z\right]}{\mathrm{Tr}\left[e^{-\beta H}\right]}\right]^2 \qquad (12)$$

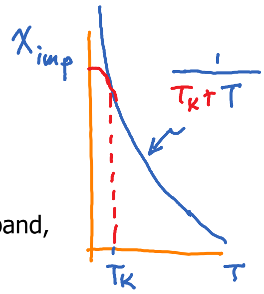
$$\boxed{\chi = \beta\left(\langle S_z^2\rangle_T - \langle S_z\rangle_T^2\right)} \qquad (13)$$

In NRG context: approximate $\langle\ \rangle_T$ by $\langle\ \rangle_{\ell T}$ of (9).

Impurity contribution: $\chi_{imp} = \chi_{tot} - \chi_{band}$ (14)

total system

only conduction band, without impurity



Specific heat

Partition function: $Z = \mathrm{Tr}\, e^{-\beta H} \equiv e^{-\beta F}$ with free energy $F = -T\ln Z$ (15)

Entropy: $$S = -\frac{\partial F}{\partial T} = \ln Z + T\,\frac{\mathrm{Tr}\left[e^{-\beta H}(-H)\right]}{Z}\underbrace{\left(\frac{\partial\beta}{\partial T}\right)}_{=-\frac{1}{T^2}} \qquad (16)$$

$$= \ln Z + u\beta, \quad \text{with} \quad u = \langle H\rangle_T \qquad (17)$$

Specific heat: $$C = \frac{\partial u}{\partial T} = \frac{\partial}{\partial T}\left[\frac{\mathrm{Tr}\,e^{-\beta H}H}{\mathrm{Tr}\,e^{-\beta H}}\right] = \beta^2\left(\langle H^2\rangle_T - \langle H\rangle_T^2\right) \qquad (18)$$

expensive numerically

alternatively: $$\boxed{C = \frac{\partial}{\partial T}\left[T(S - \ln Z)\right]} \qquad (19)$$

Impurity contribution: $C_{imp} = C_{tot} - C_{band}$ (20)

Wilson ratio: $$\boxed{R = \frac{\chi_{imp}/\chi_{band}}{C_{imp}/C_{band}}\Big|_{T=0}}$$ (universal number, independent of T_K) (21)

For Kondo model and symmetric Anderson model: $R = 2$

2. Lehmann representation of spectral functions

NRG-III.2

Goal: to compute dynamical quantities such as

$$\mathcal{A}^{BC}(\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i\omega t} \langle \hat{B}(t)\,\hat{C} \rangle_T , \qquad \langle \ldots \rangle_T = \mathrm{Tr}[\hat{\rho} \ldots] . \tag{1}$$

Let $\{|\alpha\rangle\}$ be a complete set of many-body eigenstates of H,

$$\hat{H}|\alpha\rangle = E_\alpha |\alpha\rangle , \qquad \sum_\alpha |\alpha\rangle\langle\alpha| = \mathbb{1}_{d^N \times d^N} \tag{2}$$

Then

$$\mathcal{A}^{BC}(\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i\omega t} \sum_{\alpha\beta} \langle\alpha|\,\hat{\rho}\, e^{i\hat{H}t}\hat{B}\, e^{-i\hat{H}t}|\beta\rangle\langle\beta|\hat{C}\,|\alpha\rangle \tag{3}$$

with density matrix $\hat{\rho} = e^{-\beta\hat{H}}/Z$ and partition function $Z = \sum_\alpha e^{-\beta E_\alpha}$ (4)

$$\mathcal{A}^{BC}(\omega) = \sum_{\alpha\beta} \frac{e^{-\beta E_\alpha}}{Z} \langle\alpha|\hat{B}|\beta\rangle \underbrace{\int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{it(\omega + E_\alpha - E_\beta)}}_{\delta(\omega - E_{\beta\alpha})} \langle\beta|\hat{C}|\alpha\rangle \tag{5}$$

$$E_{\beta\alpha} = E_\beta - E_\alpha$$

$$\boxed{\mathcal{A}^{BC}(\omega) = \sum_{\alpha\beta} \frac{e^{-\beta E_\alpha}}{Z} \langle\alpha|\hat{B}|\beta\rangle\, \delta(\omega - E_{\beta\alpha})\, \langle\beta|\hat{C}|\alpha\rangle} \tag{6}$$

'Lehmann representation'

Spectral sum rule:

$$\int d\omega\, \mathcal{A}^{BC}(\omega) = \sum_{\alpha\beta} \frac{e^{-\beta E_\alpha}}{Z} \langle\alpha|\hat{B}\underbrace{|\beta\rangle\langle\beta|}_{\mathbb{1}}\hat{C}|\alpha\rangle = \langle \hat{B}\,\hat{C} \rangle_T \tag{7}$$

Zero temperature

$$\mathcal{A}^{BC}(\omega)\Big|_{T=0} \overset{(6)}{=} \sum_\beta \langle g|\hat{B}|\beta\rangle\, \delta(\omega - E_{\beta g})\, \langle\beta|\hat{C}|g\rangle \tag{8}$$

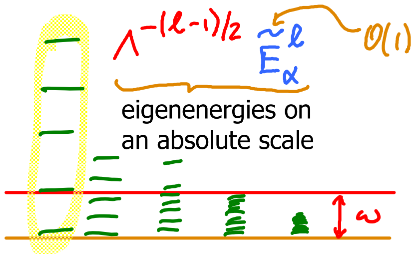
3. Single-shell and patching schemes

[Bulla2008, Sec. III.B]

NRG-III.3

NRG gives energy shells,

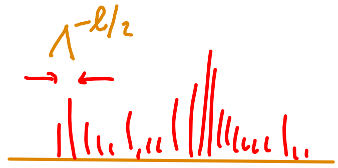
$$\tilde{H}^{\ell}|\alpha\rangle_{\ell} = \tilde{E}^{\ell}_{\alpha}|\alpha\rangle_{\ell} \qquad (1)$$



but they don't form a complete set, due to truncation.

Chose shell ℓ for which $\Lambda^{-(\ell-1)/2} \simeq \omega$

$$\mathcal{A}^{BC}(\omega)\Big|_{T=0} \overset{(6)}{=} \sum_{\beta\ell} {}_{\ell}\langle g|\hat{B}|\beta\rangle_{\ell}\, \delta(\omega - E^{\ell}_{\alpha g})\, {}_{\ell}\langle\beta|\hat{C}|g\rangle_{\ell} \qquad (2)$$



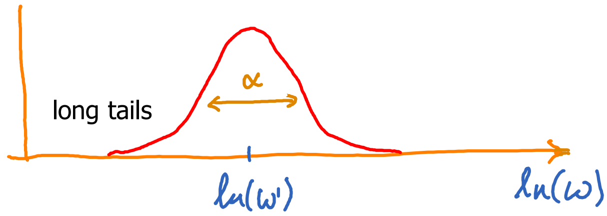
[Sometimes one can average this over several shells.]

Broaden:
$$\mathcal{A}^{BC}_{smooth}(\omega) = \int d\omega'\, K(\omega,\omega')\, \mathcal{A}^{BC}_{disc}(\omega') \qquad (3)$$

[Weichselbaum2007, supplementary information (Ref. 13)]

Log-Gaussian kernel:
$$K(\omega,\omega') = \frac{\theta(\omega\omega')}{\sqrt{\pi}\,\alpha|\omega|}\, e^{-\left(\frac{\ln|\omega/\omega'|}{\alpha} - \frac{\alpha}{4}\right)^2}, \qquad \alpha \simeq \Lambda^{-1/2} \qquad (4)$$

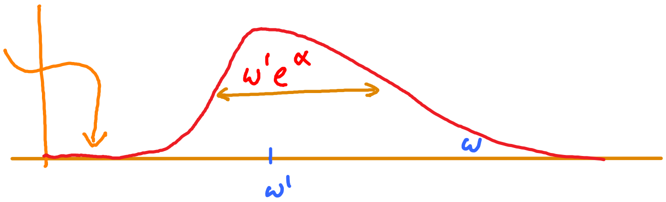
Plotted on log scale: $K(\omega,\omega')$



peak width is set by:
$\ln|\omega/\omega'| \simeq \alpha$
$\Longrightarrow \omega \simeq \omega' e^{\alpha}$

Plotted on linear scale: $K(\omega,\omega')$

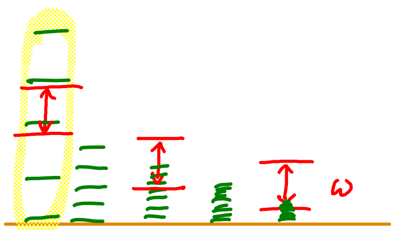
Rapid fall-off at $\omega < \omega'$
ensures that when averaging
over several shells, broadening of
high-energy shells does not spoil
resolution obtained from lower-lying shells.



long tail generates
overbroadening
at large ω

Nonzero temperature

$$\mathcal{A}^{BC}(\omega) \overset{(6)}{=} \sum_{\alpha\beta} e^{-\beta E_{\alpha}} \langle\alpha|\hat{B}|\beta\rangle\, \delta(\omega - E_{\beta\alpha})\, \langle\beta|\hat{C}|\alpha\rangle \qquad (5)$$

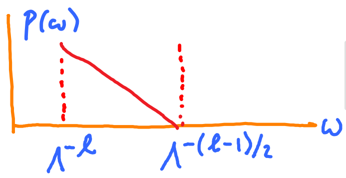


Typical 'initial state' $|\alpha\rangle$ has energy $E_{\alpha} \lesssim T$.

So we have to average over a range of shells around the one with $\Lambda^{-(\ell-1)/2} \simeq T$.

To combine their contributions, interpolation schemes ('patching rules') have been devised [Bulla2001]:

$$\mathcal{A}_{tot}(\omega) = \mathcal{A}_{\ell}(\omega)\, p(\omega) + \mathcal{A}_{\ell-1}(\omega)\,(1 - p(\omega)) \qquad (6)$$



But this is rather *ad hoc*, and does not satisfy sum rules precisely.

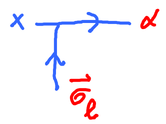
4. Graphical notation for basis change

NRG-III.4

It will be useful below to have a graphical depiction for basis changes.

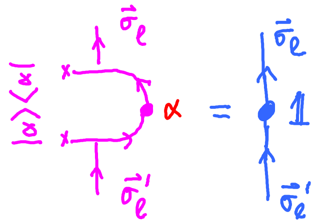
Consider a unitary transformation defined on chain of length ℓ, spanned by basis $\{|\vec\sigma_\ell\rangle\}$:

$$|\alpha\rangle = |\vec\sigma_\ell\rangle U^{\vec\sigma_\ell}{}_{\alpha} \qquad (1)$$



Unitarity guarantees resolution of identity on this subspace:

$$\sum_\alpha |\alpha\rangle\langle\alpha| = |\vec\sigma_\ell'\rangle \underbrace{U^{\vec\sigma_\ell'}{}_{\alpha}\, U^{\dagger\alpha}{}_{\vec\sigma_\ell}}_{\mathbb{1}^{\vec\sigma_\ell'}{}_{\vec\sigma_\ell}} \langle\vec\sigma_\ell| = \sum_{\vec\sigma_\ell} |\vec\sigma_\ell'\rangle \mathbb{1}^{\vec\sigma_\ell'}{}_{\vec\sigma_\ell}\langle\vec\sigma_\ell|$$

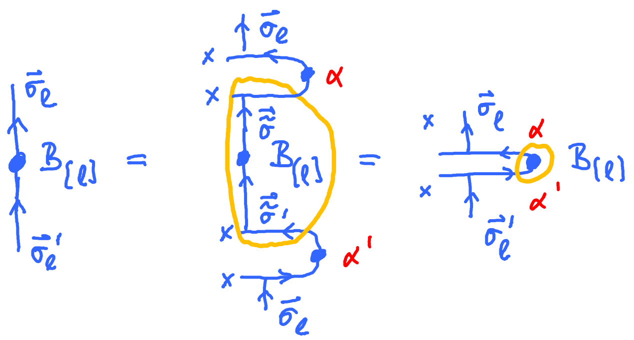


(2)

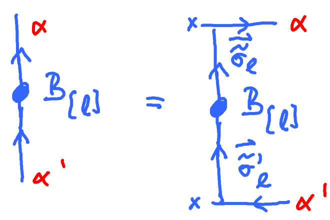
Transformation of an operator defined on this subspace:

$$\hat B = |\vec\sigma_\ell'\rangle B^{\vec\sigma_\ell'}{}_{\vec\sigma_\ell}\langle\vec\sigma_\ell| = \sum_{\alpha'\alpha} |\alpha'\rangle\langle\alpha'|\hat B|\alpha\rangle\langle\alpha| = |\alpha'\rangle B^{\alpha'}{}_{\alpha}\langle\alpha| \qquad (3)$$

Matrix elements: $B^{\alpha'}{}_{\alpha} = \langle\alpha'|\vec\sigma_\ell'\rangle B^{\vec\sigma_\ell'}{}_{\vec\sigma_\ell}\langle\vec\sigma_\ell|\alpha\rangle = U^{\dagger\alpha'}{}_{\vec\sigma_\ell'}\, B^{\vec\sigma_\ell'}{}_{\vec\sigma_\ell}\, U^{\vec\sigma_\ell}{}_{\alpha}$ (4)



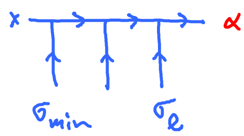
with



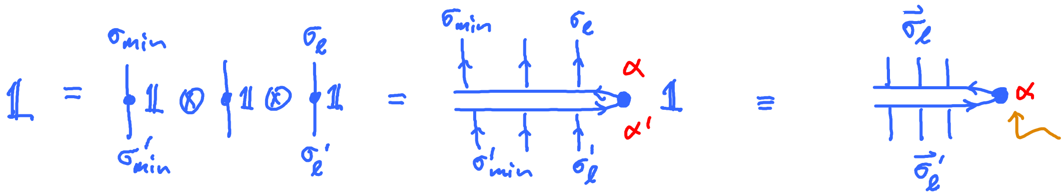
(5)

If the states $|\alpha\rangle$ are MPS:

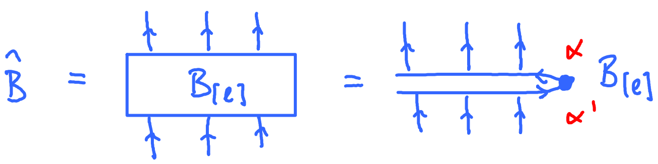
$$|\alpha\rangle = |\sigma_\ell\rangle \dots |\sigma_{min}\rangle \left(A^{\sigma_{min}} \dots A^{\sigma_\ell}\right)^{1}{}_{\alpha}$$



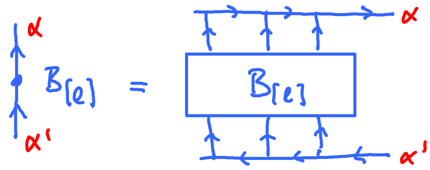
(6)



shorthand for unit matrix (7)



with



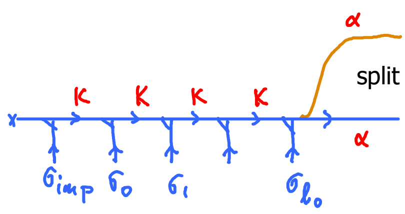
(8)

5. MPS notation for discarded/kept states [Weichselbaum2007]

Key insight by F. Anders & A. Schiller (AS): discarded states can be used to construct a complete many-body basis, suitable for use in Lehmann representation. This requires keeping track of 'environmental states'. This section describes how to do this, the next section how to construct the complete basis.

Suppose a short chain of length ℓ_0 has been diagonalized exactly (no truncation):
Then split its eigenstates into 'discarded' states (D) and 'kept' states (K).

$|\alpha\rangle^F_{\ell_0} =$

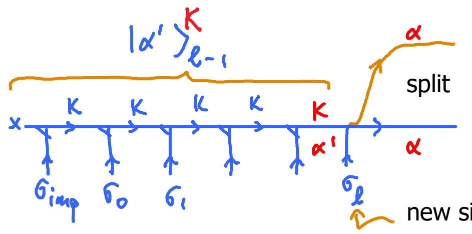


$$\equiv |\alpha\rangle^D_{\ell_0}, \quad \alpha = D_{K+1}, \dots, d^{\ell_0} \qquad (1)$$

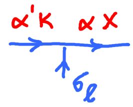
$$\equiv |\alpha\rangle^K_{\ell_0}, \quad \alpha = 1, \dots, D_K \qquad (2)$$

For $\ell > \ell_0$, iteratively use kept states as input, add one site at a time, diagonalize, and split again:

$|\alpha\rangle^X_\ell =$



$$D \equiv |\alpha\rangle^D_\ell, \quad K \equiv |\alpha\rangle^K_\ell \; \Big\} = |\sigma_\ell\rangle |\alpha'\rangle^K_{\ell-1} \left[A^K_{[\ell]X}\right]^{\alpha'\sigma_\ell}_{\alpha} = \qquad (3)$$

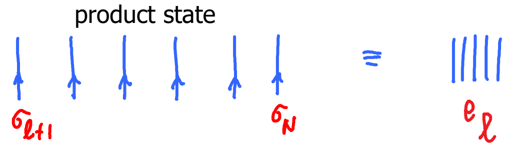


Include environment

Every state $|\alpha\rangle^X_\ell$ in shell ℓ has same 'environment', the rest of chain, with degeneracy $d^{N-\ell}$:

$$|e_\ell\rangle \equiv |\sigma_N\rangle \otimes \dots \otimes |\sigma_{\ell+1}\rangle = \qquad (4)$$

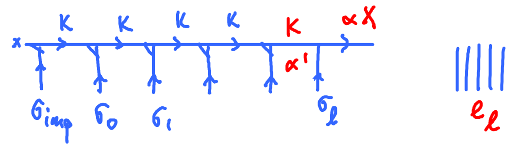
(according to our ordering convention, state spaces are added in opposite order to that of sketch)



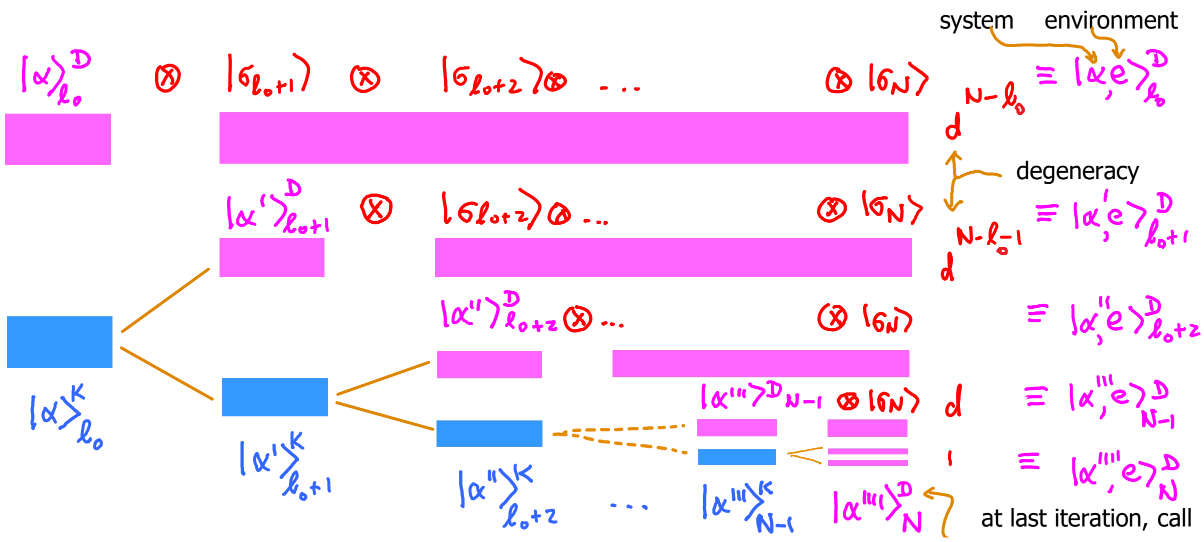
Combine shell states and environment states into states defined on entire length-N chain:

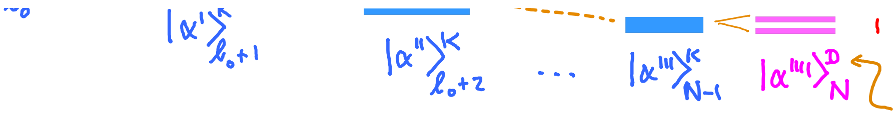
$$|\alpha, e\rangle^X_\ell \equiv |e_\ell\rangle |\alpha\rangle^X_\ell = \qquad (5)$$

shorthand for $e_\ell = (\sigma_{\ell+1}, \dots, \sigma_N)$



At last iteration, declare all states to be 'discarded': $|\alpha, e\rangle^D_N \equiv |\alpha\rangle_N$ (6)

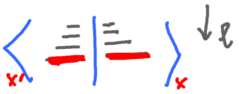




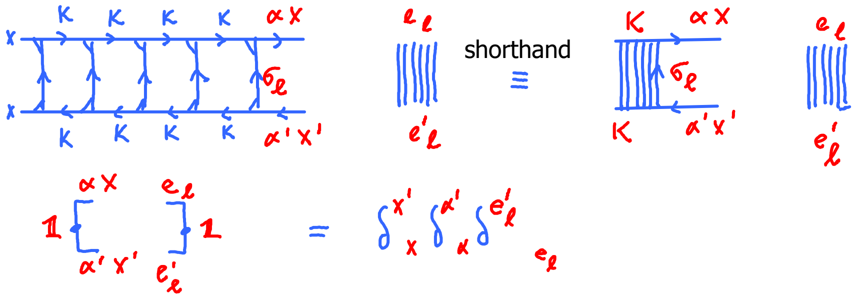
$\equiv |\alpha'''', e\rangle^D_N$ at last iteration, call all states 'discarded'

Orthogonality of kept and discarded states

'shell-diagonal X', X : $(\ell' = \ell)$

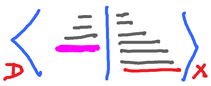


$${}^{X'}_{\ell'}\langle \alpha' e' | \alpha e\rangle^X_\ell = \quad \text{shorthand} \equiv \qquad (7)$$



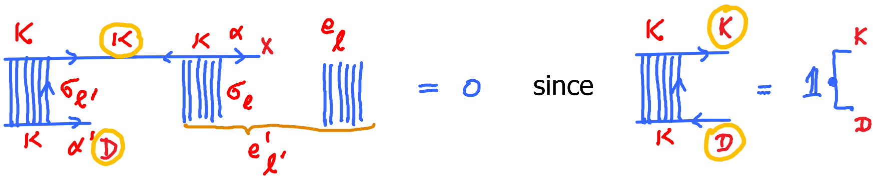
$$= \mathbb{1}\left[\;\right]^{\alpha X \; e_\ell}_{\alpha' X' \; e'_\ell}\mathbb{1} = \delta^{X'}_X \, \delta^{\alpha'}_\alpha \, \delta^{e'_\ell}_{e_\ell} \qquad (8)$$

Early D, late X

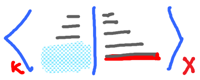


(9)

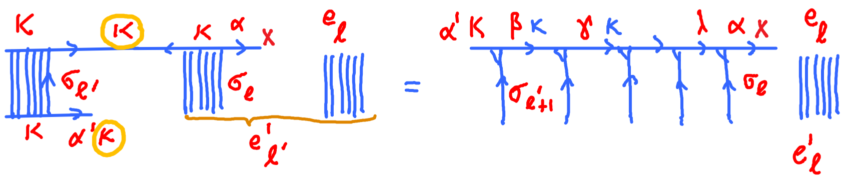
$${}^{D}_{\ell'}\langle \alpha' e' | \alpha e\rangle^X_\ell \;,\; \ell' > \ell \quad = \quad = 0 \quad \text{since} \quad = \mathbb{1}\left\{ {}^K_D \right.$$



Early K, late X:



$${}^{K}_{\ell'}\langle \alpha' e' | \alpha e\rangle^X_\ell \;,\; \ell' < \ell \quad = \quad = \qquad (10)$$



$$\equiv \left[A_{[\ell'+1]}{}^{K\sigma'_{\ell'+1}}{}_K \dots A_{[\ell]}{}^{K\sigma'_\ell}{}_D \right]^{\alpha'}{}_\alpha \; \delta^{e'_\ell}_{e_\ell} \qquad (11)$$

Rule of thumb: $\boxed{\text{off-diagonal overlaps are non-zero only for 'early K with late X'}}$

Summary:

$${}^{X'}_{\ell'}\langle \alpha' e' | \alpha e\rangle^X_\ell = \begin{cases} \delta_{X'K}\left[\left[A^K_{[\ell'+1]K}\right]^{\sigma'_{\ell'+1}} \dots \left[A^K_{[\ell]X}\right]^{\sigma_\ell} \right]^{\alpha'}{}_\alpha \; \delta_{e'e} & \text{if } \ell' < \ell \\ \delta_{X'X}\,\delta_{e'e} & \text{if } \ell' = \ell \\ \left[\left[A^{X'}_{[\ell]K}\right]^\dagger_{\sigma_\ell} \dots \left[A^K_{[\ell'+1]K}\right]_{\sigma'_{\ell'+1}} \right]^{\alpha'}{}_\alpha \; \delta_{KX}\,\delta_{e'e} & \text{if } \ell' > \ell \end{cases} \qquad (12)$$

$\ell\downarrow$ $= \delta_{X'X}$ $\neq 0$ $= 0$