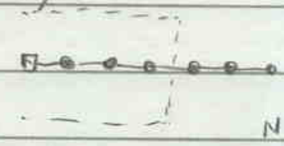
(Feb 2005)

NRG Density Matrix: recurrence relation

At iteration $\underline{\underline{N}}$, the full density matrix is given by:



$$\hat{\rho}_N = \sum_m \frac{e^{-E_m/T_N}}{Z} |m\rangle_N {}_N\langle m|$$

and the $\{|m\rangle\}$ basis spans the "full" (if you consider all of the "discarded") Hilbert space of the N-site chain. In other words, we can say

$$\hat{\rho}_N = \sum_{ij} (\rho_N)_{ij} |i\rangle_N \langle j| \quad \text{with} \quad (\rho_N)_{ij} = \frac{e^{-E_i/T_N}}{\left(\sum_i e^{-E_i/T_N}\right)} \delta_{ij}$$

In general, we can write the reduced density of states for the site $M<N$ by tracing out the "environment" degrees of freedom. For instance, let's consider

$$\hat{\rho}^{red}_M = \sum_{ij} (\rho^{red}_M)_{ij} |i\rangle_M \langle j|$$

Usually: $|i\rangle_M = \sum_K U_{iK} \underset{\text{basis}}{|K\rangle_M} = \sum_K U_{iK} \left(\sum_{K^{old}, \tilde{K}} \mathbb{C}^K_{K^{old}\tilde{K}} \underset{\text{eigenstate}}{|K^{old} \omega\rangle_{M-1}} \underset{\text{single site op in } M}{|\tilde{K}\rangle_M} \right)$

Therefore

$$|i\rangle_M = \sum_{\substack{K \\ K^{old} \tilde{K}}} U_{iK} \, \mathbb{C}_{K^{old}\tilde{K}} \, |K^{old} \omega\rangle_{M-1} |\tilde{K}\rangle_M$$

U_{iK} is the matrix coming from the diagonalization in the $|K\rangle_M$ basis and $\mathbb{C}_{K^{old}\tilde{K}}$ defines the "building" of the basis (e.g., a Clebsch-Gordon coefficient for instance. It is diagonal in the $|Q S_z\rangle$ construction).

When we "trace out" the M states, we will be doing a trace in $|\tilde{K}\rangle_M$. Let's see then:

(1) $$\boxed{\hat{\rho}^{red}_M = \sum_{ij} (\rho^{red}_M)_{ij} \sum_{\substack{K \\ K^{old} \tilde{K}}} \sum_{\substack{K' \\ K^{old'} \tilde{K}'}} U_{iK} U_{jK'} \mathbb{C}^K_{K^{old}\tilde{K}} \mathbb{C}^{*K'}_{K^{old'}\tilde{K}'} |K^{old}\rangle_{M-1} |\tilde{K}\rangle_M \langle \tilde{K}'| \langle K^{old'}|_{M-1}}$$

Ok, now let's see how we can calculate $\left(\hat{\rho}^{red}_{M-1}\right)$ from $\left(\hat{\rho}^{red}_{M}\right)$:

$$\hat{\rho}^{red}_{M-1} = Tr_{|\tilde{K}\rangle_M}\left\{\hat{\rho}^{red}_M\right\} = \sum_{\tilde{K}''} {}_M\langle\tilde{K}''|\hat{\rho}^{red}_M|\tilde{K}''\rangle_M \quad \left(\{|\tilde{K}''\rangle_M\} \text{ are the M-site basis}\right)$$

$$\begin{pmatrix}\text{* see}\\ \text{previous}\\ \text{page}\end{pmatrix} = \sum_{K^{old}, K^{old'}} \left(\sum_{\substack{ij\\ KK'\\ \tilde{K}}} (\rho^{red}_M)_{ij}(U^M_{iK})(U^M_{jK'})\, \mathbb{C}^{K}_{K^{old}\tilde{K}}\, \mathbb{C}^{*K'}_{K^{old'}\underline{\underline{\tilde{K}}}}\right) |K^{old}\rangle_{M-1}\langle K^{old'}| \qquad (2)$$

which is to be compared to

$$\hat{\rho}^{red}_{M-1} = \sum_{i^{old}\, j^{old'}} \left(\hat{\rho}^{red}_{M-1}\right)_{i^{old}\, j^{old}} |i^{old}\rangle_{M-1}\langle j^{old'}| \qquad \text{Therefore}$$

$$\boxed{\left(\hat{\rho}^{red}_{M-1}\right)^{\boxed{\text{block old}}}_{i^{old}\, j^{old}} = \sum_{\substack{i,j \Rightarrow \text{eigenstate of } M\\ K\,(K'(K))\\ (\tilde{K}'=\tilde{K})\text{sum } \tilde{K} \to \text{gives } K'\text{s}}} (\rho^{red}_M)_{ij}\,(U^M_{iK})\,(U^{*M}_{jK'})\; \mathbb{C}^{K}_{\underline{\underline{i^{old}}}\tilde{K}}\; \mathbb{C}^{*K'}_{\underline{\underline{j^{old}}}\tilde{K}'=\tilde{K}} \qquad (3)}$$

On this sum ① $\left\{\right.$ i, j run over all $\boxed{\text{eigen states}}$ on a symmetry block.

② $\left|\right.$ K run over all basis states on the symmetry block. (basis in M) (basis in M)

③ given K the only K' entering the sum are those such that $\tilde{K} = \tilde{K}'$ $\boxed{\text{* Both basis states } |K\rangle_M, |\tilde{K}\rangle_M \text{ are constructed with the same site states}}$

→ ③ implies that, if QS_z is assumed, then given K there is only one $\tilde{K}$ → thus K' is given

For (Q, S) or more general symmetries, this might not be the case.

In $(\bar{Q}, \bar{S}_z)$ → $\mathbb{C}^{K}_{K^{old}\tilde{K}} = 1$ $\left(|K\rangle_M = |K^{old}\rangle_{M-1}|\tilde{K}\rangle_M\right)$, then there is no additional sum.

What I will need is this:

⇒ [Block old → Block new 1, Block new 2, ... } something like $\text{stcf} = \text{Abasis}^M.\text{stcf}(\text{ist})$ loop in ist

$\rightarrow |i^{old}\rangle_{M-1}$ → states generated in M matrix } $\text{Aeis}^{M-1}.\text{stgen}(\text{stcf}).\text{push\_back}(\text{ist})$ // (queue with...)

⇒ Save U_{iK}, Aeis, Abasis for each M ! First thing. ✓

(3)

(April 2005)

DM-NRG in QS_z basis (Basic stuff).

In the $|QS_z\rangle$ basis, we have simply

Basis $\equiv i$; site state

$$|Q\,S_z\,\text{type scf}\rangle_N = |Q^{old}(=Q-\tilde{Q})\,S_z^{old}(=S_z-\tilde{S}_z)\,\text{scf}\rangle_{N-1} \times |\tilde{Q}\,\tilde{S}_z\,\text{type}\rangle_N$$

$$|Q\,S_z\,\omega\rangle_N = \sum_{i\,(\text{basis})} U^{QS_z}_{\omega i}\,|Q\,S_z\,i\rangle_N = \sum_i U^{QS_z}_{\omega i}\,|Q^{old}\,S_z^{old}\,\text{scf}\rangle_{N-1}\,|\tilde{Q}\,\tilde{S}_z\,\text{type}\rangle_N$$

Now:

$$\hat{\rho}_N = \sum_\omega (\hat{\rho}_N)_\omega\,|Q\,S_z\,\omega\rangle_N\langle Q\,S_z\,\omega| \qquad (\text{diagonal})\ (\hat{\rho}_N)_{\omega\omega} = e^{-E_\omega/T_N}$$

$$= \sum_{\substack{\omega\\ i\,i'}} (\hat{\rho}_N)_\omega\,U^{QS_z}_{\omega i}\,(U^{QS_z}_{\omega i'})^\dagger\,|Q^{old}\,S_z^{old}\,\text{scf}\rangle_{N-1}\,|\tilde{Q}\,\tilde{S}_z\,\text{type}\rangle_N\,\langle\tilde{Q}'\,\tilde{S}_z'\,\text{type}'|\,{}_{N-1}\langle Q^{old'}\,S_z^{old'}\,\text{scf}'|$$

$\delta_{Q^{old}+\tilde{Q},\,Q^{old'}+\tilde{Q}',\,Q}\ \delta_{S_z^{old}+\tilde{S}_z,\,S_z^{old'}+\tilde{S}_z',\,S_z}$

$Q^{old} = Q^{old'}$ since $\tilde{Q} = \tilde{Q}'$

Now:

$$\hat{\rho}_{N-1} = \mathrm{Tr}_{|\tilde{k}\rangle_N}\{\hat{\rho}_N\} = \underset{(\tilde{Q}\,\tilde{S}_z\,\text{type})}{\text{Trace in}} = \sum_{\substack{QS_z\\ \omega\in QS_z\\ i,i'\in QS_z\\ (i'\text{ such that type}=\text{type}')}} (\hat{\rho}_N)_\omega\,U^{QS_z}_{\omega i}\,(U^{QS_z}_{\omega' i'})^\dagger\,|Q^{old}\,S_z^{old}\,\text{scf}\rangle_{N-1}\,\langle Q^{old'}\,S_z^{old'}\,\text{scf}'|$$

$$\otimes\,\delta_{Q^{old}+\tilde{Q},\,Q^{old'}+\tilde{Q}',\,Q}\ \delta_{S_z^{old}+\tilde{S}_z,\,S_z^{old'}+\tilde{S}_z',\,S_z} \otimes \boxed{\delta_{\tilde{Q}\tilde{Q}'}\,\delta_{\tilde{S}_z\tilde{S}_z'}\,\delta_{\text{type type}'}}$$

?

O.K., how does the sum in i, i', ω changes when the deltas are included? From trace

- Only states with $\begin{cases} Q^{old}+\tilde{Q} = Q^{old'}+\tilde{Q}' \text{ and } \tilde{Q}=\tilde{Q}' \\ S_z^{old}+\tilde{S}_z = S_z^{old'}+\tilde{S}_z' \text{ and } \tilde{S}_z=\tilde{S}_z' \end{cases} \Rightarrow \begin{matrix} Q^{old}=Q^{old'} \\ S_z^{old}=S_z^{old'} \end{matrix}$

(diagonal block structure)

- Only $|\text{scf type}\rangle \times |\text{scf}'\text{ type}\rangle$ enter (meaning, basis states of same type) contribute.

If we write this way:

$$\hat{\rho}^{red}_{N-1} = \sum_{\substack{Q^{old}\,S_z^{old}\\ \text{scf}\in Q^{old}S_z^{old}\\ [\text{scf}'\in Q^{old}S_z^{old}]}} \underbrace{\left[(\hat{\rho}_N)_\omega\,U^{(QS_z)_N}_{\omega i}\,(U_{\omega i'})^\dagger\right]}_{=\left(\rho_N^{red\,Q^{old}S_z^{old}}\right)_{\text{scf scf}'}}\,|Q^{old}\,S_z^{old}\,\text{scf}\rangle_N\langle Q^{old}\,S_z^{old}\,\text{scf}'|$$

Who are ω, i, i'?

Let's look at the two formulae more closely:

$$\hat{\rho}^{red}_{N-1} = \sum_{|type''\rangle} \sum_{\substack{ibl \in QS_z \\ \omega \in QS_z \\ i, i' \in QS_z}} (\hat{\rho}^{QS_z}_N)_\omega (U^{QS_z}_{\omega i})(U^{QS_z}_{\omega i'})^\dagger \, |Q^{old} S_z^{old} scf\rangle_{N-1} \langle Q^{old'} S_z^{old'} scf'| \cdot \langle \tilde{Q}'' \tilde{S}_z'' type'' | \tilde{Q} \tilde{S}_z type\rangle \langle \tilde{Q}' \tilde{S}_z' type' | \tilde{Q}'' \tilde{S}_z'' type''\rangle$$

$$= \sum_{\substack{ibl \in (QS_z)_N \\ \omega \in (QS_z)_N \\ i, \in (QS_z)_N \\ [i' \text{ such that } type' = type_i \\ (\Rightarrow Q^{old} S_z^{old} = Q^{old'} S_z^{old'}!)}} (\hat{\rho}^{QS_z}_N)_\omega (U^{QS_z}_{\omega i})(U^{QS_z}_{\omega i'})^\dagger \, |Q^{old} S_z^{old} scf\rangle_{N-1} \langle Q^{old} S_z^{old} scf'|$$

which we rewrite (re-order) as:

$$\hat{\rho}^{red}_{N-1} = \sum_{\substack{ibl \text{ in } (Q^{old} S_z^{old})_{N-1} \\ scf, scf' \in Q^{old} S_z^{old}}} \underbrace{\left[\sum_{\substack{\omega, i, i' \\ \text{given} \\ scf\ scf'}} (\hat{\rho}_N)_\omega (U^{QS_z}_{\omega i})(U^{QS_z}_{\omega i'})^\dagger \right]}_{\equiv (\hat{\rho}^{red}_{N-1})_{scf\ scf'}} |Q^{old} S_z^{old} scf\rangle_{N-1} \langle Q^{old} S_z^{old} scf'|$$

How do we determine (i, i') and ω ?

Given scf: $\mapsto$ list of future states in N such that $stco\_from = scf$
scf': $\mapsto$ list of future states in N such that $stco\_from = scf'$
} and states in both lists (i) that have the same type (i')

$\downarrow$ Pairs (i, i') (basis states of N) $\to$ block n.

Each pair (i, i') is going to be in the same $(Q\ S_z)_N$ block $\mapsto$ $\omega(i,i')$ are the states in this block.

: List of pairs (i,i') $\mapsto$ list of blocks $(Q\ S_z)_N$, sum in ω within these blocks.

Thus, in general:

$$\left(\hat{\rho}^{red}_{N-1}\right)_{scf\ scf'} = \left[\sum_{\substack{\text{list pairs} \\ i, i' \\ (ibl\_list)}} \sum_{\substack{\omega \in ibl\_list \\ \omega' \in ibl\_list}} (\hat{\rho}^{red}_N)_{\omega\omega'} \, U^{ibl\_list}_{\omega i} \boxed{U^{ibl\_list}_{\omega' i'}}^\dagger \right]$$

(Feb 2009)

Green's function from density matrix in NRG

Question: How can we calculate the GF with the NRG density matrix?

G^R definition (Fetter-Walecka eq 31.47). Operators A, B $\left(\begin{smallmatrix} + \to \text{Fermion} \\ - \to \text{Boson}\end{smallmatrix}\right)$

$$G^R_{AB}(t) = -i\,\Theta(t)\,\mathrm{Tr}\left[\hat{\rho}\,[\hat{A}(t),\hat{B}(0)]_{\pm}\right] \quad \text{with} \quad \hat{\rho} = \sum \rho_m |\psi_m\rangle\langle\psi_m| \quad \boxed{\rho_m = \frac{e^{-E_m/T}}{Z}}$$

OK, How about $G^R_{AB}(\omega)$?

Notice that we'll use:

$$\Theta(t-t') = -\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}\frac{e^{-i\omega(t-t')}}{\omega+i\eta} \quad \text{(Fetter, eq (7.43))} \quad ; \quad \hat{A}(t) = e^{iHt}\hat{A}\,e^{-iHt}$$

and

$$G^R(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} G^R(\omega)\, e^{-i\omega t}\, d\omega \quad (2\pi \text{ is here...})$$

Commutator: (assume ~~fermionic~~ NOW OK operators $\hat{A}$ and $\hat{B}$).

$$[\hat{A}(t),\hat{B}]_{+} = e^{iHt}Ae^{-iHt}B \underset{(-)}{+} Be^{iHt}Ae^{-iHt} = \sum_{nn'} e^{i(E_n-E_{n'})t}\Big(|\psi_n\rangle\langle\psi_n|\hat{A}|\psi_{n'}\rangle\langle\psi_{n'}|\hat{B} + B|\psi_n\rangle\langle\psi_n|\hat{A}|\psi_{n'}\rangle\langle\psi_{n'}|\Big)$$

- $$\mathrm{Tr}\left[\hat{\rho}[\hat{A}(t),\hat{B}]_{+}\right] = \sum_{nn'} e^{i(E_n-E_{n'})t}\sum_m \rho_{mn}A_{nn'}B_{n'm} \underset{(-)}{+} \langle\psi_m|\underbrace{\hat{\rho}\hat{B}}_{\sum|\psi_{n'}\rangle\langle\psi_{n'}|}|\psi_n\rangle A_{nn'}\,\delta_{n'm}$$

$$= \sum_{nn'} e^{i(E_n-E_{n'})t}\sum_m \rho_{mn}A_{nn'}B_{n'm} \underset{(-)}{+} \rho_{n'm}B_{mn}A_{nn'}$$

Include $\Theta(t)$:

$\left\{\begin{array}{l}\bar{\omega} = \omega-(E_n-E_{n'}) \\ \omega = \bar{\omega}-(E_{n'}-E_n)\end{array}\right.$

$$G^R_{AB}(t) = -\cancel{i}\,\cancel{(-1)}\sum_{nn'}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{e^{-i(\omega-(E_n-E_{n'}))t}}{\omega+i\eta}\sum_m \rho_{mn}A_{nn'}B_{n'm} \pm \rho_{n'm}B_{mn}A_{nn'}$$

change of variables $\bar{\omega} = \omega - E_n - E_{n'}$

$$= \int_{-\infty}^{\infty}\frac{d\bar{\omega}}{2\pi}e^{-i\bar{\omega}t}\left[\sum_{\substack{nn'\\m}}\frac{\rho_{mn}A_{nn'}B_{n'm} \underset{(-)}{+} \rho_{n'm}B_{mn}A_{nn'}}{\bar{\omega}-(E_{n'}-E_n)+i\eta}\right]$$

$$\Rightarrow \boxed{G^R_{AB}(\omega) = \sum_{\substack{nn'\\m}}\frac{\rho_{mn}A_{nn'}B_{n'm} \underset{(-)}{+} \rho_{n'm}B_{mn}A_{nn'}}{\omega-(E_{n'}-E_n)+i\eta}}$$

(-) bosons

neg ω

positive ω

at iteration M, we know the energies E_i^M. The full spectrum is obtained by suming over shells. In the last shell, $\rho^{red.}$ is given by $\hat{\rho}$.

$$G_{AB}(\omega) = \sum_{\substack{M=0 \\ \text{(or MMIN?)}}}^{N} G^M_{AB}(\omega) \quad \text{where}$$

mean' in second term

$$\boxed{G^M_{AB}(\omega) = \sum_{\substack{m \\ nn'}} \underbrace{\frac{\rho^M_{mn} A^M_{nn'} B^M_{n'm}}{\omega - (E^M_{n'} - E^M_n) + i\eta}}_{\text{"positive" } \omega} \underset{(-)}{+} \underbrace{\frac{\rho^M_{nm} B^M_{mn'} A^M_{n'n}}{\omega + (E^M_{n'} - E^M_n) + i\eta}}_{\text{"negative" } \omega}}$$

where "M" indicates the matrix elements are taken over eigenstates of iteration M $|i\rangle_M$ and ρ^M_{mn} is the <u>reduced</u> <u>density</u> <u>matrix</u> at iteration M.

<u>Spectral</u> <u>density</u>:

Let's say $A = c_d$, $B = c_d^\dagger$ in the usual $\begin{Bmatrix}\text{single-impurity} \\ \text{single-channel}\end{Bmatrix}$ Anderson model. In this case, we have

$$A^M_{nn'} = \langle n|c_d|n'\rangle \quad , \quad B_{n'm} = \langle n'|c_d^\dagger|m\rangle = \left(\langle m|c_d|n'\rangle\right)^*_{\psi}$$

Thus $A^M_d(\omega) = -\frac{1}{\pi} \mathrm{Im}\, G^M_d(\omega)$ will be

$$A^M_d(\omega) = \sum_{\substack{m \\ nn'}} \rho^{red\,M}_{mn} \langle n|c_d|n'\rangle \left(\langle m|c_d|n'\rangle\right)^* \delta(\omega - (\underline{\underline{E^M_{n'} - E^M_n}}))$$

$$+ \rho^{red}_{nm} \langle n'|c_d|n\rangle \left(\langle n'|c_d|m\rangle\right)^* \delta(\omega + (E^M_{n'} - E^M_n))$$

$$A^M_d(\omega) = \sum_{nn'} \left(\sum_m \rho^M_{mn} (\langle m|c_d|n'\rangle)^*\right) . \langle n|c_d|n'\rangle \; \delta(\omega - (E^M_{n'} - E_n))$$

$$+ \left(\sum_m \rho^M_{nm} (\langle n'|c_d|m\rangle)^*\right) \langle n'|c_d|n\rangle \; \delta(\omega + (E^M_{n'} - E_n)) \quad \text{but in general:}$$

In general, though:

"positive" ω

$$A^M_{AB}(\omega, T) = \sum_{nn'} \left(\sum_m (\rho^{red}_M)_{mn} \, B^M_{n'm}\right) A^M_{nn'} \; \delta(\omega - (E^M_{n'} - E_n))$$

"negative" ω

$$+ \left(\sum_m (\rho^{red}_M)_{nm} \, B^M_{mn'}\right) A^M_{n'n} \; \delta(\omega + (E^M_{n'} - E_n))$$

$\boxed{\text{Case at } \underline{T=0}}$: $e^{-E_i/T_N} \to \delta_{0i}$ at last iteration N.

$\Rightarrow$ $\boxed{(\hat{\rho}_N(T=0))_{ij} = \frac{\delta_{0i}\delta_{ij}}{Z_N(T=0)}}$ and in this case: only $(\rho_N)_{iGS\,iGS} = 1$ survives.

$(\hat{\rho}^{red}_{N-1})_{scf\,scf'} = \sum_{\substack{\ell i \in I \\ \text{pair } i,i' \\ (ibl\_\ell is)}} U^{N\,iblGS}_{iGS\,i} (U^{N\,iblGS}_{iGS\,i'})^{+}$ $\Rightarrow$ i, i' in the same block as the ground state in iteration N

$\underline{\text{Therefore}}$: $(\rho^{red}_{N-1})_{scf\,scf'}$ will be non-zero only for blocks with states (scf, scf') in $N-1$ shell which generate $\underbrace{\text{states}}_{(i,i')}$ in the block iblGS in N with the same "itype". Note, However, that $(\rho^{red}_{N-1})_{scf\,scf'}$ $\underline{\text{will not}}$ be diagonal even in this case (contrast to the usual "Costi" or "Bulla $N, N+2$" procedure) since, given

$$\begin{cases} |i \in blGS\rangle_N = |\overset{blSCF}{scf}\rangle \otimes |type\rangle \\ |i' \in blGS\rangle_N = |\overset{blSCF}{scf'}\rangle \otimes |type\rangle \end{cases} \quad \text{and} \quad |GS\rangle = \sum_i U^{blGS}_{iGS,i} |i\rangle \quad \text{with} \begin{cases} U^{blGS}_{iGS\,i} \neq 0 \\ U^{ibl}_{iGS\,i'} \neq 0 \end{cases}$$

Then $(\rho^{red}_{N-1})_{scf\,scf'}$ is non-zero. That means That:

$$A^M_{AB}(\omega, T=0) = \sum_{nn'} \left(\sum_m (\rho^{red}_M)_{mn} B_{n'm} \right) \underline{\underline{A_{nn'}}}\, \delta(\omega - (E^M_{n'} - E_n))$$

A B

(c, c^{+})

$$\underset{(-)}{+} \left(\sum_m (\rho^{red}_M)_{nm} B^M_{mn'} \right) A_{n'n}\, \delta(\omega + (E^M_{n'} - E_n)) \quad \text{even at } T=0 \,!!!$$

while in $\underline{\underline{\text{Costi's}}}$ can be obtained by making $(\rho^{red}_M)_{mn} \to \frac{\delta_{iGS\,m}\,\delta_{mn}}{Z_M}$ $\begin{pmatrix} m \to iGS \\ n \to iGS \end{pmatrix}$

$A = \langle 0|C_+|n\rangle$

$B = \langle n|C_-|0\rangle$

$$A^{M(costi)}_{AB}(\omega, T=0) = \frac{1}{Z_M} \sum_{n'} \hat{A}_{0n'} \hat{B}_{n'0} \underbrace{\delta(\omega - E^M_{n'})}_{\text{positive}} \underset{(-)}{+} \hat{A}_{n'0} \hat{B}_{0n'} \underbrace{\delta(\omega + E^M_{n'})}_{\text{negative}}.$$

If diagonal $B = A^{+}$ thus $\hat{B}_{n0} = (\hat{A}_{0n})^{*}$]

$$A^{M(costi)}_{AA}(\omega, T=0) = \frac{1}{Z_M} \sum_n |\langle 0|\hat{A}|n\rangle|^2\, \delta(\omega - E^M_n) \underset{(-)}{+} |\langle n|\hat{A}|0\rangle|^2\, \delta(\omega + E^M_n)$$

Implementation: We write each $A^M(\omega,T)$ $\left(A(\omega t) = \sum_M A^M(\omega T)\right)$ as:

$$A^M(\omega,T) = \sum_{n'}\sum_{n} \left\{ \left[\sum_m (\hat{B})_{n'm}(\rho^{red}_M)_{mn}\right] \overset{+}{(-)} \left[\sum_{m'} (\rho^{red}_M)_{n'm'}(\hat{B})_{m'n}\right] \right\} (\hat{A})_{nn'}\,\delta(\omega-(E_{n'}-E_n))$$

We now define the following auxiliary matrices:

$$\left.\begin{aligned} \mathbb{C}^1 &= \mathbb{B}\cdot\rho^{red}_M \\ \mathbb{C}^2 &= \rho^{red}_M\cdot\mathbb{B} \end{aligned}\right\} \quad \mathrm{Sum} = \mathbb{C}^1 \overset{+}{(-)} \mathbb{C}^2$$

$$(\mathbb{A}^{\delta}(\omega))_{ij} = (\hat{\mathbb{A}})_{ij}\,\delta(\omega-(E_j-E_i))$$ and $A^M(\omega,T)$ will be given by

$$A^M(\omega,T) = \mathrm{Tr}\left\{\mathrm{Sum}\cdot\mathbb{A}^{\delta}(\omega)\right\} = \sum_{n'}\left(\mathrm{Sum}\cdot\mathbb{A}^{\delta}_{n'n'}(\omega)\right)_{n'n'}$$ (no need to calculate off-diag elements: save one loop!)

This makes things more easy to implement. For example, for $\hat{A} = c_{d\sigma}$, $B = c^{\dagger}_{d\sigma}$ we know $c_{d\sigma}$ will connect only a few pairs of blocks (ibl, ibl'). If we have N_{st} in block ibl and N_{st}' in block ibl', then $\mathbb{B} = (\hat{A}^*)^T$ will be a $N_{st}' \times N_{st}$ matrix ($\mathbb{A}$ will be $N_{st}\times N_{st}'$) and:

$$\to \begin{cases} \mathbb{C}^1(ibl', ibl) = \mathbb{B}(ibl', ibl)\cdot\rho^{red}(ibl, ibl) & (N_{st}'\times N_{st}) \\ \mathbb{C}^2(ibl', ibl) = \rho^{red}(ibl', ibl')\cdot\mathbb{B}(ibl', ibl) & (N_{st}'\times N_{st}) \end{cases}$$

(notice that the subblocks in ρ^{red} (block diagonal) are different!)

$$\Rightarrow (\mathbb{A}^{\delta}(\omega))^{i\in\; j\in}_{ibl\; ibl'} = (\mathbb{A})_{i\in ibl,\, j\in ibl'} \times \delta(\omega-(E_{j\in ibl'}-E_{i\in ibl})) \quad \Rightarrow \underline{N_{st}\times N_{st}'}$$

and $\mathrm{Sum}\cdot(\mathbb{A}^{\delta}(\omega))$ will be a $N_{st}'\times N_{st}'$ matrix (we just sum in block ibl')

Thus, given the list of blocks ibl, ibl' connected by $\hat{A}$, we have:

$$A^M(\omega,t) = \sum_{ibl,\,ibl'\in list}\;\sum_{n'\in ibl'}\left(\mathrm{Sum}(ibl', ibl)\cdot\mathbb{A}^{\delta}(\omega)(ibl, ibl')\right)_{n'n'} \quad //$$

which can be calculated.

$E_i = \bar{E}_i \times D_N$

$\delta(\omega - E_i)d\omega$

1

$(\omega/D_N - (E_i/D_N))\, d(\omega/D_N)$

$= 1$

$\int \frac{\delta(\omega - E_i)}{D_N} d\omega = 1$

(Oct 2009)

Costi's method vs DM-NRG at finite Temperature

Remembering The original way of calculating $A(\omega,T)$:

$$A^{M\,(\text{costi})}_{AB}(\omega,T) \approx \frac{1}{Z_M(T)} \sum_{nn'} e^{-\beta E^M_n} A_{nn'} B_{n'n}\, \delta(\omega - (E^M_{n'} - E^M_n)) \pm e^{-\beta E^M_{n'}} A_{n'n} B_{nn'}\, \delta(\omega + (E^M_{n'} - E_n))$$

which corresponds to approximate $\rho^{\text{red}\,M}_{mn} \approx \frac{\delta_{mn}}{Z_M(T)}$ in The DM-NRG scheme. (which is exact only in the last site)

Note that:

$$Z_M(T) = \sum_n e^{-\beta E^M_n}$$

Now, There are different ways to evaluate the double sum, some more efficient than others. An efficient way is to do-it by matrix multiplication (like in The DM-NRG scheme), where we define

$$(\mathbb{A}e1)_{nn'} \equiv e^{-\beta E^M_n} A_{nn'} \;;\; (\mathbb{A}e2)_{nn'} = e^{-\beta E_{n'}} A_{nn'}$$

$$(\mathbb{B}\delta)_{n'n} \equiv B_{n'n}\, \delta(\omega - (E^M_{n'} - E_n)) \quad \left((\mathbb{B}\delta)_{nn'} = B_{nn'}\, \delta(\omega + (E_{n'} - E_n)\right)$$

Then

$$A^M_{AB}(\omega,T) \approx \frac{1}{Z^M_M} \left\{ \text{Tr}\Big[\underbrace{(\mathbb{A}e1)\cdot(\mathbb{B}\delta) \pm ((\mathbb{B}\delta)\cdot(\mathbb{A}e2)}_{\text{sum/difference of matrices}} \Big] \right\} \qquad \text{(efficient)}$$

But, for debugging purposes, I can do this:

vector dE_n

$\hookrightarrow$ $\boxed{\text{matrix } E_i m E_j(i,j) = E_i - E_j}$ → excitations

weight $1(i,j,\omega) = (e^{-\beta E_j} A_{ji} B_{ij}) \times \delta(\omega - (E_i - E_j))$ o.k.

weight $2(i,j,\omega) = (e^{-\beta E_i} A_{ij} B_{ji}) \times \delta(\omega + (E_i - E_j)) \left(= \delta(-\omega - (E_i - E_j))\right)$ negative ω

If $E_i - E_j > 0$ → weight1 contributes to positive ω only (if δ is log Gauss)

weight 2 contributes to negative ω only) (if δ is log Gauss)

$E_i - E_j < 0$ → weight 1 contributes to negative ω

weight 2 contributes to positive ω

$\boxed{\begin{array}{l}\langle i|A|j\rangle \neq 0 \text{ and} \\ \langle j|B|i\rangle \neq 0 \Rightarrow \langle i|B^\dagger|i\rangle \neq 0\end{array}}$

In practice, we have $\begin{pmatrix}\hat{A}^\dagger \\ \hat{B}^\dagger\end{pmatrix}$ connecting only a few pairs of blocks; so we do:

$ibl = 0, NumBlocks()\,;\ jbl = 0,\ ibl.$

If $\left(A(ibl, jbl) == true\right) \mapsto$ calculate $\sum_{\substack{ist \in ibl \\ jst \in jbl}}$ weightNeg(ist, jst, ω) $\hookrightarrow$ negative ω

$E_i - E_j > 0$

$E_i - E_j < 0$ $\hookrightarrow$ positive ω

$E_i - E_j$

If $\begin{pmatrix} B(ibl, jbl) == true \\ \text{and } \omega > 0\end{pmatrix} \mapsto$ calculate $\sum_{\substack{ist \in ibl \\ jst \in jbl}}$ weightPos(ist, jst, ω) $\to$ positive ω (contribution) from ibl, jbl.

If p.h.s holds <u>then</u> contribution_Pos(jbl, ibl) = contribution_Neg(ibl, jbl)

$(-1\ 0)\ (0\ 1)$
$1\ 2\ ,\ 2\ 3$

$$A^M_{AB}(\omega, T) = \sum_{nn'} \left(\sum_m (\rho^{red}_M)_{mn} B_{n'm}\right) A_{nn'}\ \delta(\omega - (E^M_{n'} - E_n))$$

$$\pm \left(\sum_m (\rho^{red}_M)_{n'm} B_{mn}\right) A_{n'm}\ \delta(\omega + (E_{n'} - E_n))$$

Given $\underline{E_{n'} - E_n} =: \Delta E$

$\Delta E > 0 \to$ "positive ω" contribution (for log BD)

$\Delta E < 0 \to$ "negative ω" contribution (for log BD)

<u>OK</u>, <u>then</u>. Blocks connected by $\hat{A}$: $n \in ibl$, $n' \in jbl$

$$A^M_{AB}(\omega, T) = \sum_{nn'} \left[\sum_m (\rho^{red}_M)_{mn} B_{n'm}\right] A_{nn'}\ \delta(\omega - (E_{n'} - E_n)) \pm \left[\sum_m (\rho_M)_{n'm} B_{mn'}\right] A_{nn'}\ \delta(\omega + (E_n - E_{n'}))$$

$$= \sum_{nn'} \left((\mathbb{C}_1 \pm \mathbb{C}_2)_{n'n} A_{nn'}\ \delta(\omega - (E_{n'} - E_n)) \right)$$

$E_{n'} > E_n \Rightarrow$ positive weight $\sum^{+}_{n'} (\text{Sum})_{n'n} A_{nn'}$

$E_{n'} < E_n \Rightarrow$ negative weight $\sum^{-}_{n'} (\text{Sum})_{n'n} A_{nn'}$

Thing is: fix n (say $i65$) $\mapsto$ get contribution particle and hole like. It should be the same!

(April 2010)

DM-NRG in the Q, S basis

Continuing my note on DM-NRG, let's see how things work in the (QS) basis. Let's say $|QSw\rangle_N$ is an eigenstate of H_N in block (Q,S). Then, it is written in a basis $|Q, S\, i\,(\text{type scf})\rangle_N$ ("type" of the single-site basis, "scf" in the old

$$|Q\,S\,S_z\,w\rangle_N = \sum_{\hat{i}\,(\text{basis})} U^{QS}_{wi}\, |Q\,S\,S_z\,(\text{type scf})\rangle_M$$

Now, each basis state is written as (possibly) a combination of old states and site states

$$|Q\,S\,\overbrace{S_z\,(\text{type scf})}^{\equiv i}\rangle_N = \sum_{S_z^{old},\,\tilde{S}_z} \langle S^{old}\, S_z^{old}\, \tilde{S}\,\tilde{S}_z | S\, S_z\rangle\, \underbrace{|Q^{old}\, S^{old}\, S_z^{old}\,(\text{scf})\rangle_{N-1}}_{\text{old basis}} \otimes |\tilde{Q}\,\tilde{S}\,\tilde{S}_z\,(\text{type})\rangle_N$$

$(S_z^{old} + \tilde{S}_z = S_z)$

Therefore the "$\mathbb{C}^{K}_{i\,i^{old}\,\tilde{k}}$" in the DM-NRG tanks (p 1) is essentially

$$\mathbb{C}^{i}_{\text{scf type}} = \langle S^{scf}\, S_z^{scf}\, \tilde{S}^{type}\, \tilde{S}_z^{type} | S_i\, S_z^i\rangle \quad (\text{only non-zero if } S_z = S_z^{scf} + \tilde{S}_z^{type})$$

and the reduced matrix at iteration M will be given by (see eq (1) in notes

$$(1)\quad \hat{\rho}^{red}_M = \sum_{\substack{ibl\\(QS)}} \sum_{S_z} \sum_{\substack{ww'\\ \in ibl}} (\rho^{red}_M)^{QS}_{ww'} \sum_{\substack{i\,i' \in QS\\ \text{basis}}} U^{QS}_{wi} (U^{QS}_{w'i'})^* \sum_{\substack{S_z^{old}(\tilde{S}_z)\\ S_z^{old'}(\tilde{S}_z')}} \langle S^{old}\, S_z^{old}\, \tilde{S}\,\tilde{S}_z | S\, S_z\rangle \langle S^{old'}\, S_z^{old'}\, \tilde{S}'\,\tilde{S}_z' | S\, S_z\rangle^* \times |Q^{old}\, S^{old}\, S_z^{old}\,(\text{scf})\rangle_{M-1} |\tilde{Q}\,\tilde{S}\,\tilde{S}_z\,(\text{type})\rangle_M\; {}_{M-1}\langle Q^{old'}\, S^{old'}\, S_z^{old'}\,(\text{scf}')|\, {}_M\langle \tilde{Q}'\,\tilde{S}'\,\tilde{S}_z'\,(\text{type}')|$$

and, taking the trace over $\{|\tilde{Q}\,\tilde{S}\,\tilde{S}_z\rangle_M\}$

$$\hat{\rho}^{red}_{M-1} = \sum_{\substack{(\text{type}'')\\ \tilde{Q}\tilde{S}\tilde{S}_z}} {}_M\langle \tilde{Q}''\,\tilde{S}''\,\tilde{S}_z''^{(\text{type})} | \hat{\rho}^{red}_M | \tilde{Q}''\,\tilde{S}''\,\tilde{S}_z''^{(\text{type})}\rangle_M = \left(\begin{array}{l} \text{The trace} \\ \text{will imply} \end{array} \boxed{\begin{array}{c} \tilde{Q}\,\tilde{S}\,\tilde{S}_z = \tilde{Q}'\,\tilde{S}'\,\tilde{S}_z' \;(\text{type} = \text{type}') \Downarrow \\ \Downarrow\; Q^{old}\, S^{old}\, S_z^{old} = Q^{old'}\, S^{old'}\, S_z^{old'} \end{array}} \right.$$

$\boxed{\text{but}}$ scf not necessarily equal to scf'!

Some care is needed in this trace. Let's consider only the following:

$$\mathrm{Tr}_M\{\ldots\} = \sum_{\substack{\text{type}''\\ \text{bl}}} \langle \text{type}''| \sum_{\substack{S_z^{o}(\tilde{S}_z)\\ S_z^{o'}(\tilde{S}_z')}} \langle CG1\rangle\langle CG2\rangle\, |\text{scf}\rangle\, |\text{type}(\tilde{S}\,\tilde{S}_z)\rangle\langle \text{scf}'|\langle \text{type}'(\tilde{S}'\tilde{S}_z')|\, |\text{type}''\rangle = \sum_{\substack{S_z^{o}\, \tilde{S}_z\\ (\text{old } S_z!)}} |\langle S^o S_z^o\, \tilde{S}\,\tilde{S}_z | S\, S_z\rangle|^2\, |Q^o\, \underline{S^o\, S_z^o}\, \text{scf}\rangle \langle Q^o\, S^o\, S_z^o\, \text{scf}'|$$

(another trace will give 1)

We also define the "rotated" matrix: $(\rho^{red}_M)^{\text{basis}\,QSS_z}_{i\,i'} \equiv \sum_{ww' \in ibl} U^{QS_z}_{wi} (\rho^{red}_M)^{QSS_z}_{ww'} (U^{QS}_{w'i'})^*$ and we have this:

$$\boxed{(2)\quad \hat{\rho}^{red}_{M-1} = \sum_{\substack{ibl\\(QS)}} \sum_{S_z} \sum_{\substack{i\,i'\\ \in QSS_z}} (\rho^{red}_M)^{\text{basis}\,QS}_{i,i'} \times \sum_{S_z^o,\,\tilde{S}_z} |\langle S^o\, S_z^o\, \tilde{S}\,\tilde{S}_z | S\, S_z\rangle|^2\, |Q^o\, S^o\, S_z^o\, \text{scf}\rangle_{M-1} \langle Q^o\, S^o\, S_z^o\, \text{scf}'|}$$

$\boxed{i, i' \text{ have the "same types"}}$ $\boxed{(Q^o S^o), \tilde{S} \text{ defined by scf and scf' and the types (have same } \tilde{Q}, \tilde{S})}$

Note that the matrix element has an explicit sum in S_z^{old} but (ρ^{red}) does not depend on

Therefore (and This is important) we take the following aproach: ("0"→"old") by definition:

$$(3)\quad \hat{\rho}^{red}_{M-1} = \sum_{\substack{ibl\\=Q^0\ S^0}} \sum_{S_z^0} \sum_{\substack{scf,scf'\\ \in Q^0 S^0 S_z^0}} \left(\hat\rho^{red}_{M-1}\right)^{QS}_{scf\,scf'} |Q^0 S^0 S_z^0 (scf)\rangle_{M-1} \langle Q^0 S^0 S_z^0 (scf')| \qquad (3)$$

Now, the comparison: in Eq. (2) we have a sum over S_z and in eq. (3), a sum over S_z^0:

$$\text{from (2)}\quad \sum_{S_z=-S}^{S} \sum_{\substack{\tilde S_z=-\tilde S\\ (\tilde S \text{ given by type scf, scf'})}} |\langle S^0 S_z^0\ \tilde S \tilde S_z | S S_z\rangle|^2\ |Q^0 S^0 S_z^0 (scf)\rangle_{M-1} \langle Q^0 S^0 S_z^0 (scf')|$$

$$\text{from (3)}\quad \sum_{S_z^0=-S^0}^{S^0} |Q^0 S^0 S_z^0 (scf)\rangle_{M-1} \langle Q^0 S^0 S_z^0 (scf')| \qquad \text{How to compare?}$$

easy: (rearranging)

$$\boxed{(2) \to \sum_{S_z^0=-S^0}^{S^0} \cdot \left[\sum_{S_z=-S}^{S \text{ (child)}} |\langle S^0 S_z^0\ \tilde S (\tilde S_z = S_z - S_z^0) | S S_z\rangle|^2 \right] |Q^0 S^0 S_z^0 (scf)\rangle\langle Q^0 S^0 S_z^0 (scf')|}$$

SO, in terms of the "Rotated" $\left(\rho^{red}_M\right)^{QS}_{\substack{rot\\ i\,i'}} \equiv \sum_{ww' \in QS} (U_{w'i'})^* \left(\rho^{red}_M\right)^{QS}_{ww'} U_{wi}$, we have

$$\boxed{\left(\hat\rho^{red}_{M-1}\right)^{Q^0 S^0 S_z^0}_{scf\ scf'} = \sum_{\substack{\text{child states}\\ i,i'(\to QS)}} \underbrace{\left[\sum_{S_z=-S}^{S} |\langle S^0 S_z^0\ \tilde S\ \tilde S_z = S_z - S_z^0 | S S_z\rangle|^2 \right]}_{\text{should be independent of } S_z^0\text{!}} \cdot \left(\hat\rho^{red}_M\right)^{QS}_{\substack{rot(basis)\\ i,i'}}} \qquad (4)$$

(from type)

How to determine the "child states" i, i' given (scf, scf')?

Given $|Q^0 S^0 S_z^0 = S^0, scF\rangle_{M-1}$ Then $|Q\,S\,S_z = S\ i\rangle^{M}_{(i')} = \sum_{S_z^0(\tilde S_z)\ (\text{type})} \langle S^0 S_z^0\ \tilde S \tilde S_z | S S\rangle |Q^0 S^0 S_z^0\ scf_{(scf')}\rangle_{M-1} |\tilde Q \tilde S \tilde S_z (type)_{(type')}\rangle_N$

$|Q^0 S^0 S_z^0 = S^0\ scf'\rangle_{M-1}$ Then $\quad \boxed{\text{Type} = \text{type}'}$

is a "child state". Note that i and i' can implicitly involve more than one "type" but all involved "type" will have the same $\tilde S$. For instance: $|Q\ 0 \overset{S=S_z=0}{i}\rangle^{M}_{(i')} = \frac{+1}{\sqrt2} \underbrace{|0 \tfrac12 \tfrac12\rangle^{N-1}}_{scf\,(scf')} |\downarrow\rangle_{(t=2)} + \frac{1}{\sqrt2} \underbrace{|0 \tfrac12 -\tfrac12\rangle}_{scf\,(scf')} |\uparrow\rangle_{(t=1)}$

will be marked as "type = 2" and "child" of scf (scf'). Note that the sum in (4) is S_z^0-independent. Thus:

$$\boxed{\left(\rho^{red}_{M-1}\right)^{Q^0 S^0}_{scf\ scf'} = \sum_{\substack{\text{child states}\\ i,i' \to (S)}} \left[\sum_{S_z=-S}^{S} |\langle S^0 S^0\ \tilde S (\tilde S_z = S_z - S^0) | S S_z\rangle|^2 \right] \cdot \left(\hat\rho^{red}_M\right)^{QS}_{\substack{rot(basis)\\ i,i'}}} \qquad (5)$$

(from "type")

and that does it!

Complete Fock Space (CFS) method

The idea is to calculate the retarded Green's function with the CFS implementation

$$G_{A,B}(t) = -i\,\Theta(t)\,\mathrm{Tr}\{\hat{\rho}\,[\hat{A}(t),\hat{B}(0)]_{\pm}\} \qquad (\pm) \begin{matrix}\to \text{Fermion}\\ \to \text{Boson}\end{matrix}$$

using $\hat{\rho} = \frac{1}{Z} e^{-\beta H} = \sum_m \rho_m |\Psi_m\rangle\langle\Psi_m|$, where $\rho_m = \frac{e^{-\beta E_m}}{Z}$

Using the Lehmann representation, we get (see Feb 2009 note).

$$G^{M}_{A,B}(\omega) = \sum_{\substack{nn'\\m}} \frac{\rho^M_{mn} A^M_{nn'} B^M_{n'm} \pm \rho^M_{n'm} B^M_{mn} A^M_{nn'}}{\omega - (E^M_{n'} - E^M_{n}) + i\eta} \qquad \begin{matrix}+ \to \text{Fermion}\\ - \to \text{Boson}\end{matrix} \qquad (1)$$

for a given NRG iteration M and $G_{AB}(\omega) = \sum_{M=0}^{N} G^M_{AB}(\omega)$ "

In the CFS procedure, we split (1) in 3 parts.

The first contribution comes from $M=N$ only, where $\rho^N_{mn} = \frac{e^{-E_n/T}}{Z}\delta_{mn}$

$$G^{N\,(i)}_{A,B}(\omega) = \sum_{nn'} \frac{A^N_{nn'} B^N_{n'n} e^{-E^N_n/T} \pm B^N_{n'n} A^N_{nn'} e^{-E^N_{n'}/T}}{\omega - (E^N_{n'} - E^N_n) + i\eta} \qquad \text{(all states at iteration } N \text{ are "discarded")}$$

The next two contributions come from the fact that $\hat{\rho}\,|n\,(\text{disc})\rangle_M = 0$ for $M<N$

We have $(M = M_{min}, N-1)$ only $\rho_{mn} \Rightarrow \langle m\,(\text{kept})|\rho|n\,(\text{kept})\rangle$ are nonzero!

$$G^{M}_{A,B} = \underbrace{\sum_{\substack{n(k)\,n'(d)\\m(k)}} \frac{\rho^M_{m(k)n(k)} A^M_{n(k)n'(d)} B^M_{n'(d)m(k)}}{\omega - (E_{n'(d)} - E_{n(k)}) + i\eta}}_{\text{"positive" } \omega \quad \text{"}G^{(iii)}\text{" in Anders'}} \underbrace{\pm \sum_{\substack{n(k)\\n'(d)\\m(k)}} \frac{\rho^M_{n(k)m(k)} B^M_{m(k)n'(d)} A^M_{n'(d)n(k)}}{\omega + (E_{n'(d)} - E_{n(k)}) + i\eta}}_{\text{"}G^{(ii)}\text{" in Ander's}}$$

Notice that $A^M_{n(k)n'(d)}$ involves only kept states in block i and discarded states in "block j".

Switching $n \leftrightarrow n'$ in the second sum

$$G^M_{A,B} = \sum_{n(k)n'(d)} \left(\sum_{m(k)} B^M_{n'(d)m(k)} \rho_{m(k)n(k)}\right) \frac{A^M_{n(k)n'(d)}}{\omega - (E_{n'(d)} - E_{n(k)}) + i\eta} \pm$$

$$\pm \sum_{n(k)n'(d)} \left(\sum_{m'(k)} \rho_{n'(k)m'(k)} B_{m'(k)n(d)}\right) \frac{A_{n(d)n'(k)}}{\omega - (E_{n'(k)} - E_{n(d)}) + i\eta}$$

Implementation: The spectral function at iteration M will be given by

$$\rho^{M}_{CFS}(\omega,T) = \sum_{n(k)} \sum_{n'(d)} \left\{ \left[\sum_{m(k)} (\hat{B})_{n'(d)m(k)} (\rho^{red}_{M})_{m(k)n(k)} \right] \hat{A}_{n(k)n'(d)}\, \delta(\omega - (E_{n'(d)} - E_{n(k)})) \right.$$

$$\pm \sum_{n(k)} \sum_{n'(d)} \left\{ \left[\sum_{m'(k)} (\rho^{red}_{M})_{n'(k)m'(k)} (\hat{B})_{m'(k)n(d)} \right] \hat{A}_{n(d)n'(k)}\, \delta(\omega - (E_{n'(k)} - E_{n(d)}))\right.$$

↑ THIS WILL BE < 0!

Notice that the matrices "A" in the two sums are not the same (as opposed to the usual DM-NRG approach). In matrix form, we need:

$$\mathbb{C}^1 = \mathbb{B}_{d,k} \cdot \rho_{kk} \quad ; \quad \mathbb{A}^{\delta}_1(\omega) = (A)_{i(k)j(d)}\, \delta(\omega - E^{(d)}_j - E^{(k)}_i)$$

$$\mathbb{C}^2 = \rho_{kk}\, \mathbb{B}_{k,d} \quad ; \quad \mathbb{A}^2_2(\omega) = (A)_{i(d)j(k)}\, \delta(\omega - E^{(k)}_j - E^{(d)}_i)$$

and

$$\rho^{M}_{CFS}(\omega,T) = \sum_{n'(d)} \sum_{n(k)} (\mathbb{C}_1)_{n'n} (\mathbb{A}^{\delta}_1)_{nn'} + \sum_{n(k)} \sum_{n'(d)} (\mathbb{C}_2)_{nn'} (\mathbb{A}^{\delta}_2)_{n'n} = \underset{(disc)}{Tr}\{\mathbb{C}_1 \cdot \mathbb{A}^{\delta}_1(\omega)\} + \underset{(kept)}{Tr}\{\mathbb{C}_2 \cdot \mathbb{A}^{\delta}_2(\omega)\}$$

Who are these matrices? Given blocks (ibl, ibl') that are connected by $\hat{A}$ ($\langle ibl | \hat{A} | ibl' \rangle \neq 0$), with states $N_{ibl} = N_{ibl,k} + N_{ibl,d}$; $N_{ibl'} = N_{ibl',k} + N_{ibl',d}$ we have:

$$\begin{cases} \mathbb{C}^1(ibl', ibl) = B(ibl',d, ibl,k)\ \rho(ibl,k, ibl,k) & \leftarrow \overset{size}{(N_{ibl',d} \times N_{ibl,k})} \\ \mathbb{C}^2(ibl', ibl) = \rho(ibl',k, ibl',k)\ B(ibl',k, ibl,d) & \leftarrow \overset{size}{(N_{ibl',k} \times N_{ibl,d})} \end{cases}$$

and

$$\begin{cases} \mathbb{A}^{\delta}_1(\omega) = A(ibl,k, ibl',d) & \rightarrow (N_{ibl,k} \times N_{ibl',d}) \\ \mathbb{A}^{\delta}_2(\omega) = A(ibl,d, ibl',k) & \rightarrow (N_{ibl,d} \times N_{ibl',k}) \end{cases} \quad \delta(\omega - E' - E)$$

Thus we need a routine that, given blocks ibl, ibl' of an operator produces BLAS matrices. (ibl,(k,d), ibl'(k,d)) → (4 combinations).

What if there are no kept or discarded states in a given block?

$N_{ibe,k} = 0$ or $N_{ibe',d} = 0$ $\Rightarrow$ $\Rightarrow$ $\mathbb{C}_1 = 0$, terms 2 $\mathbb{C}_2$ only

$N_{ibe,d} = 0$ or $N_{ibe',k} = 0$ $\Rightarrow$ $\Rightarrow$ $\mathbb{C}_2 = 0$ terms 1 $\mathbb{C}_1$ only

$N_{ibe,k} \neq 0$ AND $N_{ibe',d} \neq 0$ $\rightarrow$ calculate $\mathbb{C}_1$

$N_{ibe,d} \neq 0$ AND $N_{ibe',k} \neq 0$ $\rightarrow$ calculate $\mathbb{C}_2$