

# Optimisation of the L-neighbour approach (1)

In the LN approach

$$F_{i_L \dots i_1}^{(s+1)} = \sum_{e=0,1} G_{i_L \dots i_e} F_{i_L \dots i_e}^{(s)}$$

with the initial  $F_{i_L \dots i_1}^{(1)} = M_{i_1 i_0}$

and

$$G_{i_L \dots i_e} = M_{i_e} e^{\delta_{e1} (K_0 + 2\delta_{i_1 1} K_1 + \dots + 2\delta_{i_{L-1} 1} K_L)}$$

and the polarisation has the form

$$P_{i_N i_0}(t) = e^{\delta_{i_N 1} K_0} F_{0 \dots 0 i_N}^{(N)}$$

Here  $i=0$  ( $i=1$ ) corresponds to the cavity (exciton) state.

Let us first introduce at each iteration  $s$  a normal matrix array  $F$ :

$$F_{i_L \dots i_1}^{(s)} = \overline{F}_{nm}$$

This is not necessarily the case and will not be the case for some iterations, but let us ~~take~~ <sup>choose</sup> for clarity  $n$  and  $m$  such that

in  $n$ -array the values of  $i_1$  to  $i_{L/2}$  do not change  
in  $m$ -array the values of  $i_{L/2+1}$  to  $i_L$  do not change

For example,

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$$m = 2^{\frac{L}{2}-1} i_{\frac{L}{2}} + 2^{\frac{L}{2}-2} i_{\frac{L}{2}-1} + \dots + 2^0 i_1$$

so  $m$  depends on  $i_{\frac{L}{2}} \dots i_1$  only

$$n = 2^{\frac{L}{2}-1} i_L + 2^{\frac{L}{2}-2} i_{L-1} + \dots + 2^0 i_{\frac{L}{2}+1}$$

so  $n$  depends on  $i_L \dots i_{\frac{L}{2}+1}$  only

At this point one has to introduce arrays of  $i_p$ , with  $p = 1, \dots, L$

Assuming for simplicity the ~~size~~  $n$ - and  $m$ -arrays are of the same size  $\bar{N}$ , these can be 2D arrays

$$i_p[0 \dots 1][0 \dots \bar{N}] \quad \text{with } \bar{N} = 2^{\frac{L}{2}-1} \text{ (L even)}$$

where the first index says whether  $i_p$  belongs to  $n$  or  $m$  and the second is  $n$  or  $m$  itself. For example if  $i_p$  belongs to  $n$ -array, then

$$i_p[0][n] = 0 \text{ or } 1 \text{ (dependent on } n)$$

$$i_p[1][m] = 2 \text{ (or any other number)}$$

the latter indicating that  $m$ -array is independent of  $i_p$ . See also an example in the Appendix.

Let us now rewrite the recursive formula as

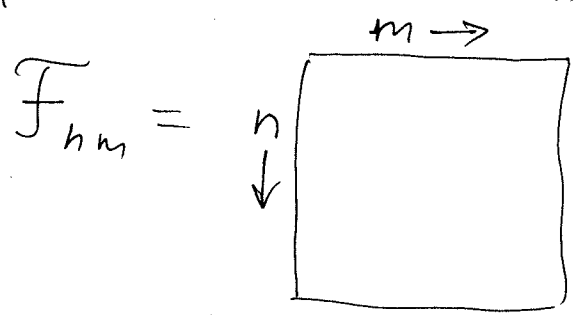
$$F_{p i_L \dots i_2}^{(s+1)} = \sum_e Q_{pe}^{(L)} Q_{i_2 e}^{(L-1)} \dots Q_{i_{s-2} e}^{(2)} Q_{i_{s-1} e}^{(1)} F_{i_2 \dots i_2 e}^{(s)}$$

where  $l=i_1$  and  $p$  take the values of 0 or 1 and

$$Q_{ie}^{(r)} = e^{\sum_{i=1}^{i_1} \delta_{i1} 2K_r} \quad (1 < r \leq L)$$

$$Q_{ie}^{(1)} = M_{ie} e^{\sum_{i=1}^{i_1} K_0} e^{\sum_{i=1}^{i_1} \delta_{i1} 2K_1} \quad (r=1)$$

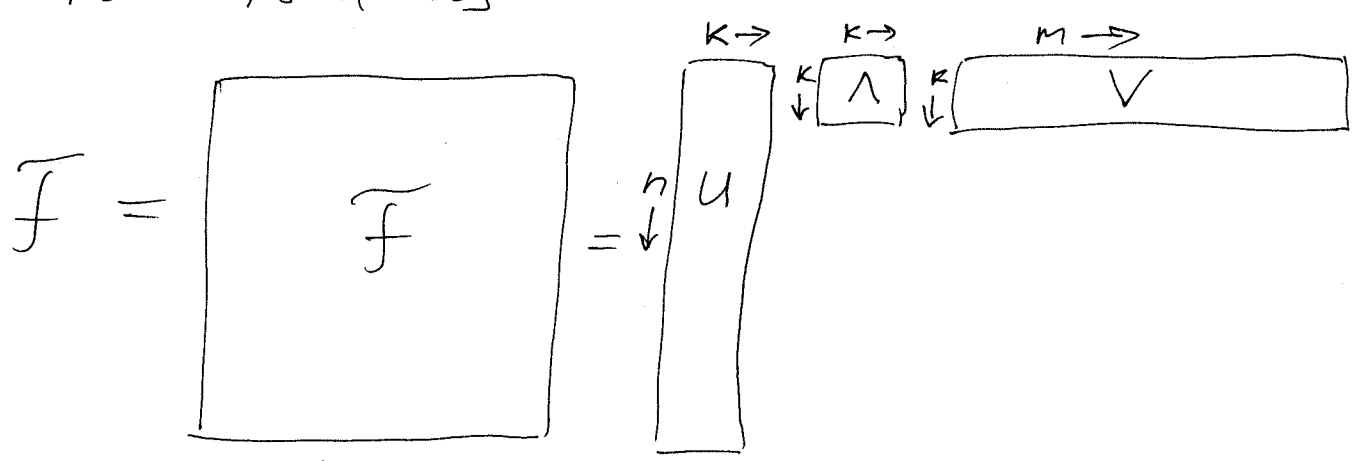
To implement this, we take the SVD of normal matrix



$i_1 - i_{L/2}$  not changing in  $n$

$i_{L/2+1} - i_L$  not changing in  $m$

representing  $F_{i_L \dots i_1}^{(s)}$ , which can be visualised as



and written as

$$F_{nm} = \sum_k U_{nk} \Lambda_k V_{km}$$

Let us separate  $i_1=0$  and  $i_1=1$  elements of  $F$ :

$$F_{nm'}^{(0)} = \sum_k U_{nk} \Lambda_k V_{km'}^{(0)}$$

$$F_{nm'}^{(1)} = \sum_k U_{nk} \Lambda_k V_{km'}^{(1)}$$

so  $F_{nm} = F_{nm}^{(0)}$  if  $i_1 = 0$

and  $F_{nm} = F_{nm}^{(1)}$  if  $i_1 = 1$

Since  $n$ -array does not depend on  $i_1$

$U_{nk}$  is the same in both cases

but  $V_{km}^{(0)} = V_{km}$  if  $i_1 = 0$

and  $V_{km}^{(1)} = V_{km}$  if  $i_1 = 1$

Clearly  $m'$ -array is 2 times shorter than  $m$ -array as it is independent of  $01$  (but  $m$ -array depends on  $i_1$ )

Then multiply  $U_{nk}$  <sup>with  $Q$ s</sup> to obtain two new matrices:

$$\tilde{U}_{nk}^{(0)} = Q_{i_2 0}^{(L-1)} \cdots Q_{i_{\frac{L}{2}+1} 0}^{(L/2)} U_{nk}$$

$$\tilde{U}_{nk}^{(1)} = Q_{i_2 1}^{(L-1)} \cdots Q_{i_{\frac{L}{2}+1} 1}^{(L/2)} U_{nk}$$

again corresponding to  $i_1 = 0$  and  $i_1 = 1$ , respectively. Similarly,

$$\tilde{V}_{km}^{(0,p)} = Q_{p0}^{(L)} Q_{i_{\frac{L}{2} 0}^{(\frac{L}{2}-1)} \cdots Q_{i_2 0}^{(1)} V_{km}^{(0)}$$

$$\tilde{V}_{km}^{(1,p)} = Q_{p1}^{(L)} Q_{i_{\frac{L}{2} 1}^{(\frac{L}{2}-1)} \cdots Q_{i_2 1}^{(1)} V_{km}^{(1)}$$

with  $p = 0$  or  $1$ , introducing a new index, due to  $G$ .

Now a new  $\tilde{F}_{nm'}^{(p)}$  representing  $F_{p i_1 \dots i_2}^{(s+1)}$  takes the form

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$$\tilde{F}_{nm'}^{(p)} = \sum_k \left( \tilde{U}_{nk}^{(0)} \Lambda_k \tilde{V}_{km'}^{(0,p)} + \tilde{U}_{nk}^{(1)} \Lambda_k \tilde{V}_{km'}^{(1,p)} \right)$$

We can introduce a new matrix  $\tilde{F}_{nm}$  on step  $s+1$  as a product of matrices:

$$\tilde{F} = \begin{bmatrix} \tilde{U}^{(0)} \\ \tilde{U}^{(1)} \end{bmatrix} \begin{bmatrix} \Lambda & & \\ & \Lambda & \\ & & \tilde{V}^{(0,0)} & \tilde{V}^{(0,1)} \\ & & \tilde{V}^{(1,0)} & \tilde{V}^{(1,1)} \end{bmatrix}$$

Clearly the  $m$ -array is now restored to accommodate the new index  $p$ . At this stage all the arrays  $ip[][]$  should be redefined, in order to go from

$$F_{p i_1 \dots i_2}^{(s+1)} \rightarrow F_{i_1 \dots i_2 i_1}^{(s+1)}$$

The new  $F$  has the form of SVD with a double size of the diagonal matrix and can be optimised by applying SVD to different parts of  $F$ .

For instance, one can SVD the matrix 6

$$\begin{bmatrix} \Lambda \\ \Lambda \end{bmatrix} \begin{bmatrix} \tilde{V}^{(0,0)} & \tilde{V}^{(0,1)} \\ \tilde{V}^{(1,0)} & \tilde{V}^{(1,1)} \end{bmatrix} = A \begin{bmatrix} \Lambda_1 \\ V_1 \end{bmatrix}$$

where  $\Lambda_1$  has a smaller size due to the threshold condition that

if  $|\lambda_k| < \varepsilon$  then  $\lambda_k = 0$

Next, one can apply an SVD to

$$\begin{bmatrix} \tilde{U}^{(0)} \\ \tilde{U}^{(1)} \end{bmatrix} A \begin{bmatrix} \Lambda_1 \end{bmatrix} = U_2 \begin{bmatrix} \Lambda_2 \\ B \end{bmatrix}$$

This procedure can be repeated several times until matrices  $A$  and  $B$  are reduced to their minimal size. After that we can go from  $F^{(s+1)}$  to  $F^{(s+2)}$

Clearly, at some point (for some  $s$ ) the index  $i_1 = e$  will be found in the  $n$ -array. In this case one should do with matrix  $U$  the same what was done with  $V$ , and vice versa.

Arrays  $ip[][]$  should be reorganised for each  $s$ .

The SVD of the initial tensor ( $s=1$ )  
is analytical:

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$$F_{i_2 \dots i_1}^{(1)} = M_{i_1 i_0} = F_{nm}$$

where  $i_0$  is fixed. Then

$$F_{nm} = \sum_k U_{nk} \Lambda_k V_{km}$$

with

$$U_{n0} = 1 \quad \Lambda_k = \delta_{k0} \quad V_{0m} = M_{i_1 i_0}$$

so  $\Lambda$  is a  $1 \times 1$  matrix.

Appendix: Example of  $F_{i_4 i_3 i_2 i_1}$  tensor

$m = 2i_2 + i_1$        $n = 2i_4 + i_3$

$\tilde{F} = \begin{matrix} & \begin{matrix} (i_2, i_1) = \\ 00 & 01 & 10 & 11 \end{matrix} \\ \begin{matrix} (i_4, i_3) = \\ 00 \\ 01 \\ 10 \\ 11 \end{matrix} & \begin{bmatrix} & & & \\ & & & \\ & & & \\ & & & \end{bmatrix} \end{matrix} = U \Lambda V$

Separating  $i_1=0$  elements, obtain:

$\tilde{F}^{(0)} = \begin{matrix} & 00 & 10 \\ \begin{matrix} 00 \\ 01 \\ 10 \\ 11 \end{matrix} & \begin{bmatrix} & \\ & \\ & \\ & \end{bmatrix} \end{matrix} = \begin{matrix} & K \rightarrow \\ \begin{matrix} 00 \\ 01 \\ 10 \\ 11 \end{matrix} & \begin{bmatrix} & & & \\ & & & \\ & & & \\ & & & \end{bmatrix} U \end{matrix} \times \Lambda \times \begin{matrix} \downarrow K \\ \begin{matrix} 00 & 1,0 \\ & \end{matrix} \\ \begin{bmatrix} & \\ & \\ & \\ & \end{bmatrix} V^{(0)} \end{matrix}$

Here it is assumed  $\Lambda$  has the maximum size ( $4 \times 4$  in this case).

However, for the whole procedure to work one probably has to require that  $\Lambda$  is 4 times smaller than its maximum size (i.e.  $2 \times 2$  in this case)

Or maybe this is not needed because of the SVD applied, see page 6.