Normalized A-matrices MPS

scientific mode. matrix product states. for a sum of single particle states on a chain, I want to write normalized A-matrices. how can this be done directly

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Assume an open chain with a local "vacuum/occupied" basis $\{|0\rangle, |1\rangle\}$ and a **one-particle** state

$$|\psi\rangle = \sum_{j=1}^{N} c_j\,|0\cdots 1_j \cdots 0\rangle, \qquad \sum_{j=1}^{N} |c_j|^2 = 1.$$

Then there is an **exact bond-dimension** $D \le 2$ MPS whose site tensors are **left-normalized** in the standard sense

$$\sum_{\sigma\in\{0,1\}} (A_\sigma^{[j]})^\dagger A_\sigma^{[j]} = I,$$

for all sites except (typically) the last one in a left-canonical gauge. homepages.phy... +1

Direct closed-form left-canonical A-matrices

Define cumulative weights

$$q_j := \sum_{k=1}^{j} |c_k|^2, \quad q_0 := 0.$$

(If some initial $q_j = 0$ because $c_1 = \cdots = c_j = 0$, then keep bond dimension 1 up to the first nonzero coefficient; the formulas below apply once $q_j > 0$.)

Use open-boundary dimensions $D_1 = 1$, $D_j = 2$ for $2 \le j \le N$, $D_{N+1} = 1$. Then set:

- **Site** $j = 1$ (row vectors 1×2; requires $q_1 > 0$):

$$A_0^{[1]} = \begin{bmatrix} 1 & 0 \end{bmatrix}, \qquad A_1^{[1]} = \begin{bmatrix} 0 & \frac{c_1}{q_1} \end{bmatrix}.$$

- **Sites** $2 \le j \le N-1$ (matrices 2×2; requires $q_j > 0$):

$$A_0^{[j]} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{q_{j-1}}{q_j} \end{bmatrix}, \qquad A_1^{[j]} = \begin{bmatrix} 0 & \frac{c_j}{q_j} \\ 0 & 0 \end{bmatrix}.$$

- **Site** $j = N$ (column vectors 2×1):

$$A_0^{[N]} = \begin{bmatrix} 0 \\ q_{N-1} \end{bmatrix}, \qquad A_1^{[N]} = \begin{bmatrix} c_N \\ 0 \end{bmatrix}.$$

What this guarantees (exactly)

1. **Correct amplitudes:** Contracting $A_{\sigma_1}^{[1]} \cdots A_{\sigma_N}^{[N]}$ produces coefficient c_j iff the string $\sigma_1 \cdots \sigma_N$ has a single "1" at site j; otherwise it gives 0. (This follows from the triangular "one-excitation" structure of the $A_1^{[j]}$ blocks and the final vectors.)
2. **Left-normalization:** For every $j < N$,

$$(A_0^{[j]})^\dagger A_0^{[j]} + (A_1^{[j]})^\dagger A_1^{[j]} = I_2,$$

i.e. the tensors are left-normalized in the standard canonical-form condition. homepages.phy... +1
(The last site is where the overall norm “lands” in a purely left-canonical gauge; this is the usual situation discussed in canonical-form constructions. homepages.phy...)

3. **State is normalized** provided $\sum_j |c_j|^2 = 1$ (equivalently $q_N = 1$).

If you want the **right-canonical** analogue (or a mixed-canonical Γ–Λ form with explicit Schmidt values on each bond), it can be written just as directly using tail sums $\sum_{k=j}^N |c_k|^2$, but the above is the minimal “direct normalized A-matrices” construction for the one-particle sector.

give me the gamma-lambda form

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Take a chain with local basis $\{|0\rangle, |1\rangle\}$ and the normalized one-particle state

$$|\psi\rangle = \sum_{j=1}^{N} c_j \, |0 \cdots 1_j \cdots 0\rangle, \qquad \sum_{j=1}^{N} |c_j|^2 = 1.$$

In Vidal’s Γ–Λ form (open boundaries),

$$|\psi\rangle = \sum_{\{\sigma\}} \Gamma^{[1]\sigma_1} \Lambda^{[1]} \Gamma^{[2]\sigma_2} \Lambda^{[2]} \cdots \Lambda^{[N-1]} \Gamma^{[N]\sigma_N} \, |\sigma_1 \cdots \sigma_N\rangle,$$

where each $\Lambda^{[j]}$ is diagonal and contains the Schmidt coefficients across bond $j|j+1$. www2.physik.uni... +2

Schmidt values $\Lambda^{[j]}$ (bond dimension $D \le 2$)

Define cumulative weights

$$p_j := \sum_{k=1}^{j} |c_k|^2, \qquad r_j := \sum_{k=j+1}^{N} |c_k|^2 = 1 - p_j.$$

Then the Schmidt rank across any cut is at most 2, with Schmidt coefficients r_j and p_j. Set

$$\Lambda^{[j]} = \mathrm{diag}(\; r_j, \; p_j), \qquad j = 1, \ldots, N-1.$$

(If $r_j = 0$ or $p_j = 0$ for some bond, the Schmidt rank drops to 1 there; equivalently, you delete the corresponding row/column rather than divide by zero.) www2.physik.uni... +1

Explicit Γ tensors (one consistent gauge)

Use the bond-index ordering $\alpha = 0$ (“particle to the right of the cut”) and $\alpha = 1$ (“particle to the left of the cut”). Then:

- **Site** 1 (1×2 row vectors)

$$\Gamma_0^{[1]} = \begin{bmatrix} 1 & 0 \end{bmatrix}, \qquad \Gamma_1^{[1]} = \begin{bmatrix} 0 & c_1 \end{bmatrix}.$$

- **Sites** $2 \le j \le N-1$ (2×2 matrices)

$$\Gamma_0^{[j]} = \begin{bmatrix} \dfrac{1}{r_{j-1}} & 0 \\ 0 & \dfrac{1}{p_{j-1}} \end{bmatrix}, \qquad \Gamma_1^{[j]} = \begin{bmatrix} 0 & \dfrac{c_j}{r_{j-1}} \\ 0 & 0 \end{bmatrix}.$$

- **Site** N (2×1 column vectors)

$$\Gamma_0^{[N]} = \begin{bmatrix} 0 \\ \dfrac{1}{p_{N-1}} \end{bmatrix}, \qquad \Gamma_1^{[N]} = \begin{bmatrix} \dfrac{c_N}{r_{N-1}} \\ 0 \end{bmatrix}.$$

With these Γ's and the $\Lambda^{[j]}$ above, the contraction $\Gamma^{[1]}\Lambda^{[1]}\Gamma^{[2]}\cdots\Lambda^{[N-1]}\Gamma^{[N]}$ reproduces exactly the amplitudes c_j on the one-particle basis states and zero elsewhere; normalization is inherited from $\sum_j |c_j|^2 = 1$. www2.physik.uni... +1