Appendix A: Mathematical proof for stack operation of two MPS

For simplicity, we consider performing the stack operation of two MPS: $|\psi_\alpha\rangle, |\psi_\beta\rangle$, which can be written as

$$\big[|\psi_\alpha\rangle,\ \ |\psi_\beta\rangle\big] = |\psi_\alpha\rangle \otimes |0\rangle + |\psi_\beta\rangle \otimes |1\rangle \tag{A1}$$

and

$$|\psi_\alpha\rangle = \sum_{\{\boldsymbol{\sigma}\}} \mathrm{Tr}\left[M_\alpha^{\sigma_0} M_\alpha^{\sigma_1} \dots M_\alpha^{\sigma_{n-1}}\right] |\sigma_0, \dots, \sigma_{n-1}\rangle \tag{A2}$$
$$|\psi_\beta\rangle = \sum_{\{\boldsymbol{\sigma}\}} \mathrm{Tr}\left[M_\beta^{\sigma_0} M_\beta^{\sigma_1} \dots M_\beta^{\sigma_{n-1}}\right] |\sigma_0, \dots, \sigma_{n-1}\rangle$$

are the two MPS's. We seek to find a new MPS $|\phi\rangle$ which exactly represents the stacked operation from Eq. (A1). We denote the new MPS as

$$|\phi\rangle = \sum_{\{\boldsymbol{\sigma}\}} \mathrm{Tr}\left[\tilde{M}^{\sigma_0} \tilde{M}^{\sigma_1} \dots \tilde{M}^{\sigma_{n-1}}\right] |\sigma_0, \dots, \sigma_{n-1}\rangle \tag{A3}$$

To see the detailed structure of each $\tilde{M}^{\sigma_i}$ in the above expression, we expand both terms on the right-hand side of Eq. (A1)

$$\begin{aligned}
&|\psi_\alpha\rangle|0\rangle \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (A4)\\
&= \sum_{\sigma_0,\dots,\sigma_{n-1}} \mathrm{Tr}\left[M_\alpha^{\sigma_0} M_\alpha^{\sigma_1} \dots M_\alpha^{\sigma_{n-1}}\right] |\sigma_0, \dots, \sigma_{n-1}\rangle|0\rangle\\
&= \sum_{\sigma_0,\dots,\sigma_n} \mathrm{Tr}\left[M_\alpha^{\sigma_0} M_\alpha^{\sigma_1} \dots M_\alpha^{\sigma_{n-1}}\right] \delta_0^{\sigma_n} |\sigma_0, \dots, \sigma_{n-1}\rangle|\sigma_n\rangle\\
&= \sum_{\sigma_0,\dots,\sigma_n} \mathrm{Tr}\left[M_\alpha^{\sigma_0} M_\alpha^{\sigma_1} \dots M_\alpha^{\sigma_{n-1}} \Delta_0^{\sigma_n}\right] |\sigma_0, \dots, \sigma_{n-1}, \sigma_n\rangle
\end{aligned}$$

where $\Delta_0^{\sigma_n} = \delta_0^{\sigma_n}\mathbb{I}$, and $\mathbb{I}$ is the identity matrix of which the row size is the same as the column size of the previous site matrix $M_\sigma^{\sigma_{n-1}}$.

Similarily, we have

$$\begin{aligned}
&|\psi_\beta\rangle|1\rangle \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (A5)\\
&= \sum_{\sigma_0,\dots,\sigma_n} \mathrm{Tr}\left[M_\beta^{\sigma_0} M_\beta^{\sigma_1} \dots M_\beta^{\sigma_{n-1}} \Delta_1^{\sigma_n}\right] |\sigma_0, \dots, \sigma_{n-1}, \sigma_n\rangle
\end{aligned}$$

By summing up Eq. (A4) and (A5), we obtain

$$\begin{aligned}
&|\psi_\alpha\rangle \otimes |0\rangle + |\psi_\beta\rangle \otimes |1\rangle \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (A6)\\
&= \sum_{\{\boldsymbol{\sigma}\}} \mathrm{Tr}\left[M_\alpha^{\sigma_0} M_\alpha^{\sigma_1} \dots M_\alpha^{\sigma_{n-1}} \Delta_0^{\sigma_n}\right] |\sigma_0, \dots, \sigma_{n-1}, \sigma_n\rangle\\
&+ \sum_{\{\boldsymbol{\sigma}\}} \mathrm{Tr}\left[M_\beta^{\sigma_0} M_\beta^{\sigma_1} \dots M_\beta^{\sigma_{n-1}} \Delta_1^{\sigma_n}\right] |\sigma_0, \dots, \sigma_{n-1}, \sigma_n\rangle\\
&= \sum_{\{\boldsymbol{\sigma}\}} \mathrm{Tr}\left[M_\alpha^{\sigma_0} M_\alpha^{\sigma_1} \dots M_\alpha^{\sigma_{n-1}} \Delta_0^{\sigma_n}\right.\\
&\left. + M_\beta^{\sigma_0} M_\beta^{\sigma_1} \dots M_\beta^{\sigma_{n-1}} \Delta_1^{\sigma_n}\right] |\sigma_0, \sigma_1, \dots, \sigma_{n-1}, \sigma_n\rangle\\
&= \sum_{\{\boldsymbol{\sigma}\}} \mathrm{Tr}\left\{\begin{bmatrix} M_\alpha^{\sigma_0} \\ M_\beta^{\sigma_0} \end{bmatrix}^T \begin{bmatrix} M_\alpha^{\sigma_0} & 0 \\ 0 & M_\beta^{\sigma_0} \end{bmatrix} \cdots\right.\\
&\left.\begin{bmatrix} M_\alpha^{\sigma_{n-1}} & 0 \\ 0 & M_\beta^{\sigma_{n-1}} \end{bmatrix} \begin{bmatrix} \Delta_0^{\sigma_n} & 0 \\ 0 & \Delta_1^{\sigma_n} \end{bmatrix}\right\} |\sigma_0, \sigma_1, \dots, \sigma_{n-1}, \sigma_n\rangle\\
&= \sum_{\{\boldsymbol{\sigma}\}} \mathrm{Tr}\left[\tilde{M}^{\sigma_0} \tilde{M}^{\sigma_1} \dots \tilde{M}^{\sigma_{n-1}} \tilde{\Delta}^{\sigma_n}\right] |\sigma_0, \sigma_1, \dots, \sigma_{n-1}, \sigma_n\rangle\\
&= \sum_{\{\boldsymbol{\sigma}\}} \mathrm{Tr}\left[\tilde{M}^{\sigma_0} \tilde{M}^{\sigma_1} \dots \tilde{M}^{\sigma_{n-1}}\right] |\sigma_0, \sigma_1, \dots, \sigma_{n-1}, \sigma_n\rangle
\end{aligned}$$

Note that for the first site σ_0, the resulting matrix $\tilde{M}^{\sigma_0}$ is stacked in row geometry [see the first site of the resulting stacked MPS in Fig. 4], all the other matrices $\tilde{M}^{\sigma_j} (j = 1, \cdots, n-1)$ are block diagonal [Fig. 4], as the stack operation is essentially equivalent to a direct sum of local matrices. In the final step of the above equation, to maintain the form of the stacked MPS as shown in Eq. (A3), we have absorbed $\tilde{\Delta}^{\sigma_n}$ into $\tilde{M}^{\sigma_{n-1}}$ and reformulate it as

$$\begin{aligned}
&\tilde{M}^{\sigma_{n-1}} \to \tilde{M}^{\sigma_{n-1}} \tilde{\Delta}^{\sigma_n} \qquad\qquad\qquad\qquad\qquad (A7)\\
&= \begin{bmatrix} M_\alpha^{\sigma_{n-1}} & 0 \\ 0 & M_\beta^{\sigma_{n-1}} \end{bmatrix} \begin{bmatrix} \Delta_0^{\sigma_n} & 0 \\ 0 & \Delta_1^{\sigma_n} \end{bmatrix}\\
&= \begin{bmatrix} M_\alpha^{\sigma_{n-1}} \Delta_0^{\sigma_n} & 0 \\ & M_\beta^{\sigma_{n-1}} \Delta_1^{\sigma_n} \end{bmatrix}
\end{aligned}$$

which is still block diagonal, but each block with size $D \times 1$.

The above process is the stack operation for two MPS, and it is easy to extrapolate to the stack operation of n MPS. For simplicity, we assign MPS with the same auxiliary dimension D for each bond. It is not necessary as they can be different. One only needs to change the diagonal block indices from (D, D) to (D_i, D_j).