Schmidt Decomposition of Matrix Product State

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Consider a quantum system which consists of N_s sites, each having a D-dimensional Hilbert space. A translation-invariant matrix product state (MPS) with periodic boundary condition is specified by a set of $\chi \times \chi$ matrices A_i for $i = 1, \dots, D$. Such a state can be expressed as

$$|\psi\rangle = \sum_{i_1,\dots,i_{N_s}} \mathrm{Tr}[A_{i_1} \cdots A_{i_{N_s}}] |i_1 i_2 \cdots i_{N_s}\rangle.$$

Divide the system into two regions p and q, where p contains the sites from 1 to N_p, and q the rest ($N_p + N_q = N_s$). We notate

$$\vec{i}_p = (i_1, \dots, i_{N_p}), \quad \vec{i}_q = (i_{N_p+1}, \dots, i_{N_s}).$$

Now we write

$$|\psi\rangle = Tr[B_{\vec{i}_p} C_{\vec{i}_q}] |\vec{i}_p\rangle \otimes |\vec{i}_q\rangle = |\psi\rangle = (B_{\vec{i}_p})_{\alpha\beta} (C_{\vec{i}_q})_{\beta\alpha} |\vec{i}_p\rangle \otimes |\vec{i}_q\rangle$$

for

$$B_{\vec{i}_p} := A_{i_1} \cdots A_{i_{N_p}}, \quad C_{\vec{i}_q} := A_{i_{N_p+1}} \cdots A_{i_{N_s}}.$$

The density matrix ρ_p is given by $\rho_p = \mathrm{Tr}_q[|\psi\rangle\langle\psi|]$, so

$$(\rho_p)_{\vec{i}_p \vec{j}_p} = \langle \vec{i}_p | \rho_p | \vec{j}_p \rangle = \sum_{\vec{i}_q} (\langle \vec{i}_p | \otimes \langle \vec{i}_q |) |\psi\rangle\langle\psi| (|\vec{j}_p\rangle \otimes |\vec{i}_q\rangle) = (B_{\vec{i}_p})_{\alpha\beta} (B^*_{\vec{j}_p})_{\gamma\delta} \sum_{\vec{i}_q} (C_{\vec{i}_q})_{\beta\alpha} (C^*_{\vec{i}_q})_{\delta\gamma}.$$

The transfer matrix $\mathbb{E}$ is defined as

$$\mathbb{E} := \sum_{i=1}^{D} A_i \otimes A_i^*,$$

so

$$\mathbb{E}_{(\alpha\gamma)(\beta\delta)} = \sum_{i=1}^{D} (A_i)_{\alpha\beta} (A_i^*)_{\gamma\delta}.$$

Hence,

$$\sum_{\vec{i}_q} (C_{\vec{i}_q})_{\beta\alpha} (C^*_{\vec{i}_q})_{\delta\gamma} = (\mathbb{E}^{N_q})_{(\beta\delta)(\alpha\gamma)}.$$

This means that

$$(\rho_p)_{\vec{i}_p \vec{j}_p} = (B_{\vec{i}_p})_{\alpha\beta} (\mathbb{E}^{N_q})^{\mathrm{T}}_{(\alpha\gamma)(\beta\delta)} (B^*_{\vec{j}_p})_{\gamma\delta}.$$

We reformat the matrix indices, where

$$\mathscr{B}_{\vec{i}_p(\alpha\beta)} := (B_{\vec{i}_p})_{\alpha\beta}, \quad \mathscr{Q}_{(\alpha\beta)(\gamma\delta)} := (\mathbb{E}^{N_q})^{\mathrm{T}}_{(\alpha\gamma)(\beta\delta)}.$$

Then

$$(\rho_p)_{\vec{i}_p \vec{j}_p} = \mathscr{B}_{\vec{i}_p(\alpha\beta)} \mathscr{Q}_{(\alpha\beta)(\gamma\delta)} \mathscr{B}^*_{\vec{j}_p(\gamma\delta)} \implies \rho_p = \mathscr{B}\mathscr{Q}\mathscr{B}^\dagger.$$

In terms of nonzero eigenvalues, the multiplication order does not matter, so ρ_p shares the same nonzero eigenvalues with $\mathscr{B}^\dagger \mathscr{B} \mathscr{Q}$. We can figure out the product $\mathscr{B}^\dagger \mathscr{B}$:

$$(\mathscr{B}^\dagger \mathscr{B})_{(\alpha\beta)(\gamma\delta)} = \sum_{\vec{i}_p} \mathscr{B}^*_{\vec{i}_p(\alpha\beta)} \mathscr{B}_{\vec{i}_p(\gamma\delta)} = \sum_{\vec{i}_p} (B^*_{\vec{i}_p})_{\alpha\beta} (B_{\vec{i}_p})_{\gamma\delta} = (\mathbb{E}^{N_p})_{(\gamma\alpha)(\delta\beta)}.$$

Therefore,

$$(\mathscr{B}^\dagger \mathscr{B} \mathscr{Q})_{(\alpha\beta)(\gamma\delta)} = (\mathbb{E}^{N_p})_{(\epsilon\alpha)(\zeta\beta)} (\mathbb{E}^{N_q})_{(\zeta\delta)(\epsilon\gamma)}.$$