# 1 Introduction

$$|\Psi\rangle = \sum_{i_1=1}^{d_1}\sum_{i_2=1}^{d_2}\cdots\sum_{i_N=1}^{d_N}\Psi_{i_1,i_2,\ldots,i_N}\,|i_1\rangle\otimes|i_2\rangle\otimes\cdots\otimes|i_N\rangle \tag{1}$$

$$T \in \mathbb{C}^{\chi_1\times\chi_2\times\cdots\times\chi_n} \tag{2}$$

$$T_{i_1,i_2,\ldots,i_n} \in \mathbb{C}, \quad i_j \in \{1,2,\ldots,\chi_j\} \tag{3}$$

$$c = \sum_{\alpha=1}^{\chi} A_\alpha B_\alpha \tag{4}$$

$$C_{ij} = \sum_{\alpha=1}^{\chi_2} A_{i\alpha}B_{\alpha j} \tag{5}$$

$$\Psi_{i_1,i_2,\cdots,i_N} \coloneqq \sum_{\alpha_1=1}^{\chi_1}\sum_{\alpha_2=1}^{\chi_2}\cdots\sum_{\alpha_{N-1}=1}^{\chi_{N-1}} T^{[1],i_1}_{1,\alpha_1}T^{[2],i_2}_{\alpha_1,\alpha_2}\cdots T^{[N],i_N}_{\alpha_{N-1},1} \tag{6}$$

$$d^N \to N\chi^2 d \tag{7}$$

$$W \in \mathbb{C}^{n\times m},\ n \geq m \tag{8}$$

$$W^\dagger W = \mathbb{1} \tag{9}$$

$$WW^\dagger = \mathbb{P}, \quad \mathbb{P}^2 = \mathbb{P} \tag{10}$$

$$U \in \mathbb{C}^{n\times n} \tag{11}$$

$$U^\dagger U = \mathbb{1} \tag{12}$$

$$UU^\dagger = \mathbb{1} \tag{13}$$

$$\langle\Psi|\hat{O}_n|\Psi\rangle = \tag{14}$$

$$|\Psi(\Delta t)\rangle = \hat{U}\left(\Delta t\right)|\Psi\rangle = e^{-i\Delta t\hat{H}}\,|\Psi\rangle \tag{15}$$

$$\hat{H} = \sum_{j\text{ even}} \hat{h}^{[j,j+1]} + \sum_{j\text{ odd}} \hat{h}^{[j,j+1]} =: \hat{H}_{\text{even}} + \hat{H}_{\text{odd}} \tag{16}$$

$$\hat{U}(\Delta t) = e^{-i\Delta t\left(\hat{H}_{\text{even}}+\hat{H}_{\text{odd}}\right)} = \underbrace{e^{-i\Delta t\hat{H}_{\text{even}}}e^{-i\Delta t\hat{H}_{\text{odd}}}}_{\hat{U}^{\text{TEBD1}}(\Delta t)} + \mathcal{O}\left(\Delta t^2\right) \tag{17}$$

$$e^{-i\Delta t\hat{H}_{\text{even}}} = e^{-i\Delta t\sum_{j\ \text{even}}\hat{h}^{[j,j+1]}} = \prod_{j\ \text{even}} e^{-i\Delta t\hat{h}^{[j,j+1]}} \tag{18}$$

$$\Psi_{i_1,i_2,\cdots,i_N} \coloneqq \mathcal{C}\left(T^{[1],i_1}, T^{[2],i_2}, \ldots, T^{[N],i_N}\right) \tag{19}$$

$$\Lambda^{[n]}B^{[n+1]} \approx A^{[n]}\Lambda[n+1] \tag{20}$$

$$\Lambda^{[n]} \approx A^{[n]}\Lambda \tag{21}$$

$$\|\Lambda^{[n]} - A^{[n]}\Lambda\| \tag{22}$$

$$\hat{H} = \underbrace{\sum_{x=1}^{L_x}\hat{H}_x}_{\text{columns}} + \underbrace{\sum_{y=1}^{L_y}\hat{H}_y}_{\text{rows}} \tag{23}$$

$$\||\Psi\rangle - |\Psi'\rangle\| = \sqrt{\langle\Psi|\Psi\rangle + \langle\Psi'|\Psi'\rangle - 2\langle\Psi'|\Psi\rangle} \tag{24}$$

$$= \sqrt{2 - 2\,\mathrm{Re}\,\langle\Psi'|\Psi\rangle} \tag{25}$$

$$(T'_{\text{opt}}, W'_{1,\text{opt}}, W'_{2,\text{opt}}) = \underset{T,W'_1,W'_2}{\operatorname{argmax}}\,\mathrm{Re}\,\langle\Psi'|\Psi\rangle \tag{26}$$

$$T'^{\dagger}T' = \mathbb{1}, \quad W_1'^{\dagger}W_1' = \mathbb{1}, \quad \|W_2'\|_{\text{F}} = 1 \tag{27}$$

$$f_{\text{trunc}}\left(U,\theta\right) = \sqrt{\sum_{\mu=\chi+1}^{\chi D^2} S_\mu^2} \tag{28}$$

$$f_{\text{Rényi}}\left(U,\theta,\alpha\right) = \frac{1}{1-\alpha}\log\mathrm{Tr}\left(\rho^\alpha\right) = \frac{1}{1-\alpha}\log\left(\sum_{\mu=1}^{\chi D^2} S_\mu^{2\alpha}\right) \tag{29}$$

$$\rho = \mathrm{Tr}_{(j,r)}(|\tilde{\theta}\rangle\langle\tilde{\theta}|) \tag{30}$$

$$\mathrm{Tr}\,\rho^2 \tag{31}$$

$$\mathcal{O}(N_{\text{iter}}D^9) \tag{32}$$

$$\mathcal{O}(N_{\mathrm{iter}} N_{\mathrm{tCG}} D^9) \tag{33}$$

$$\mathcal{O}(D^9) \rightarrow \mathcal{O}(D^8 + N_{\mathrm{svd}}) \tag{34}$$

$$\mathcal{O}(D^9) \rightarrow \mathcal{O}(D^8) \tag{35}$$

$$|\Psi\rangle = \hat{U}^{[i,j]}(\Delta t)\,|\Psi\rangle \tag{36}$$

$$(T'_{i,\mathrm{opt}}, T'_{j,\mathrm{opt}}, W'_{1,\mathrm{opt}}, W'_{2,\mathrm{opt}}, W'_{3,\mathrm{opt}}) = \tag{37}$$

$$\underset{T'_i, T'_j, W'_1, W'_2, W'_3}{\mathrm{argmax}} \quad \mathrm{Re}\,\langle\Psi'|\,\hat{U}^{[i,j]}(\Delta t)\,|\Psi\rangle \tag{38}$$

$$\hat{U}(\Delta t) = \hat{U}^{\mathrm{TEBD1}}(\Delta t) + \mathcal{O}(\Delta t^2) \tag{39}$$

$$\hat{U}(\Delta t) = \hat{U}^{\mathrm{TEBD2}}(\Delta t) + \mathcal{O}(\Delta t^3) \tag{40}$$

$$g \approx 3.04438 \tag{41}$$

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