Hamiltonian quantum dynamics via optimized quantum circuits

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abstract

I. INTRODUCTION

[1, 2], [3]

II. METHOD

Let U denote the reference (ground truth) unitary map we try to approximate, for example a time step Δ governed by a given quantum Hamiltonian H (in units of $\hbar = 1$):

$$U = \mathrm{e}^{-iH\Delta t}. \tag{1}$$

Our goal is to approximate U by a variational quantum circuit. We designate the overall unitary transformation effected by the circuit as V, and quantify the approximation error by the Frobenius norm distance between U and V. Expanding the latter and using that U and V are unitary leads to

$$\begin{aligned} \|V - U\|_{\mathrm{F}}^2 &= \mathrm{Tr}\big[(V-U)^\dagger (V-U)\big] \\ &= 2\,\mathrm{Tr}[I] - 2\,\mathrm{Re}\,\mathrm{Tr}[VU^\dagger], \end{aligned} \tag{2}$$

where I denotes the identity matrix. Minimizing the Frobenius distance is thus equivalent to

$$\max_V \mathrm{Re}\,\mathrm{Tr}[VU^\dagger]. \tag{3}$$

We can re-write Eq. (3) as follows: Let $\{|\psi_j\rangle, \mathrm{e}^{-i\lambda_j}\}$ with $\lambda_j \in \mathbb{R}$ be the spectral decomposition of U, such that

$$U = \sum_j \mathrm{e}^{-i\lambda_j} |\psi_j\rangle \langle\psi_j|. \tag{4}$$

When regarding U as time step matrix, the eigenvalues λ_j are the (energy) eigenvalues of H scaled by Δt. In terms of the spectral decomposition, the target function in Eq. (3) reads

$$\mathrm{Re}\,\mathrm{Tr}[VU^\dagger] = \sum_j \mathrm{Re}\left(\mathrm{e}^{i\lambda_j} \langle\psi_j| V |\psi_j\rangle\right). \tag{5}$$

The states $|\psi_j\rangle$ can thus be interpreted as inputs to the quantum circuit V, as illustrated in Fig. 1.

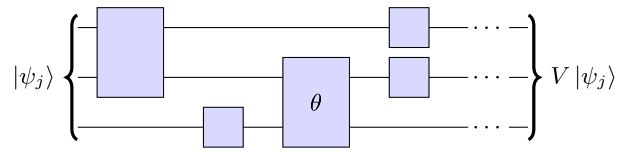

FIG. 1. Schematic excerpt of a parametrized quantum circuit with input state $|\psi_j\rangle$. The blue boxes represent unitary circuit gates, and $\theta \in \mathbb{R}$ is a variational parameter (e.g., the angle of a rotation gate).

The derivative of the target function with respect to a parameter θ is thus

$$\frac{\partial}{\partial\theta} \mathrm{Re}\,\mathrm{Tr}[VU^\dagger] = \sum_j \mathrm{Re}\left(\mathrm{e}^{i\lambda_j} \langle\psi_j| \frac{\partial}{\partial\theta} V |\psi_j\rangle\right). \tag{6}$$

As noted before [4], this expression can be efficiently evaluated (separately for each j) by "backpropagation" through the circuit, analogous to artificial neural networks: one applies the adjoint circuit gates in reverse order to $\mathrm{e}^{i\lambda_j}\langle\psi_j|$ until reaching the gate parametrized by θ.

(Describe light-cone considerations)

Alternative formulation based on spectral filtering?

Projection onto subspace of eigenstates, indexed by $S = \{j_1, j_2, \dots\}$:

$$P = \sum_{j\in S} |\psi_j\rangle \langle\psi_j|. \tag{7}$$

By construction, P commutes with U. Then

$$\begin{aligned} &\|P(V-U)P\|_{\mathrm{F}}^2 \\ &\quad = \|PVP\|_{\mathrm{F}}^2 + \|PUP\|_{\mathrm{F}}^2 - 2\,\mathrm{Re}\,\mathrm{Tr}[VPU^\dagger P]. \end{aligned} \tag{8}$$

Additional term

$$\|PVP\|_{\mathrm{F}}^2 = \mathrm{Tr}\big[PV^\dagger PV\big] = \sum_{j,k\in S} |\langle\psi_k| V |\psi_j\rangle|^2. \tag{9}$$

Similar to Eq. (5),

$$\mathrm{Re}\,\mathrm{Tr}[VPU^\dagger P] = \sum_{j\in S} \mathrm{Re}\left(\mathrm{e}^{i\lambda_j} \langle\psi_j| V |\psi_j\rangle\right). \tag{10}$$

Alternative approaches described in Fig. 2 and Fig. 3.

Translation-invariant MPO Ansatz:

$$W = \mathrm{e}^{-i\theta A\otimes A/2} \cdot (\mathrm{e}^{-i\varphi A/2} \otimes \mathrm{e}^{-i\varphi A/2}) \tag{11}$$

with $A \in \mathbb{C}^{2\times 2}$ a Hermitian, traceless matrix, and parameters $\theta, \varphi \in \mathbb{R}$.

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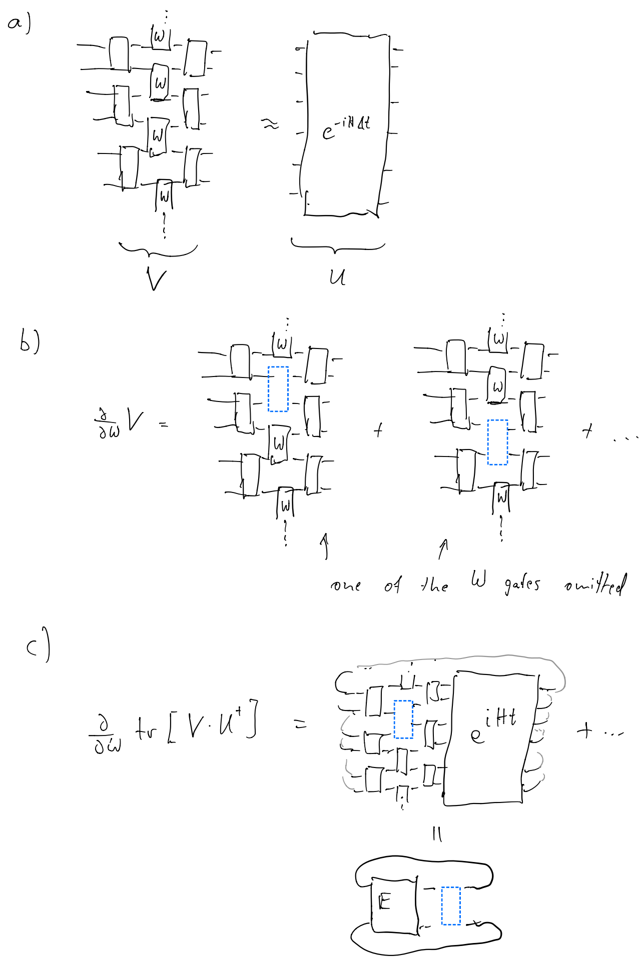

FIG. 2. (a) Approximation of the exact unitary time step $e^{-iH\Delta t}$ by a variational "brickwall" quantum circuit. (b) The gradient with respect to the internal W matrices results from omitting this matrix from the circuit. (c) Inserted into the objective function, the gradient can be represented as contraction with an "environment" tensor E.

III. NUMERICAL SIMULATIONS

(Compare with direct Trotter approximation?)

Compare spectra

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[3] M. Heyl, P. Hauke, and P. Zoller, Quantum localization bounds Trotter errors in digital quantum simulation, Sci. Adv. **5**, eaau8342 (2019).

[4] X.-Z. Luo, J.-G. Liu, P. Zhang, and L. Wang, Yao.jl: Extensible, efficient framework for quantum algorithm design, Quantum **4**, 341 (2020).

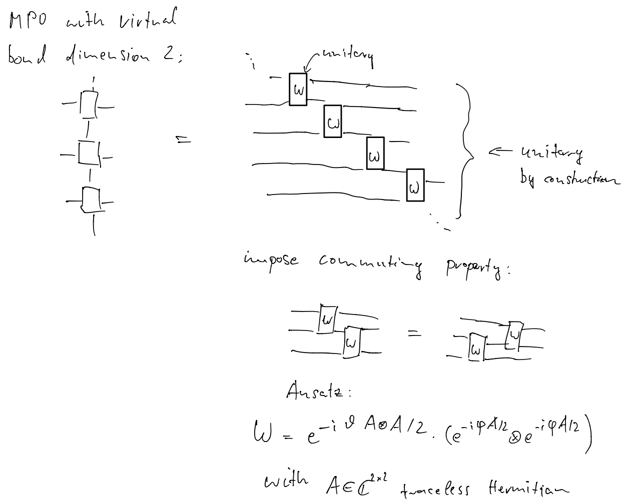

FIG. 3. Matrix product operator (MPO) written as translation invariant quantum circuit. The commuting property ensures symmetry with respect to upwards and downwards direction.