Riemannian quantum circuit optimization based on matrix product operators

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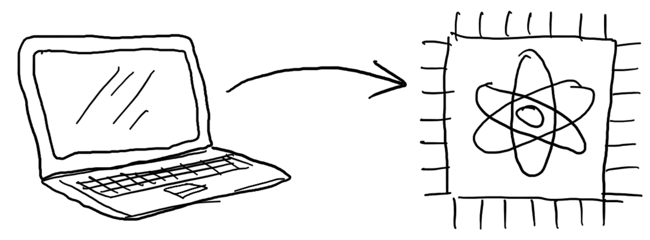
Goal

Classically optimize a quantum circuit to approximate the time evolution for time Δt

Treat problem classically for short Δt



Execute on quantum hardware for $\Delta t \gg 1$

Methods

- Start with a brickwall circuit that implements a Trotter step
- Approximate the reference as a higher-order Trotterization and express it as a **matrix product operator (MPO)**
- Evaluate cost function and gradient using **tensor network methods**
- Use **Riemannian optimization** to incorporate the unitary constraint of the quantum gates

Results

Spin chains

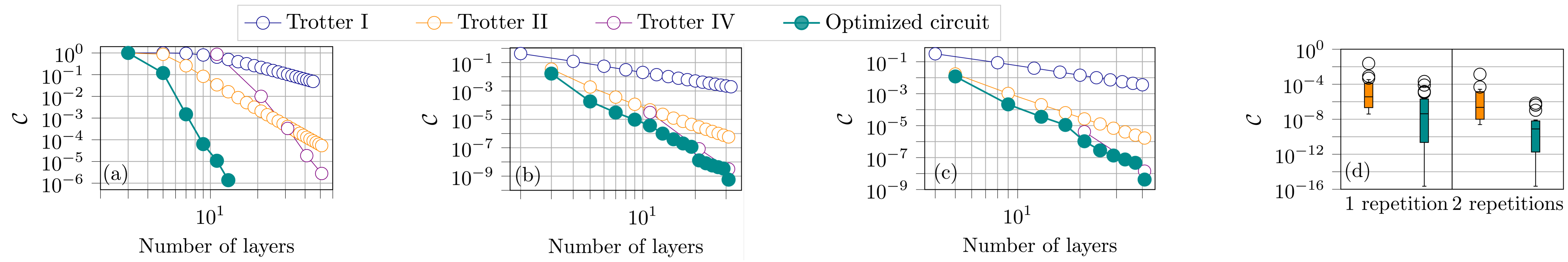
a) Transverse-field Ising model (50 sites, *J=1, g=0.75, h=0.6, t=2*): up to 4 orders of magnitude improvement

b) Heisenberg model (50 sites, *J=(1,1,-1/2), h=(3/4,0,0), t=0.25*): up to 1 order of magnitude improvement

Fermionic systems

c) Spinful Fermi-Hubbard chain (50 qubits, *T=1, V=4, t=0.3*): up to a factor of 6 improvement

d) Molecular Hamiltonian (LiH, 6 orbitals, diagonal interaction): up to 8 orders of magnitude improvement



By combining **Riemannian optimization** and **tensor network** methods, we improve the accuracy of Trotter circuits up to **four orders of magnitude**.

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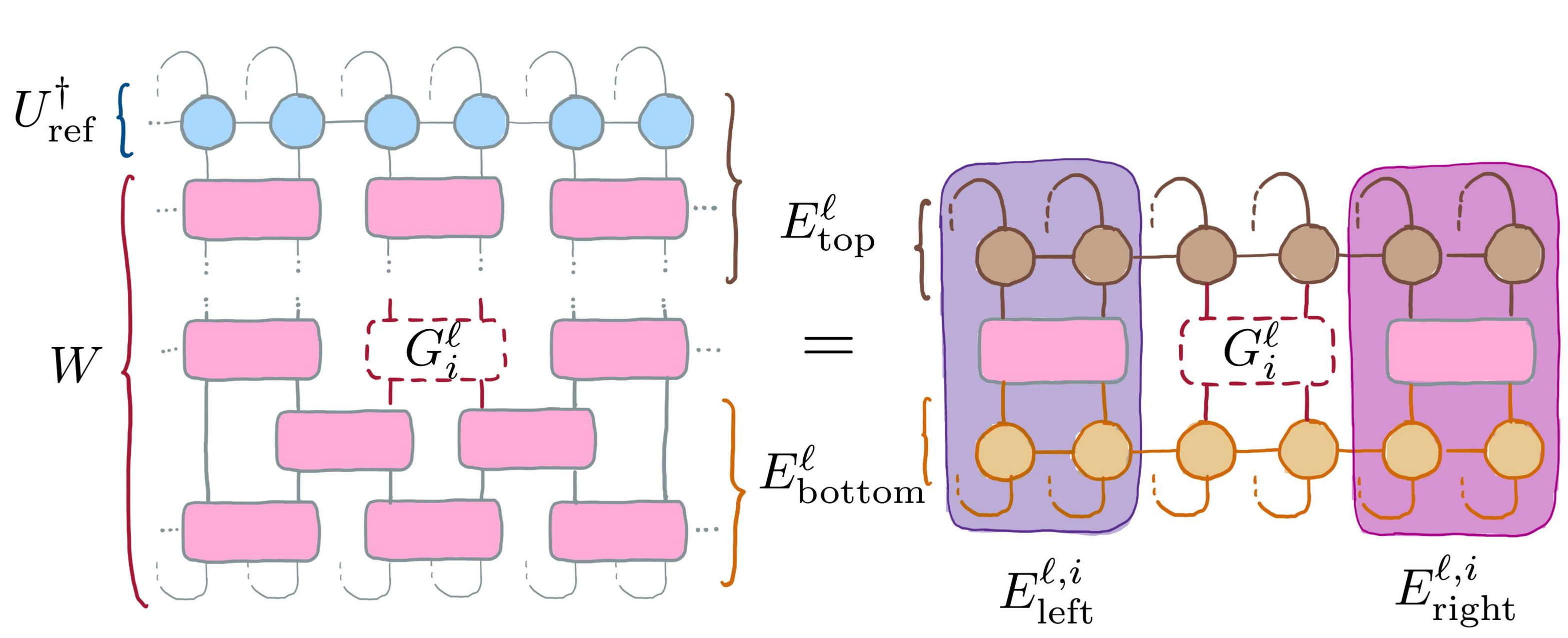
Optimization problem

- Optimization statement: $G_{\text{opt}} = \underset{G \in \mathcal{U}(4)^{\times N}}{\arg\min}\, \mathcal{C}(U_{\text{ref}}, W)$
- Cost function: Hilbert-Schmidt test

$$\mathcal{C}(U_{\text{ref}}, W) = 1 - \frac{1}{d^2}\left|\operatorname{Tr}(U_{\text{ref}}^{\dagger} W)\right|^2$$

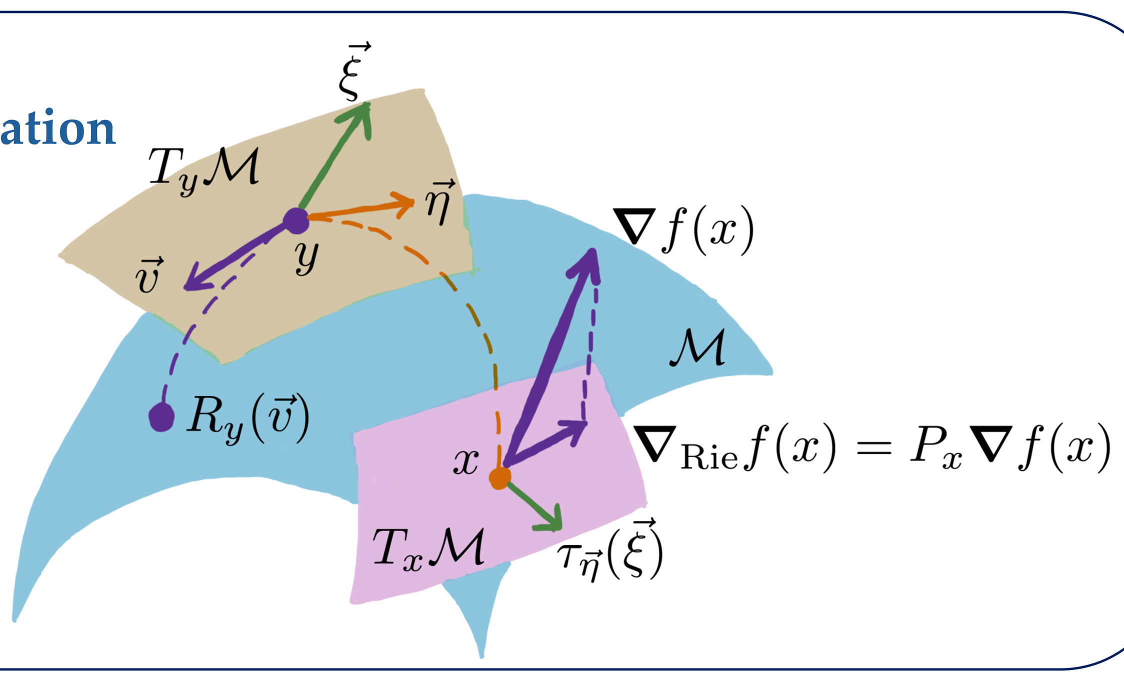
- Evaluation of $\partial_{G_\ell} \operatorname{Tr}(U_{\text{ref}}^{\dagger} W)$ using tensor networks



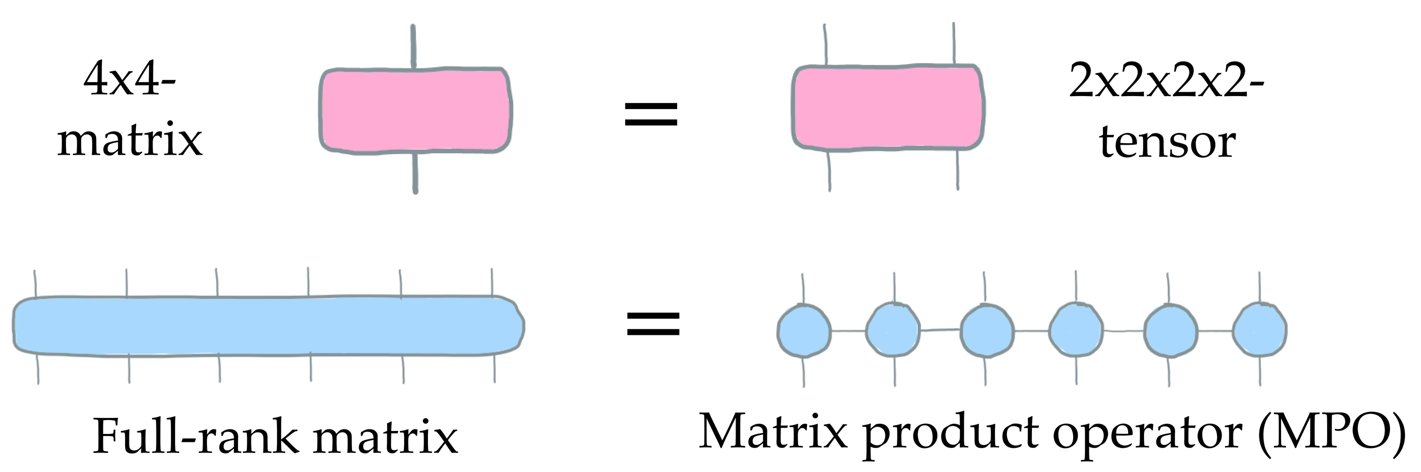
Riemannian optimization

Optimization on the manifold of unitary 4x4-matrices

Modified version of ADAM



Tensor network methods



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