Aspects of quantum simulation of the Fermi-Hubbard model
(arXiv:2212.07556 and arXiv:2306.10603)

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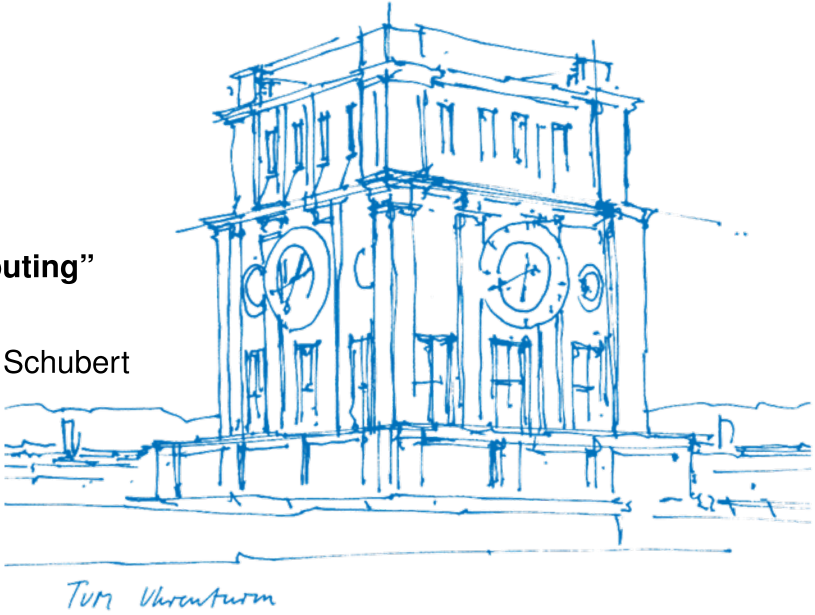
October 3, 2023

IPAM Workshop
”Mathematical and Computational Challenges in Quantum Computing”

joint work with Ayse Kotil, Rahul Banerjee, Qunsheng Huang, Ansgar Schubert



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Open Day and "Maustag" at Max Planck Institute of Quantum Optics

03 October 2023 - 10:00

Public

On 3 October, the Max Planck Institute of Quantum Optics (MPQ), Munich Center for

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creating quantum computers atom by atom

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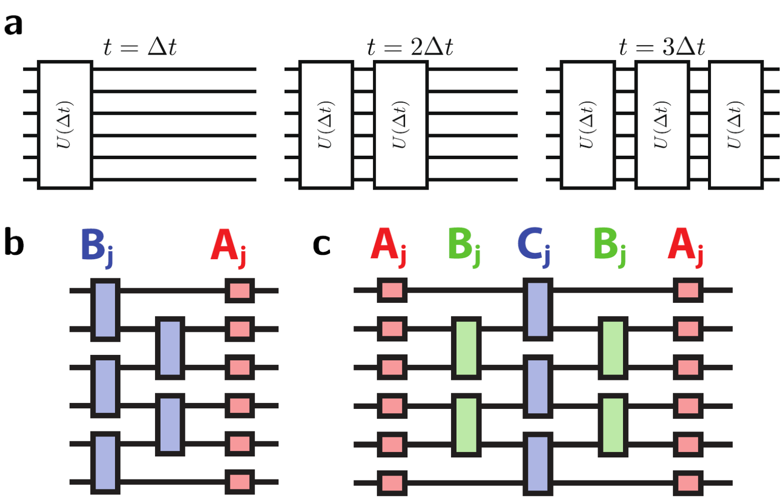
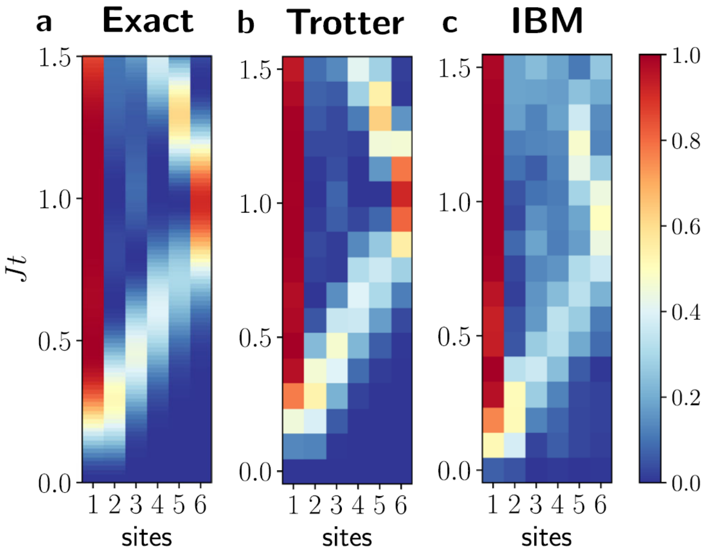
Motivation: Quantum simulation

Goal: realize time evolution operator e^{-iHt} of target Hamiltonian H





Smith, Kim, Pollmann, Knolle. “Simulating quantum many-body dynamics on a current digital quantum computer”. npj Quantum Information 5, 106 (2019)
B. Chiaro et al. “Growth and preservation of entanglement in a many-body localized system”. arXiv:1910.06024

Trotter error with commutator scaling for the Fermi-Hubbard model

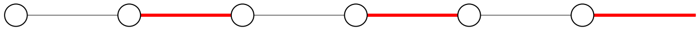
(arXiv:2306.10603)

Lie-Trotter product formulas

Example: even-odd partitioning of a Hamiltonian H:

$$H = A + B, \quad A = H_{\text{even}}, \quad B = H_{\text{odd}}$$

(a) “even” hopping terms A



(b) “odd” hopping terms B

Lie-Trotter:

$$\mathcal{S}_1(t) = e^{-itB} e^{-itA} \quad \rightsquigarrow \quad e^{-itH} = \mathcal{S}_1(t) + \mathcal{O}(t^2)$$

Strang (second-order Suzuki):

$$\mathcal{S}_2(t) = e^{-i\frac{t}{2}A} e^{-itB} e^{-i\frac{t}{2}A} \quad \rightsquigarrow \quad e^{-itH} = \mathcal{S}_2(t) + \mathcal{O}(t^3)$$

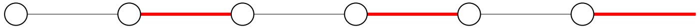
Higher-order generalizations possible

Lie-Trotter product formulas

Example: even-odd partitioning of a Hamiltonian H:

$$H = A + B, \quad A = H_{\text{even}}, \quad B = H_{\text{odd}}$$

(a) “even” hopping terms A



(b) “odd” hopping terms B

Lie-Trotter:

$$\mathcal{S}_1(t) = \mathrm{e}^{-itB}\,\mathrm{e}^{-itA} \quad \rightsquigarrow \quad \mathrm{e}^{-itH} = \mathcal{S}_1(t) + \mathcal{O}(t^2)$$

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Higher-order generalizations possible

Appearance of commutators:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\,t}\mathcal{S}_1(t) &= -iB\,\mathcal{S}_1(t) + \mathrm{e}^{-itB}(-iA)\,\mathrm{e}^{-itA}\\ &= -i(A+B)\,\mathcal{S}_1(t) + [\mathrm{e}^{-itB}, -iA]\,\mathrm{e}^{-itA}\\ &= -iH\,\mathcal{S}_1(t) + [\mathrm{e}^{-itB}, -iA]\,\mathrm{e}^{-itA}\end{aligned}$$

$\rightsquigarrow$ variation-of-parameters formula:

$$\mathcal{S}_1(t) = \mathrm{e}^{-itH} + \int_0^t \mathrm{d}\,\tau\,\mathrm{e}^{-i(t-\tau)H}\,[\mathrm{e}^{-itB}, -iA]\,\mathrm{e}^{-i\tau A}$$

Resolve matrix exponential inside commutator:

$$\begin{aligned}[\mathrm{e}^{tX}, Y] &= \mathrm{e}^{tX}\int_0^t \mathrm{d}\,\tau\,\mathrm{e}^{-\tau X}[X, Y]\,\mathrm{e}^{\tau X}\\ &= \int_0^t \mathrm{d}\,\tau\,\mathrm{e}^{\tau X}[X, Y]\,\mathrm{e}^{-\tau X}\,\mathrm{e}^{tX}\end{aligned}$$

A. M. Childs et al. “Theory of Trotter error with commutator scaling”. Phys. Rev. X 11, 011020 (2021)

Higher-order error bounds with small prefactors

Theorem (Higher-order error bounds with small prefactors, arXiv:2306.10603)

Let $\mathcal{S}_p$ be a product formula of order p in the representation $\mathcal{S}_p(t) = \mathrm{e}^{-itA_K} \cdots \mathrm{e}^{-itA_1}$, and let $s \in \{1, \dots, K\}$. Then

$$\left\|\mathcal{S}_p(t) - \mathrm{e}^{-itH}\right\| \leq \frac{t^{p+1}}{(p+1)!}\left(\sum_{j=2}^{s} \sum_{\substack{q_j+\cdots+q_s=p \\ q_j\neq 0}} \binom{p}{q_j, \dots, q_s} \left\|\mathrm{ad}_{A_s}^{q_s} \cdots \mathrm{ad}_{A_j}^{q_j} B_j\right\| + \sum_{j=s+1}^{K} \sum_{\substack{q_{s+1}+\dots \\ +q_j=p \\ q_j\neq 0}} \binom{p}{q_{s+1}, \dots, q_j} \left\|\mathrm{ad}_{A_{s+1}}^{q_{s+1}} \cdots \mathrm{ad}_{A_j}^{q_j} B_j\right\|\right)$$

with

$$B_j = \sum_{\ell=1}^{j-1} A_\ell, \quad j = 2, \dots, K.$$

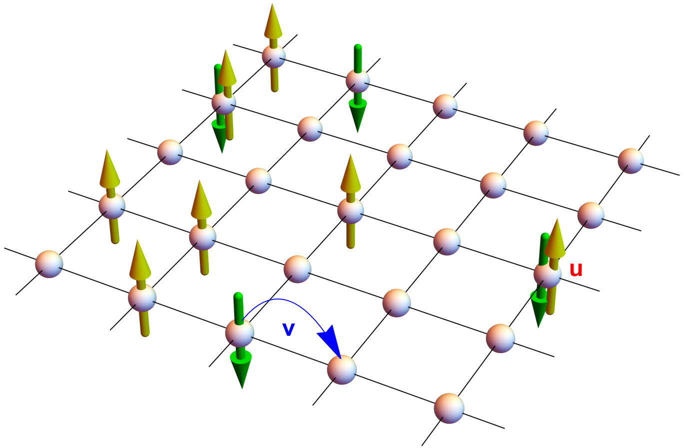
Note: $\mathrm{ad}_A B = [A, B]$ denoting the *adjoint action*, and ad_A^q its q-fold application, e.g., $\mathrm{ad}_A^3 B = [A, [A, [A, B]]]$

Generalizes Childs et al. (2021), Appendix M

A. Schubert, C. B. Mendl "Trotter error with commutator scaling for the Fermi-Hubbard model". arXiv:2306.10603 (2023)
A. M. Childs et al. "Theory of Trotter error with commutator scaling". Phys. Rev. X 11, 011020 (2021)

Fermi-Hubbard model

$$H_{\mathrm{FH}} = v \sum_{\langle i,j \rangle,\sigma} \left(a^{\dagger}_{i\sigma} a_{j\sigma} + a^{\dagger}_{j\sigma} a_{i\sigma} \right) + u \sum_{i \in \Lambda} n_{i\uparrow} n_{i\downarrow}$$



hopping term: $h_{ij\sigma} = a^{\dagger}_{i\sigma} a_{j\sigma} + a^{\dagger}_{j\sigma} a_{i\sigma}$, number operator: $n_{i\sigma} = a^{\dagger}_{i\sigma} a_{i\sigma}$, signed hopping term: $\tilde{h}_{ij\sigma} = a^{\dagger}_{i\sigma} a_{j\sigma} - a^{\dagger}_{j\sigma} a_{i\sigma}$

Fermi-Hubbard model on a one-dimensional lattice

Lattice $\Lambda = \mathbb{Z}_{/L}$ with L even and $\Lambda' = (2\mathbb{Z})_{/L}$; $H_{\text{FH}} = H_1 + H_2 + H_3$ with

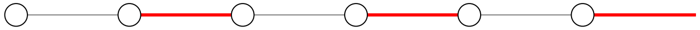
$$H_1 = v \sum_{i \in \Lambda'} \sum_{\sigma \in \{\uparrow,\downarrow\}} h_{i,i+1,\sigma},$$

$$H_2 = v \sum_{i \in \Lambda'} \sum_{\sigma \in \{\uparrow,\downarrow\}} h_{i-1,i,\sigma},$$

$$H_3 = u \sum_{i \in \Lambda'} \left(n_{i,\uparrow} n_{i,\downarrow} + n_{i+1,\uparrow} n_{i+1,\downarrow} \right).$$

Each H_γ is translation invariant with respect to Λ', i.e., by a shift of two sites.

(a) hopping terms in H_1



(b) hopping terms in H_2

(c) interaction terms in H_3

Evaluating commutators

Commutators of elementary operators:
Number operators always commute: for all lattice sites $i, j \in \Lambda$ and $\sigma, \tau \in \{\uparrow, \downarrow\}$,

$$[n_{i\sigma}, n_{j\tau}] = 0.$$

For $i, j, k \in \Lambda$ with $i \neq j$ and $j \neq k$ and $\sigma \in \{\uparrow, \downarrow\}$,

$$[h_{ij\sigma}, h_{jk\sigma}] = \tilde{h}_{ik\sigma},$$
$$[\tilde{h}_{ij\sigma}, \tilde{h}_{jk\sigma}] = \tilde{h}_{ik\sigma},$$
$$[h_{ij\sigma}, \tilde{h}_{jk\sigma}] = \begin{cases} 2\left(n_{i\sigma} - n_{j\sigma}\right), & i = k \\ h_{ik\sigma}, & i \neq k \end{cases}$$

as well as, for $i \neq j$,

$$[h_{ij\sigma}, n_{j\sigma}] = \tilde{h}_{ij\sigma},$$
$$[\tilde{h}_{ij\sigma}, n_{j\sigma}] = h_{ij\sigma}$$

Evaluating commutators

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$$[h_{ij\sigma}, h_{jk\sigma}] = \tilde{h}_{ik\sigma},$$
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$$[\tilde{h}_{ij\sigma}, n_{j\sigma}] = h_{ij\sigma}$$

https://github.com/qc-tum/fermi_hubbard_commutators

General commutator relations:

$$[A, B_1 + \dots + B_n] = [A, B_1] + \dots + [A, B_n]$$

and

$$\begin{aligned}[A, B_1 \cdots B_n] = [A, B_1]B_2 \cdots B_n \\ + B_1[A, B_2]B_3 \cdots B_n + \dots \\ + B_1 \cdots B_{n-1}[A, B_n]\end{aligned}$$

$\rightsquigarrow$ commutators can be expressed solely in terms of sums and products of $h_{ij\sigma}$, $\tilde{h}_{ij\sigma}$ and $n_{i\sigma}$

Sublattice Λ' translations:

$$\left[\sum_{i\in\Lambda'} A_i, \sum_{k\in\Lambda'} B_k\right] = \sum_{i\in\Lambda'} \left[A_i, \sum_{\ell\in\Lambda'} B_{i+\ell}\right]$$

Fermi-Hubbard model on a one-dimensional lattice (cont.)

Nested commutators (example):

$$[H_1,[H_2,H_1]] = 2v^3 \sum_{i\in\Lambda'} \sum_{\sigma\in\{\uparrow,\downarrow\}} \left(h_{i-2,i+1,\sigma} - h_{i-1,i,\sigma}\right),$$

$$[H_2,[H_3,H_1]] = v^2 u \sum_{i\in\Lambda'} \sum_{\sigma\in\{\uparrow,\downarrow\}} \Big(\left(h_{i-1,i+1,\sigma} - h_{i,i+2,\sigma}\right) \cdot \left(n_{i,\bar\sigma} - n_{i+1,\bar\sigma}\right) + \tilde h_{i-1,i,\sigma} \cdot \tilde h_{i,i+1,\bar\sigma} + \tilde h_{i,i+1,\sigma} \cdot \tilde h_{i+1,i+2,\bar\sigma} \Big),$$

Upper bound on the spectral norm *per lattice site*:

$$\frac{1}{|\Lambda|} \|[H_1,[H_2,H_1]]\| \le |v|^3 \sum_{\sigma\in\{\uparrow,\downarrow\}} \left\| h_{-2,1,\sigma} - h_{-1,0,\sigma} \right\| = 4|v|^3$$

Final error bound for Strang splitting:

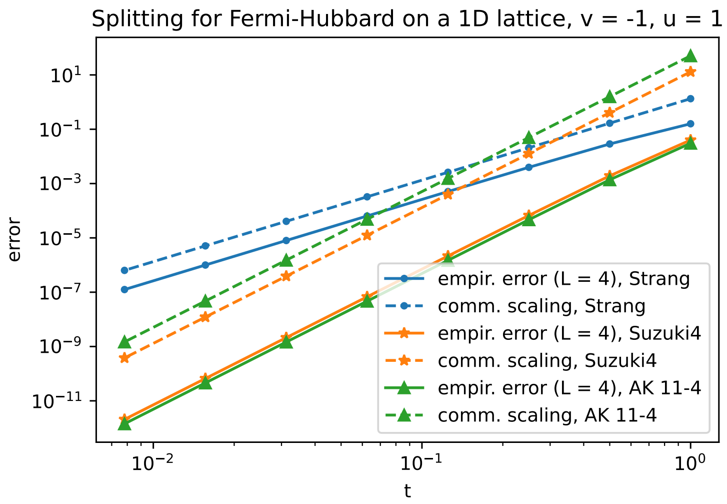
$$\frac{1}{|\Lambda|} \left\| \mathcal{S}_2(t) - e^{-itH_{\mathrm{FH}}} \right\| \le \frac{t^3}{6} \left(3|v|^3 + 4|v|^2|u| + |v||u|^2 \right)$$

Fermi-Hubbard model on a one-dimensional lattice (cont.)

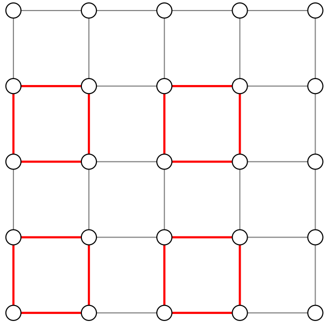
Final error bound for fourth-order Suzuki method:

$$\frac{1}{|\Lambda|}\left\|\mathcal{S}_4(t) - e^{-itH_{\text{FH}}}\right\| \leq t^5\big(1.3405|v|^5 + 8.8233|v|^4|u| + 2.3945|v|^3|u|^2 + 0.4137|v|^2|u|^3 + 0.06001|v||u|^4\big)$$

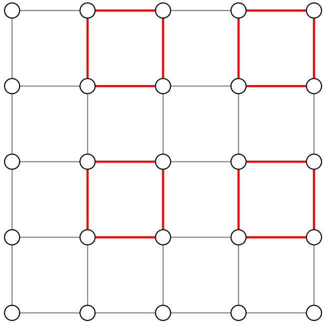
Comparison with empirical error:



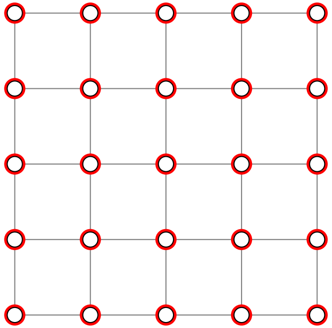
Fermi-Hubbard model on a two-dimensional square lattice



(a) hopping terms in H_1



(b) hopping terms in H_2



(c) interaction terms in H_3

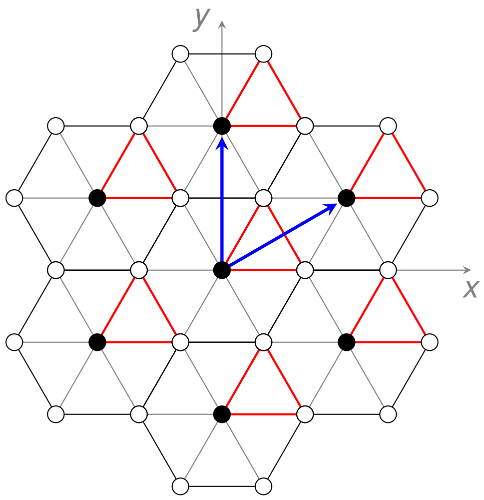
For Strang splitting:

$$\frac{1}{|\Lambda|}\left\|\mathcal{S}_2(t) - \mathrm{e}^{-itH_{\mathrm{FH}}}\right\| \leq \frac{t^3}{6}\left(4.4142|v|^3 + 8.0889|v|^2|u| + 1.3062|v||u|^2\right)$$

For fourth-order Suzuki formula:

$$\frac{1}{|\Lambda|}\left\|\mathcal{S}_4(t) - \mathrm{e}^{-itH_{\mathrm{FH}}}\right\| \leq t^5\big(2.1485|v|^5 + 92.1642|v|^4|u| + 14.3445|v|^3|u|^2 + 1.0712|v|^2|u|^3 + 0.07938|v||u|^4\big)$$

Fermi-Hubbard model on a triangular lattice



For Strang splitting:

$$\frac{1}{|\Lambda|}\left\|\mathcal{S}_2(t) - e^{-itH_{\mathrm{FH}}}\right\| \leq \frac{t^3}{6}\left(39.4721|v|^3 + 20.1594|v|^2|u| + 1.9546|v||u|^2\right)$$

For fourth-order Suzuki formula:

$$\frac{1}{|\Lambda|}\left\|\mathcal{S}_4(t) - e^{-itH_{\mathrm{FH}}}\right\| \leq t^5\big(124.815|v|^5 + 493.917|v|^4|u| + 60.4106|v|^3|u|^2 + 2.9855|v|^2|u|^3 + 0.1206|v||u|^4\big)$$

A. Schubert, C. B. Mendl “Trotter error with commutator scaling for the Fermi-Hubbard model”. arXiv:2306.10603 (2023)

Riemannian quantum circuit optimization for Hamiltonian simulation

(arXiv:2212.07556)

Ansatz brick wall circuit

Goal: approximate time evolution operator

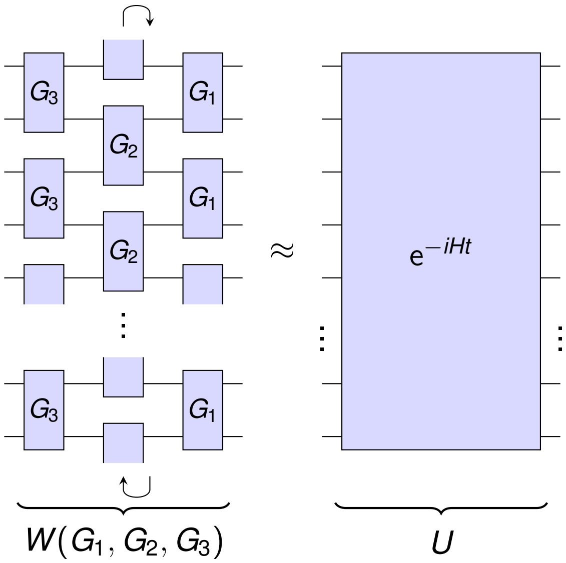
$$U = \mathrm{e}^{-iHt}$$

Optimize gates in brick wall Ansatz circuit, assuming translation invariance:

$$G_{\mathrm{opt}} = \underset{G \in \mathcal{U}(m)^{\times n}}{\operatorname{argmin}} \|W(G) - U\|_{\mathrm{F}}^2$$

with $\mathcal{U}(m)$: unitary $m \times m$ matrices

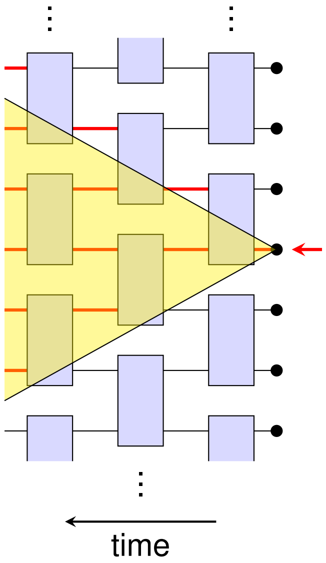
Circuit topology inherited from Trotter splitting



A. Kotil, R. Banerjee, Q. Huang, C. B. Mendl. "Riemannian quantum circuit optimization for Hamiltonian simulation". arXiv:2212.07556 (2022)

Light cone considerations

For translation invariant systems, only need to optimize up to system sizes L containing the causal light cone of physical correlations (Lieb-Robinson bounds)



M. Heyl, P. Hauke, P. Zoller. “Quantum localization bounds Trotter errors in digital quantum simulation”. Sci. Adv. 5, eaau8342 (2019)
J. Haah et al.. “Quantum algorithm for simulating real time evolution of lattice Hamiltonians”. SIAM J. Comput. FOCS18, 250–284 (2021)
R. Mansuroglu et al. “Variational Hamiltonian simulation for translational invariant systems via classical pre-processing”. Quantum Sci. Technol. 8 (2023)
A. Kotil, R. Banerjee, Q. Huang, C. B. Mendl. “Riemannian quantum circuit optimization for Hamiltonian simulation”. arXiv:2212.07556 (2022)

Target function

Goal:

$$G_{\text{opt}} = \underset{G \in \mathcal{U}(m)^{\times n}}{\operatorname{argmin}} \|W(G) - U\|_{\mathrm{F}}^2$$

with $U = \mathrm{e}^{-iHt}$ and brick wall circuit $W(G)$
⇝ equivalent to minimizing

$$f : \mathcal{U}(m)^{\times n} \to \mathbb{R}, \quad f(G) = -\operatorname{Re} \operatorname{Tr}[U^\dagger W(G)]$$

with $\mathcal{U}(m)$: manifold of unitary $m \times m$ matrices

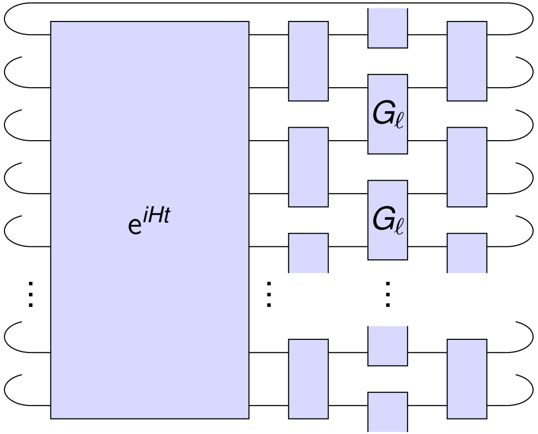
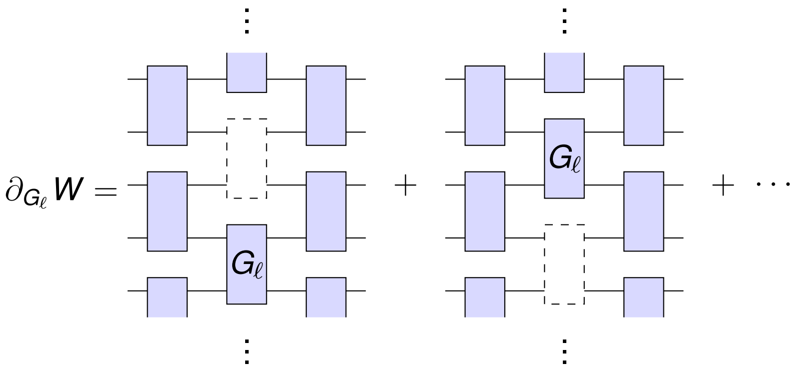


Figure: Tensor diagram representation of $\operatorname{Tr}[U^\dagger W(G)]$.

A. Kotil, R. Banerjee, Q. Huang, C. B. Mendl. "Riemannian quantum circuit optimization for Hamiltonian simulation". arXiv:2212.07556 (2022)

Gradient computation on manifold of unitary matrices

Derivative of W with respect to G_ℓ:



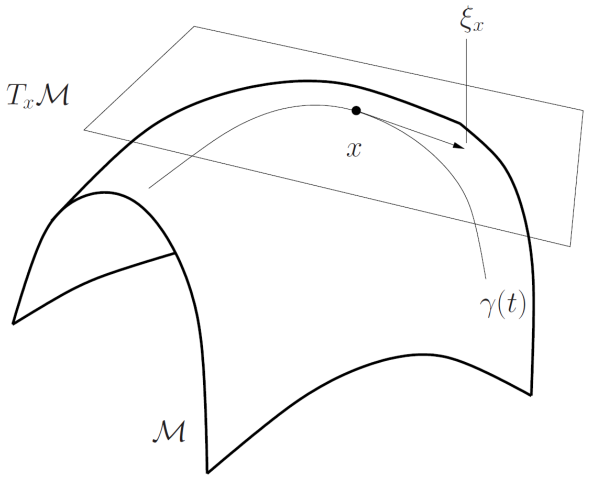


Figure: Source: Absil (2008)

Projecting gradient vectors onto unitary tangent space:

$$\operatorname{grad} f(V) = P_V \operatorname{grad} \bar{f}(V)$$

with $P_V X = V \operatorname{skew}(V^\dagger X)$ and $\operatorname{skew}(A) = \frac{1}{2}(A - A^\dagger)$
Second derivative (gradient as vector field):

$$\nabla_X \xi = P_V(D\xi(V)[X])$$

P.-A. Absil, R. Mahony, R. Sepulchre. “Optimization Algorithms on Matrix Manifolds”. Princeton University Press (2008)

Riemannian trust-region algorithm

Riemannian trust-region algorithm based on quadratic approximation:

$$\hat{m}_G(X) = f(G) + \langle \operatorname{grad} f(G), X \rangle + \frac{1}{2} \langle \operatorname{Hess} f(G)[X], X \rangle$$

for $X \in T_G \mathcal{U}^{\times n}$, with the Riemannian Hessian

$$\operatorname{Hess} f(G)[X] = \nabla_X \operatorname{grad} f(G)$$

Retraction on $\mathcal{U}$: polar decomposition ($V \in \mathcal{U}$):

$$R : T\mathcal{U} \to \mathcal{U}, \quad R_V(\xi) = q_{\text{polar}}(V + \xi),$$

with $q_{\text{polar}}(A)$: unitary matrix from polar decomposition of A

https://github.com/qc-tum/rqcopt

Algorithm 10 Riemannian trust-region (RTR) meta-algorithm

Require: Riemannian manifold $(\mathcal{M}, g)$; scalar field f on $\mathcal{M}$; retraction R from $T\mathcal{M}$ to $\mathcal{M}$ as in Definition 4.1.1.
Parameters: $\bar{\Delta} > 0$, $\Delta_0 \in (0, \bar{\Delta})$, and $\rho' \in [0, \frac{1}{4})$.
Input: Initial iterate $x_0 \in \mathcal{M}$.
Output: Sequence of iterates $\{x_k\}$.

```
for k = 0, 1, 2, ... do
    Obtain η_k by (approximately) solving (7.6);
    Evaluate ρ_k from (7.7);
    if ρ_k < 1/4 then
        Δ_{k+1} = 1/4 Δ_k;
    else if ρ_k > 3/4 and ||η_k|| = Δ_k then
        Δ_{k+1} = min(2Δ_k, Δ̄);
    else
        Δ_{k+1} = Δ_k;
    end if
    if ρ_k > ρ' then
        x_{k+1} = R_x η_k;
    else
        x_{k+1} = x_k;
    end if
end for
```

T. Steihaug. "The conjugate gradient method and trust regions in large scale optimization". SIAM J. Numer. Anal. 20, 626–637 (1983)

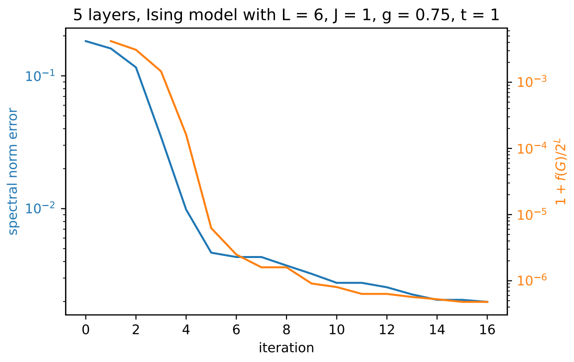
P.-A. Absil, R. Mahony, R. Sepulchre. "Optimization Algorithms on Matrix Manifolds". Princeton University Press (2008)

Optimization results and comparison with Trotter splitting

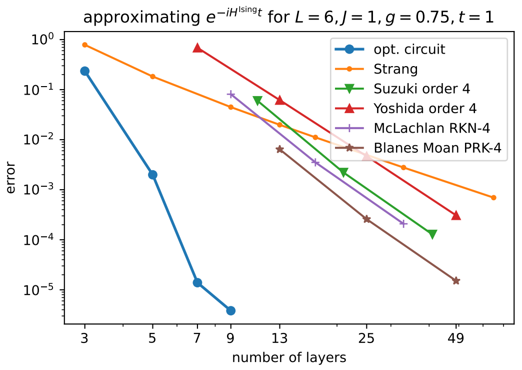
Transverse-field Ising model Hamiltonian on 1D lattice $\mathbb{Z}_{/(L)}$ and periodic boundary conditions:

$$H^{\text{Ising}} = \sum_{j=0}^{L-1} \left(J Z_j Z_{j+1} + g X_j \right)$$

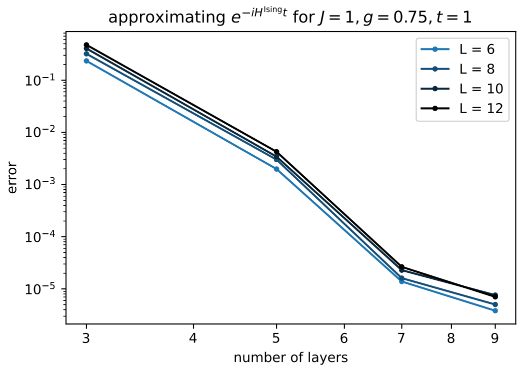
(here $J = 1$, $g = 0.75$, time step $t = 1$, optimization for system size $L = 6$)



(a) Progress of Riemannian trust-region iteration



(b) Approximation error and comparison with Trotter



(c) Extrapolation to larger systems

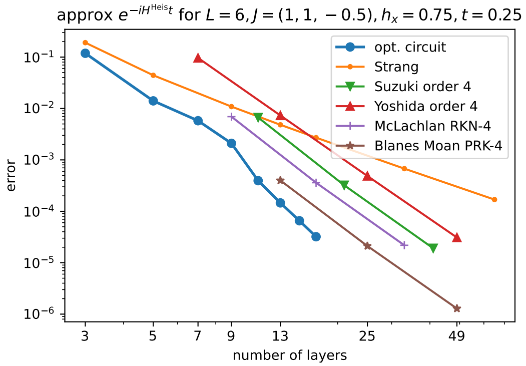
A. Kotil, R. Banerjee, Q. Huang, C. B. Mendl. “Riemannian quantum circuit optimization for Hamiltonian simulation”. arXiv:2212.07556 (2022)

Optimization results and comparison with Trotter splitting

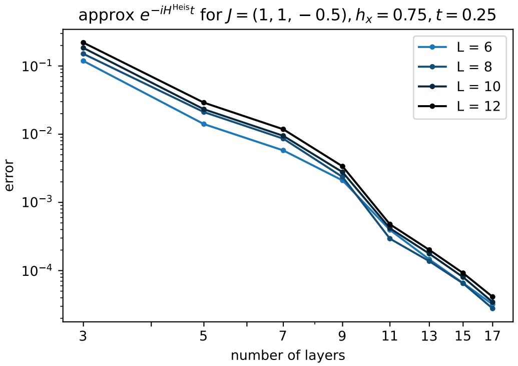
Heisenberg-type Hamiltonian on 1D lattice $\mathbb{Z}_{/(L)}$ and periodic boundary conditions:

$$H^{\text{Heis}} = \sum_{j=0}^{L-1} \sum_{\alpha=1,2,3} \left(J_\alpha \sigma_j^\alpha \sigma_{j+1}^\alpha + h_\alpha \sigma_j^\alpha\right)$$

(here $\vec{J} = (1, 1, -\frac{1}{2})$, $\vec{h} = (\frac{3}{4}, 0, 0)$, time step $t = \frac{1}{4}$, optimization for system size $L = 6$)



(d) Approximation error and comparison with Trotter

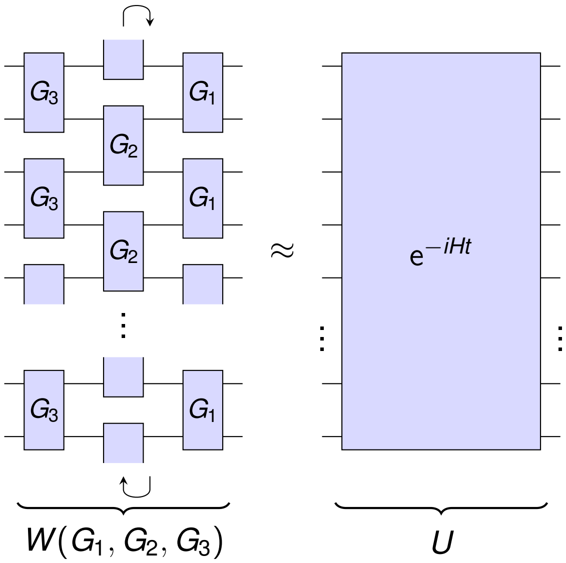


(e) Extrapolation to larger systems

A. Kotil, R. Banerjee, Q. Huang, C. B. Mendl. "Riemannian quantum circuit optimization for Hamiltonian simulation". arXiv:2212.07556 (2022)

Conclusions and outlook

- Application to Fermi-Hubbard model
  ⇝ B.Sc. thesis by Peter Ridilla
- Implementation for HPC: caching, . . .
  ⇝ M.Sc. thesis by Fabian Putterer
- Run optimizations for 2D lattice geometries
- Generalization to non-unitary target matrices, block-encoding, . . .



https://github.com/qc-tum/rqcopt

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