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Exploring High-Order Product Formulas for Real-Time Evolution

Marko Maležič, Johann Ostmeyer

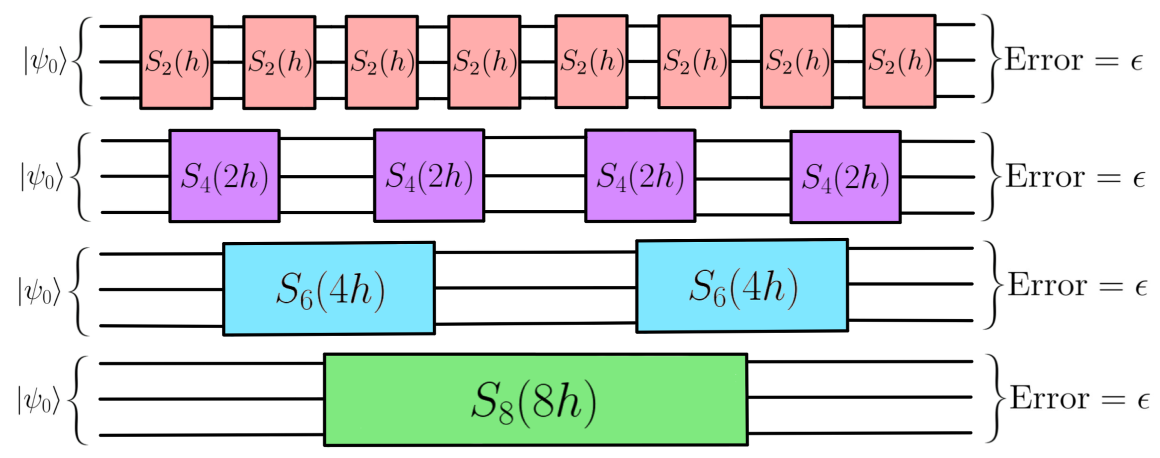
Helmholtz-Institut für Strahlen und Kernphysik, University of Bonn

Introduction and Motivation

Accurate long-time quantum simulations are challenging in complex systems. Errors accumulate with simulation time in both classical and quantum hardware. The errors are in part due to time discretizations using Trotter–Suzuki schemes. While quantum computers still suffer problems like decoherence and gate depth limitations, improving the efficiency of Trotterizations could help reduce the accumulated error (M. Maležič and J. Ostmeyer [1]).

[1]: 2601.18756

Efficiency: Same error, fewer gates

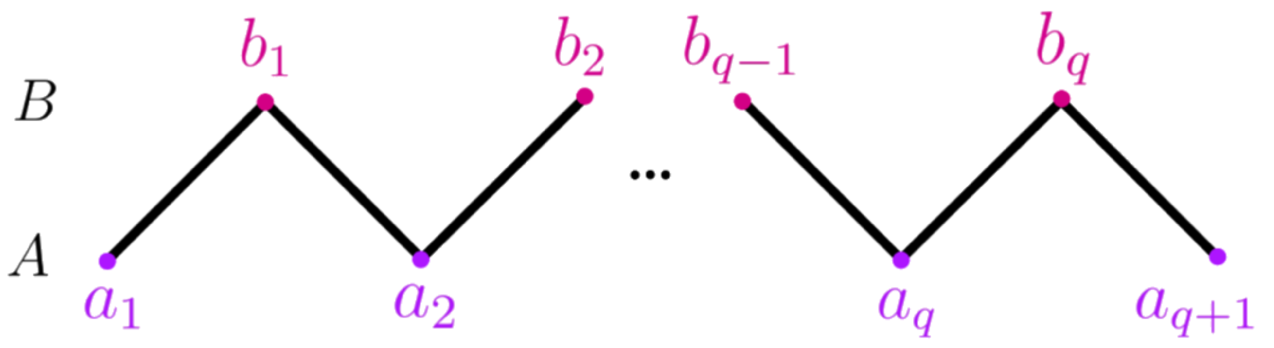


Trotter-Suzuki decompositions

- The time evolution operator $U(t) = e^{iHt}$ solves the Schrödinger equation by evolving an initial state to some time t: $|\psi(t)\rangle = U(t)|\psi(0)\rangle$.
- In absence of analytic solutions for large complex systems, scalability is exchanged for discretization error using Trotterizations: $U(t) \approx [S_n(h)]^{t/h}$.
- Construction of high order schemes from scratch (Omelyan [2]):
$$e^{a_1 Ah} e^{b_1 Bh} \cdots e^{b_q Bh} e^{a_{q+1} Ah} = e^{(A+B)h + O_1 h + O_3 h^3 + O_5 h^5},$$
where we assume symmetric parameters ($a_1 = a_{q+1}$, $b_1 = b_q$).

[2]: Omelyan et al. (2002)

- Schemes are characterized by the number of cycles q (Leapfrog has 1 cycle).



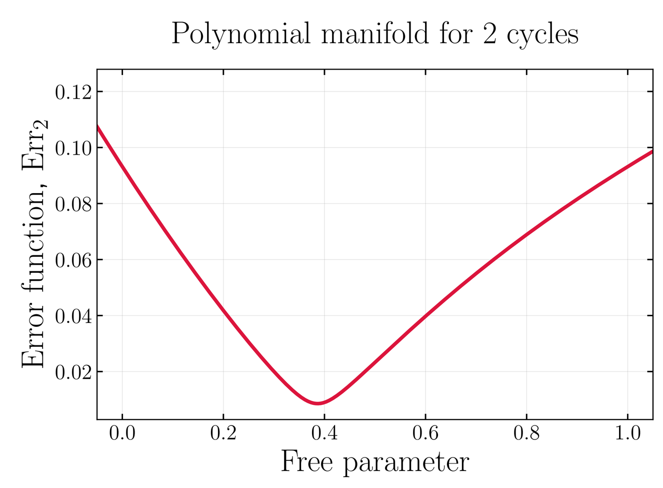
- Order operators: $O_1 = (\nu - 1)A + (\sigma - 1)B$, $O_3 = \alpha C_1 + \beta C_2$, $O_5 = \sum_{k=1}^{6} \gamma_k D_k$
- A scheme is valid if, $\nu = \sigma = 1$, which is guaranteed by: $\sum_i a_i = \sum_i b_i = 1$.
- Order $n = 4$ is satisfied by the constraints: $\alpha(a_i, b_i) = \beta(a_i, b_i) = 0$, while order $n = 6$ is satisfied by: $\gamma_j(a_i, b_i) = 0$.
- "A decomposition is efficient if its leading order errors are small compared to the number of cycles q it requires."

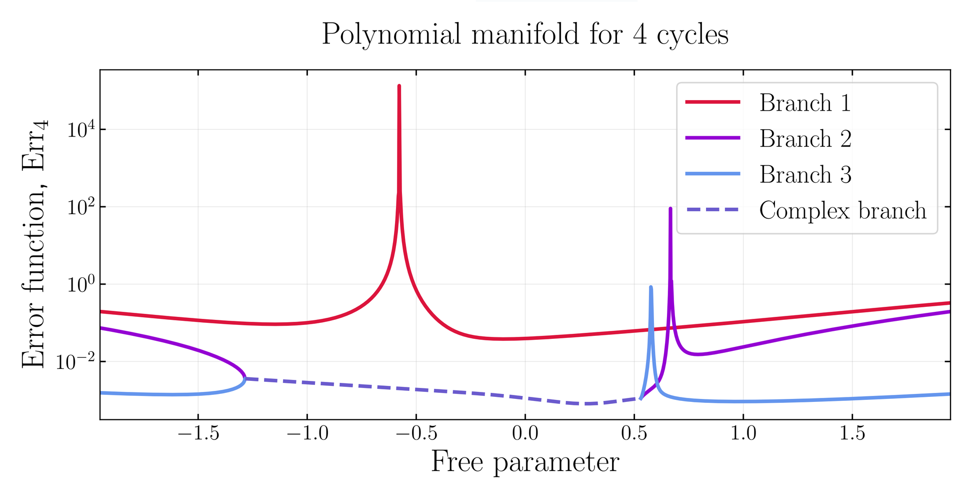
$$\mathrm{Err}_2(a_i, b_i) = \sqrt{|\alpha|^2 + |\beta|^2}, \quad \mathrm{Err}_4(a_i, b_i) = \sqrt{\sum_{k=1}^{6} |\gamma_k|^2}$$

- Efficiency per order: $\mathrm{Eff}_2 = \frac{1}{q^2 \mathrm{Err}_2}$, $\quad \mathrm{Eff}_4 = \frac{1}{q^4 \mathrm{Err}_4}$, $\quad \cdots \quad \mathrm{Eff}_n = \frac{1}{q^n \mathrm{Err}_n}$

Error Manifold Minimization

- After imposing the constraints, the polynomial manifold of the error function $\mathrm{Err}_n(a_i, b_i)$ needs to be minimized, in order to obtain the theoretically most efficient scheme.
- In practice, we use a numerical optimizer, e.g. the Levenberg-Marquard algorithm, to find the minima of the manifold.



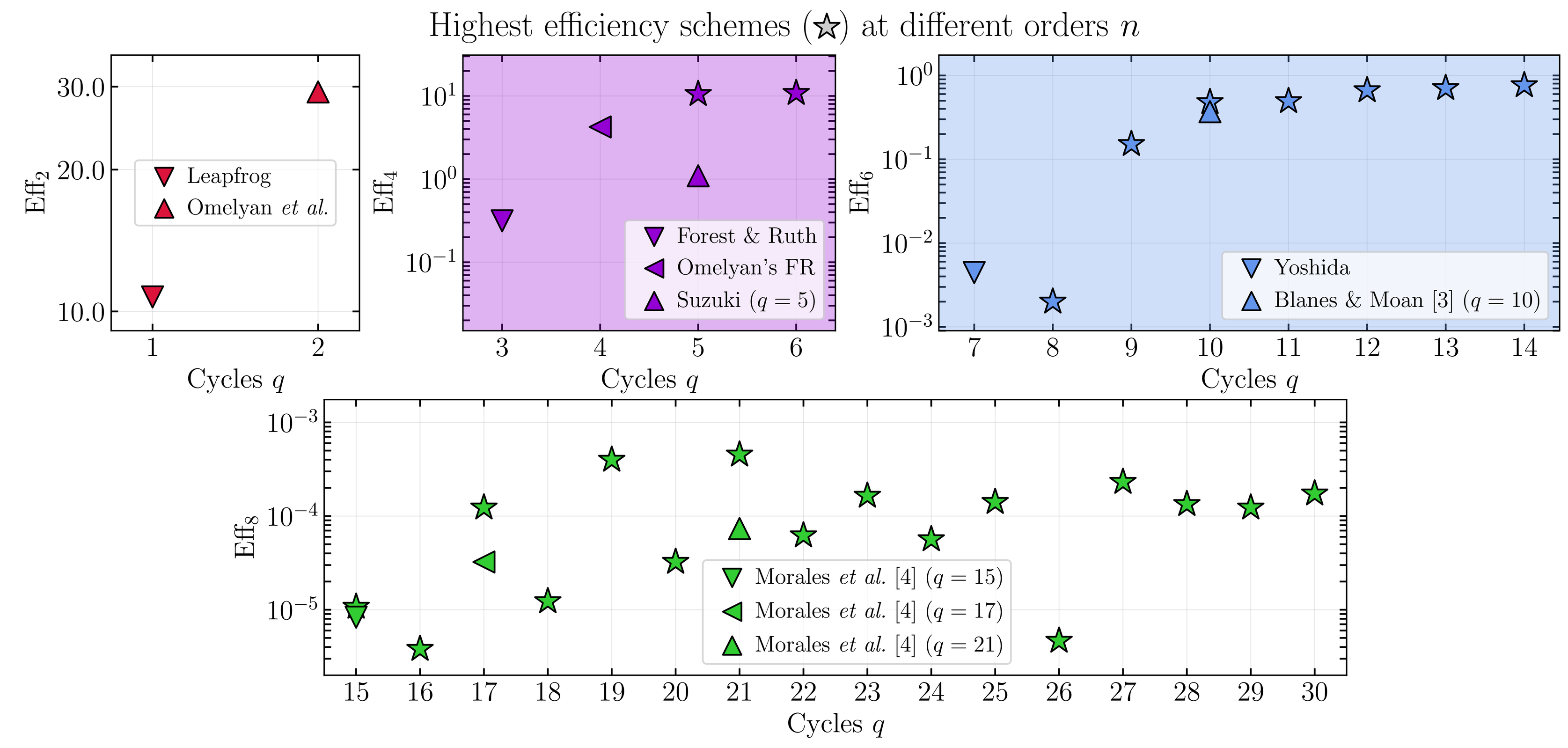


Results - Theoretical efficiency

- Improved theoretical efficiency of novel schemes compared to historical decompositions for orders $n = 4, 6$ and 8.
- A lack of clear plateau for 8^{th} order schemes suggests top most efficient schemes remain unexplored.

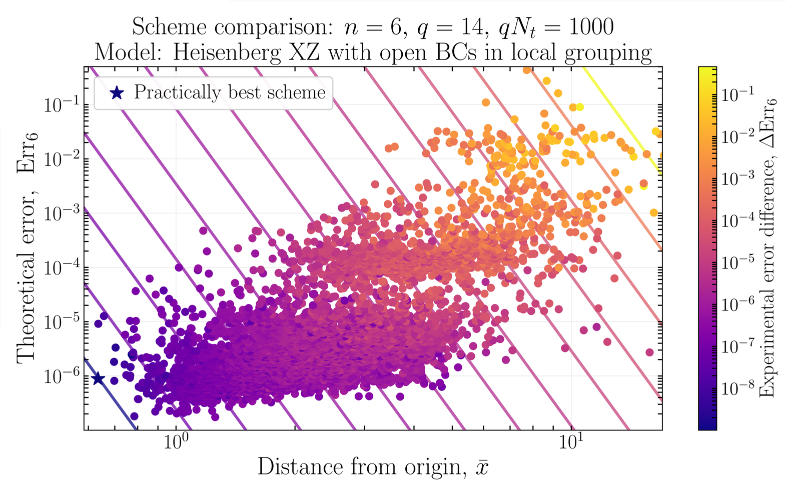
[3]: Blanes and Moan (2002)

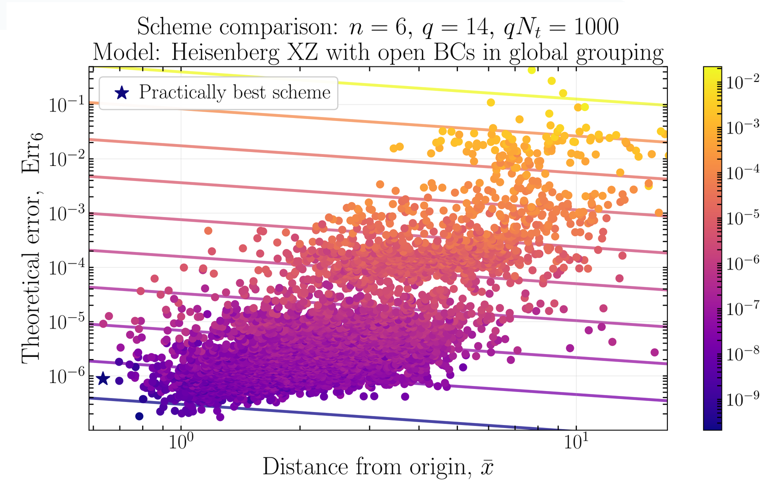
[4]: Morales et al. (2025)



Results - Practical performance

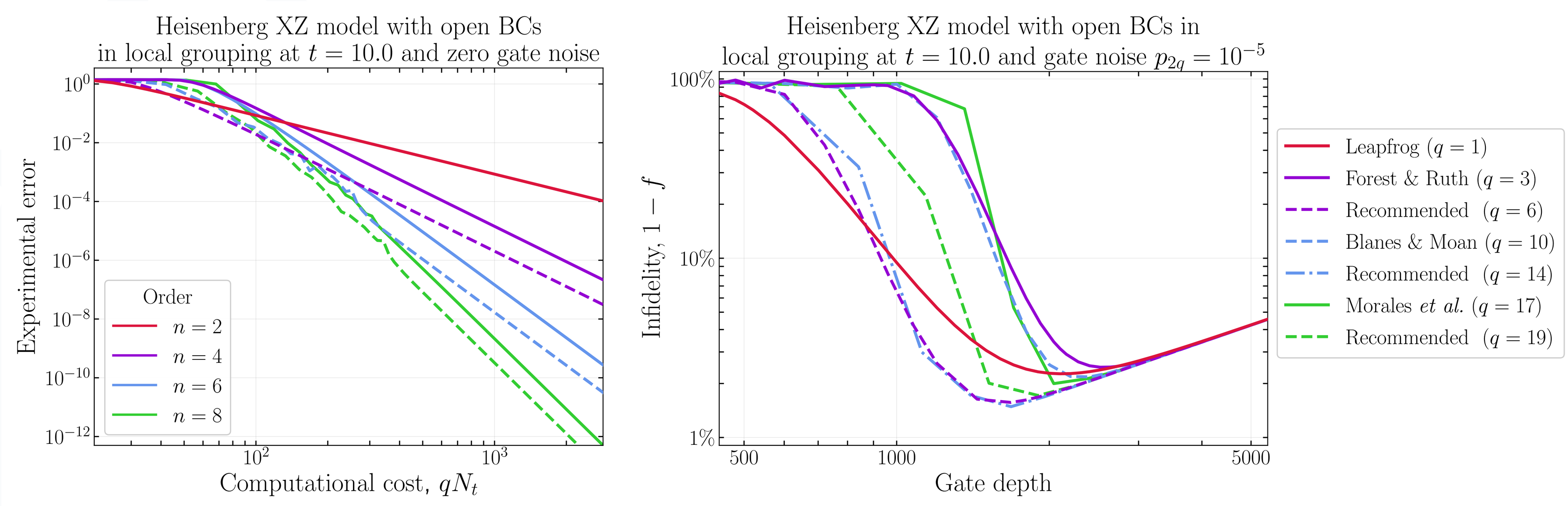
- Numerical experiments on the Heisenberg XZ model give insight into the practical performance of new schemes.
- Along with the theoretical efficiency, uniformity of scheme parameters is believed to reduce the accumulated error. Uniformity can be studied by calculating the distance from the origin point, where all parameters are equal:
$$\bar{x}^2 = 2 \sum_i^q (c_i - 1/2q)^2$$
- The impact of uniformity depends on the ordering of non-commuting operators. In the local ordering ($H = \sum_i^L h_i^x + h_i^y + h_i^z$) uniformity matters much more than in the global ($H = \sum_\alpha h_0^\alpha + h_1^\alpha + \cdots$), based on the way the experimental error changes with the theoretical error and the distance from the origin $\bar{x}$.





- Top performant schemes at higher orders match the 2^{nd} order scheme at low computational cost, and improve on previously established schemes at higher cost.
- Preliminary simulations on noisy circuits with the use of our new package qiskit-omelyan [5] for construction of product formulas, show expected improvement due to reduced gate depth.

[5]: github.com/MarkoMalezic/qiskit-omelyan



Outlook

- Fully explore order $n = 8$ at high cycles q.
- Further study noise models in other physical systems.
- Research of non-unitary schemes with complex parameters.

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