A04: Optimising the Real-Time Evolution of Quantum Spin Chains with Higher-Order Trotter Techniques

Marko Maležič, **Johann Ostmeyer**

Helmholtz-Institut für Strahlen- und Kernphysik, University of Bonn, Germany

September 30, 2024

Schrödinger equation and time evolution

$$\mathrm{i}\,\frac{\partial}{\partial t}\left|\psi\right\rangle = H\left|\psi\right\rangle \qquad\qquad (\hbar = 1)$$

Schrödinger equation and time evolution

$$\mathrm{i}\,\frac{\partial}{\partial t}\,|\psi\rangle = H\,|\psi\rangle \qquad\qquad (\hbar = 1)$$

- Real time evolution

$$|\psi(t)\rangle = \mathrm{e}^{-\mathrm{i}\,Ht}\,|\psi(0)\rangle$$

Schrödinger equation and time evolution

$$\mathrm{i}\,\frac{\partial}{\partial t}\,|\psi\rangle = H\,|\psi\rangle \qquad\qquad (\hbar = 1)$$

- Real time evolution
- Imaginary time evolution $\qquad |\psi_0\rangle = \lim_{\tau\to\infty} \mathrm{e}^{-H\tau}\,|\psi\rangle$

Schrödinger equation and time evolution

$$\mathrm{i}\,\frac{\partial}{\partial t}\left|\psi\right\rangle = H\left|\psi\right\rangle \qquad (\hbar = 1)$$

- Real time evolution
- Imaginary time evolution
- Symplectic integration

$$\dot{x} = \frac{\partial H}{\partial p}$$

$$\dot{p} = -\frac{\partial H}{\partial x}$$

Suzuki-Trotter decomposition

[Suzuki *CommunMathPhys* **51** (1976); Trotter *ProcAMS* **4** (1959)]

$$H = \sum_{i}^{\Lambda} A_i \,, \quad A_i A_j \neq A_j A_i$$

Suzuki-Trotter decomposition

[Suzuki *CommunMathPhys* **51** (1976); Trotter *ProcAMS* **4** (1959)]

$$H = \sum_{i}^{\Lambda} A_i \,, \quad A_i A_j \neq A_j A_i$$

$$U(h) \equiv \mathrm{e}^{\mathrm{i}\, Hh}$$

Suzuki-Trotter decomposition

[Suzuki *CommunMathPhys* **51** (1976); Trotter *ProcAMS* **4** (1959)]

$$H = \sum_{i}^{\Lambda} A_i \,, \quad A_i A_j \neq A_j A_i$$

$$U(h) \equiv \mathrm{e}^{\mathrm{i}\, H h}$$

$$U(h) = \mathrm{e}^{\mathrm{i}\, A_1 h}\, \mathrm{e}^{\mathrm{i}\, A_2 h} \cdots \mathrm{e}^{\mathrm{i}\, A_\Lambda h} + \mathcal{O}\left(h^2\right)$$

Suzuki-Trotter decomposition

[Suzuki *CommunMathPhys* **51** (1976); Trotter *ProcAMS* **4** (1959)]

$$H = \sum_{i}^{\Lambda} A_i \,, \quad A_i A_j \neq A_j A_i$$

$$U(h) \equiv \mathrm{e}^{\mathrm{i}\, H h}$$

$$U(h) = \mathrm{e}^{\mathrm{i}\, A_1 h}\, \mathrm{e}^{\mathrm{i}\, A_2 h} \dots \mathrm{e}^{\mathrm{i}\, A_\Lambda h} + \mathcal{O}\left(h^2\right)$$

$$U(h) = \mathrm{e}^{\mathrm{i}\, A_1 h/2}\, \mathrm{e}^{\mathrm{i}\, A_2 h/2} \dots \mathrm{e}^{\mathrm{i}\, A_\Lambda h/2}\, \mathrm{e}^{\mathrm{i}\, A_\Lambda h/2} \dots \mathrm{e}^{\mathrm{i}\, A_2 h/2}\, \mathrm{e}^{\mathrm{i}\, A_1 h/2} + \mathcal{O}\left(h^3\right)$$

Suzuki-Trotter decomposition

[Suzuki *CommunMathPhys* **51** (1976); Trotter *ProcAMS* **4** (1959)]

$$H = \sum_{i}^{\Lambda} A_i\,, \quad A_i A_j \neq A_j A_i$$

$$U(h) \equiv \mathrm{e}^{\mathrm{i}\,Hh}$$

$$U(h) = \mathrm{e}^{\mathrm{i}\,A_1 h}\,\mathrm{e}^{\mathrm{i}\,A_2 h} \cdots \mathrm{e}^{\mathrm{i}\,A_\Lambda h} + \mathcal{O}\left(h^2\right)$$

$$U(h) = \mathrm{e}^{\mathrm{i}\,A_1 h/2}\,\mathrm{e}^{\mathrm{i}\,A_2 h/2} \cdots \mathrm{e}^{\mathrm{i}\,A_\Lambda h/2}\,\mathrm{e}^{\mathrm{i}\,A_\Lambda h/2} \cdots \mathrm{e}^{\mathrm{i}\,A_2 h/2}\,\mathrm{e}^{\mathrm{i}\,A_1 h/2} + \mathcal{O}\left(h^3\right)$$

$$\vdots$$

Error estimation and efficiency [Omelyan et al. *CPC* **146** (2002), *CPC* **151** (2003)]

$$\mathrm{e}^{(A+B)h+\mathcal{O}_1\,h+\mathcal{O}_3\,h^3+\mathcal{O}_5\,h^5+\cdots} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$

Error estimation and efficiency [Omelyan et al. *CPC* **146** (2002), *CPC* **151** (2003)]

$$\mathrm{e}^{(A+B)h+\mathcal{O}_1\,h+\mathcal{O}_3\,h^3+\mathcal{O}_5\,h^5+\cdots} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$

$$\mathcal{O}_1 = (\nu-1)A + (\sigma-1)B, \quad \nu = \sum_i a_i, \sigma = \sum_i b_i$$

Error estimation and efficiency [Omelyan et al. *CPC* **146** (2002), *CPC* **151** (2003)]

$$\mathrm{e}^{(A+B)h+\mathcal{O}_1\,h+\mathcal{O}_3\,h^3+\mathcal{O}_5\,h^5+\cdots} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$

$$\mathcal{O}_1 = (\nu-1)A + (\sigma-1)B, \quad \nu = \sum_i a_i, \sigma = \sum_i b_i$$

$$\mathcal{O}_3 = \alpha[A,[A,B]] + \beta[B,[A,B]]$$

Error estimation and efficiency [Omelyan et al. *CPC* **146** (2002), *CPC* **151** (2003)]

$$\mathrm{e}^{(A+B)h+\mathcal{O}_1\,h+\mathcal{O}_3\,h^3+\mathcal{O}_5\,h^5+\cdots} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$

$$\mathcal{O}_1 = (\nu-1)A + (\sigma-1)B, \quad \nu = \sum_i a_i,\, \sigma = \sum_i b_i$$

$$\mathcal{O}_3 = \alpha[A,[A,B]] + \beta[B,[A,B]]$$

$$\begin{aligned}\mathcal{O}_5 = {}& \gamma_1[A,[A,[A,[A,B]]]] + \gamma_2[A,[A,[B,[A,B]]]] \\ &+ \gamma_3[B,[A,[A,[A,B]]]] + \gamma_4[B,[B,[B,[A,B]]]] \\ &+ \gamma_5[B,[B,[A,[A,B]]]] + \gamma_6[A,[B,[B,[A,B]]]]\end{aligned}$$

Error estimation and efficiency [Omelyan et al. *CPC* **146** (2002), *CPC* **151** (2003)]

$$e^{(A+B)h+\mathcal{O}_1 h+\mathcal{O}_3 h^3+\mathcal{O}_5 h^5+\cdots} = e^{Aa_1 h}\, e^{Bb_1 h} \cdots e^{Bb_q h}\, e^{Aa_{q+1} h}$$

$$\mathcal{O}_1 = (\nu - 1)A + (\sigma - 1)B, \quad \nu = \sum_i a_i, \sigma = \sum_i b_i$$

$$\mathcal{O}_3 = \alpha[A,[A,B]] + \beta[B,[A,B]]$$

$$\begin{aligned}\mathcal{O}_5 = {} & \gamma_1[A,[A,[A,[A,B]]]] + \gamma_2[A,[A,[B,[A,B]]]] \\ & + \gamma_3[B,[A,[A,[A,B]]]] + \gamma_4[B,[B,[B,[A,B]]]] \\ & + \gamma_5[B,[B,[A,[A,B]]]] + \gamma_6[A,[B,[B,[A,B]]]]\end{aligned}$$

$$\mathrm{Eff}_2 = \frac{1}{q^2\sqrt{|\alpha|^2 + |\beta|^2}}$$

Error estimation and efficiency [Omelyan et al. *CPC* **146** (2002), *CPC* **151** (2003)]

$$\mathrm{e}^{(A+B)h+\mathcal{O}_1\,h+\mathcal{O}_3\,h^3+\mathcal{O}_5\,h^5+\cdots} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$

$$\begin{aligned}
\mathcal{O}_1 &= (\nu-1)A+(\sigma-1)B, \quad \nu=\textstyle\sum_i a_i,\, \sigma=\sum_i b_i \\
\mathcal{O}_3 &= \alpha[A,[A,B]]+\beta[B,[A,B]] \\
\mathcal{O}_5 &= \gamma_1[A,[A,[A,[A,B]]]]+\gamma_2[A,[A,[B,[A,B]]]] \\
&\quad+\gamma_3[B,[A,[A,[A,B]]]]+\gamma_4[B,[B,[B,[A,B]]]] \\
&\quad+\gamma_5[B,[B,[A,[A,B]]]]+\gamma_6[A,[B,[B,[A,B]]]]
\end{aligned}$$

$$\mathrm{Eff}_2 = \frac{1}{q^2\sqrt{|\alpha|^2+|\beta|^2}}$$

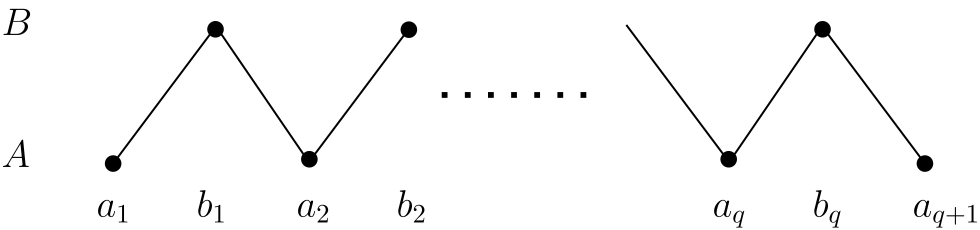
$$\mathrm{Eff}_4 = \frac{1}{q^4\sqrt{\sum_{j=1}^{6}|\gamma_j|^2}}$$

Decompositions into 2 operators

$$\mathrm{e}^{(A+B)h+\mathcal{O}\left(h^{n+1}\right)} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\,\mathrm{e}^{Aa_2h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$

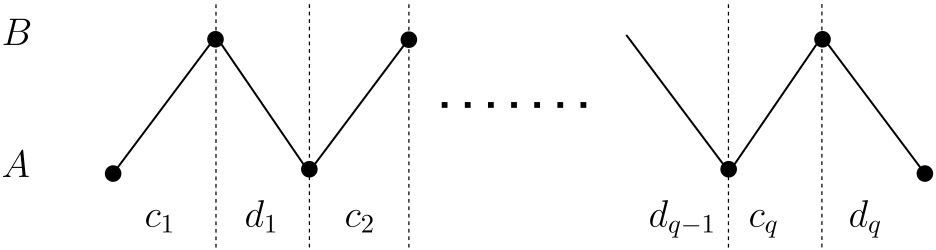
Decompositions into 2 operators

$$\mathrm{e}^{(A+B)h+\mathcal{O}\left(h^{n+1}\right)} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\,\mathrm{e}^{Aa_2h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$



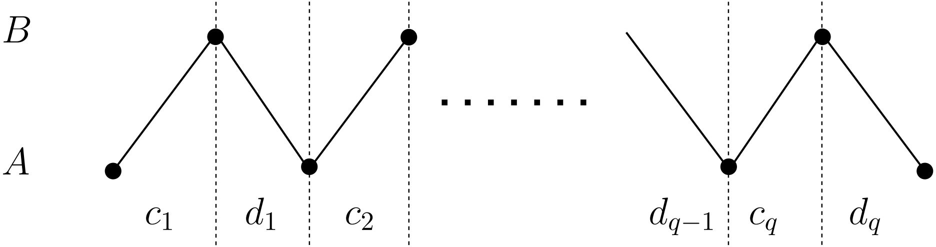
Decompositions into 2 operators

$$\mathrm{e}^{(A+B)h+\mathcal{O}\left(h^{n+1}\right)} = \mathrm{e}^{Aa_1 h}\,\mathrm{e}^{Bb_1 h}\,\mathrm{e}^{Aa_2 h}\cdots\mathrm{e}^{Bb_q h}\,\mathrm{e}^{Aa_{q+1} h}$$



Decompositions into 2 operators

$$\mathrm{e}^{(A+B)h+\mathcal{O}\left(h^{n+1}\right)} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\,\mathrm{e}^{Aa_2h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$
$$= \mathrm{e}^{Ac_1h}\,\mathrm{e}^{Bc_1h}\,\mathrm{e}^{Bd_1h}\,\mathrm{e}^{Ad_1h}\cdots\mathrm{e}^{Bd_qh}\,\mathrm{e}^{Ad_qh}$$

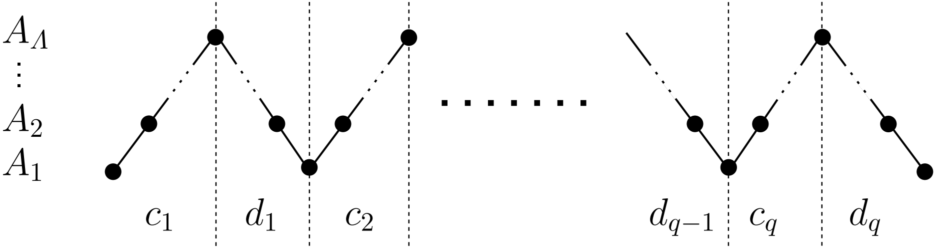


$$c_1 = a_1\,, \qquad d_1 = b_1 - c_1\,,$$
$$c_2 = a_2 - d_1\,, \qquad d_2 = b_2 - c_2\,,$$
$$\vdots \qquad \vdots$$

Decompositions into Λ operators [JO *JPhysA* **56** (2023)]

$$\mathrm{e}^{h\sum_{k=1}^{\Lambda} A_k + \mathcal{O}\left(h^{n+1}\right)}$$

$$= \left(\prod_{k=1}^{\Lambda} \mathrm{e}^{A_k c_1 h}\right)\left(\prod_{k=\Lambda}^{1} \mathrm{e}^{A_k d_1 h}\right)\cdots\left(\prod_{k=1}^{\Lambda} \mathrm{e}^{A_k c_q h}\right)\left(\prod_{k=\Lambda}^{1} \mathrm{e}^{A_k d_q h}\right)$$

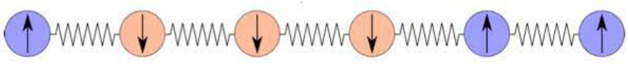


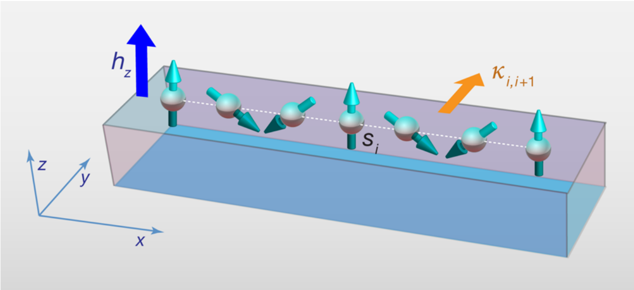
Classical and quantum spin chains

- Classical Ising model

Classical and quantum spin chains

- Classical Ising model





- Quantum Heisenberg model

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$H = \sum_{i=1}^{L} \left(S_i \cdot S_{i+1} + h_i S_i^z \right) \ ,$$

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$H = \sum_{i=1}^{L} \left(S_i \cdot S_{i+1} + h_i S_i^z \right) ,$$

$$\mathrm{e}^{\mathrm{i}\, Ht} \equiv U(t) = U(h)^{t/h}$$

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$H = \sum_{i=1}^{L} \left(S_i \cdot S_{i+1} + h_i S_i^z \right) ,$$

$$\begin{aligned} \mathrm{e}^{\mathrm{i}\,Ht} &\equiv U(t) = U(h)^{t/h} \\ &= \mathcal{U}(h)^{t/h} + \mathcal{O}\left(h^n\right) , \end{aligned}$$

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$H = \sum_{i=1}^{L} \left(S_i \cdot S_{i+1} + h_i S_i^z \right) ,$$

$$\mathrm{e}^{\mathrm{i}\,Ht} \equiv U(t) = U(h)^{t/h}$$

$$= \mathcal{U}(h)^{t/h} + \mathcal{O}\left(h^n\right) ,$$

$$\mathcal{U}(h) = \mathrm{e}^{\mathrm{i}\,H_1^x c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^y c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^z c_1 h}$$

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$
\begin{aligned}
H &= \sum_{i=1}^{L} \left(S_i \cdot S_{i+1} + h_i S_i^z \right) , \\
\mathrm{e}^{\mathrm{i}\, H t} &\equiv U(t) = U(h)^{t/h} \\
&= \mathcal{U}(h)^{t/h} + \mathcal{O}\left(h^n\right) , \\
\mathcal{U}(h) &= \mathrm{e}^{\mathrm{i}\, H_1^x c_1 h} \mathrm{e}^{\mathrm{i}\, H_1^y c_1 h} \mathrm{e}^{\mathrm{i}\, H_1^z c_1 h} \mathrm{e}^{\mathrm{i}\, H_2^x c_1 h} \mathrm{e}^{\mathrm{i}\, H_2^y c_1 h} \mathrm{e}^{\mathrm{i}\, H_2^z c_1 h}
\end{aligned}
$$

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

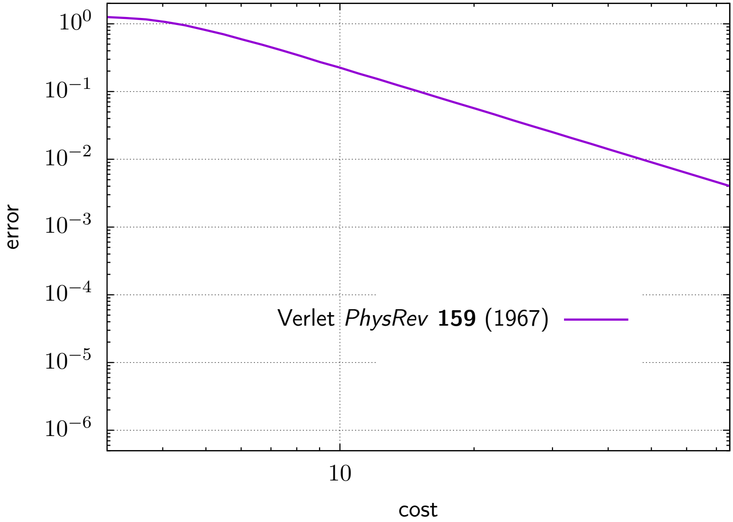
$$
\begin{aligned}
H &= \sum_{i=1}^{L} \left(S_i \cdot S_{i+1} + h_i S_i^z \right) \,, \\
\mathrm{e}^{\mathrm{i}\,Ht} &\equiv U(t) = U(h)^{t/h} \\
&= \mathcal{U}(h)^{t/h} + \mathcal{O}\left(h^n\right) \,, \\
\mathcal{U}(h) &= \mathrm{e}^{\mathrm{i}\,H_1^x c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^y c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^z c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^x c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^y c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^z c_1 h} \dots \mathrm{e}^{\mathrm{i}\,H_1^z d_q h} \mathrm{e}^{\mathrm{i}\,H_1^y d_q h} \mathrm{e}^{\mathrm{i}\,H_1^x d_q h} \,,
\end{aligned}
$$

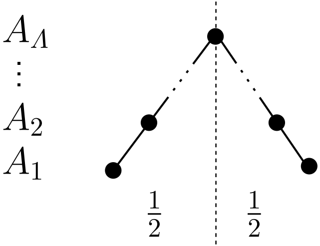
Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$
\begin{aligned}
H &= \sum_{i=1}^{L} \left(S_i \cdot S_{i+1} + h_i S_i^z\right) \,, \\
\mathrm{e}^{\mathrm{i}\,Ht} &\equiv U(t) = U(h)^{t/h} \\
&= \mathcal{U}(h)^{t/h} + \mathcal{O}\left(h^n\right) \,, \\
\mathcal{U}(h) &= \mathrm{e}^{\mathrm{i}\,H_1^x c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^y c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^z c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^x c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^y c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^z c_1 h} \dots \mathrm{e}^{\mathrm{i}\,H_1^z d_q h} \mathrm{e}^{\mathrm{i}\,H_1^y d_q h} \mathrm{e}^{\mathrm{i}\,H_1^x d_q h} \,, \\
\text{error} &\propto \left\| U(t) - \mathcal{U}(h)^{t/h} \right\|
\end{aligned}
$$

Benchmarking the Heisenberg model

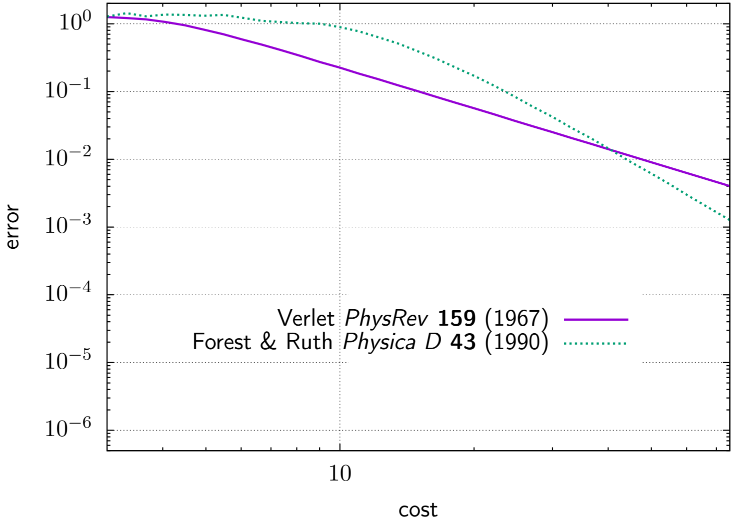


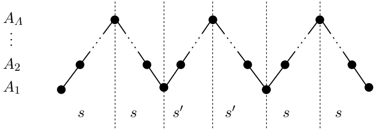


order $= 2$,

cycles $= 1$

Benchmarking the Heisenberg model





$$s = \frac{1}{2(2-\sqrt[3]{2})}$$

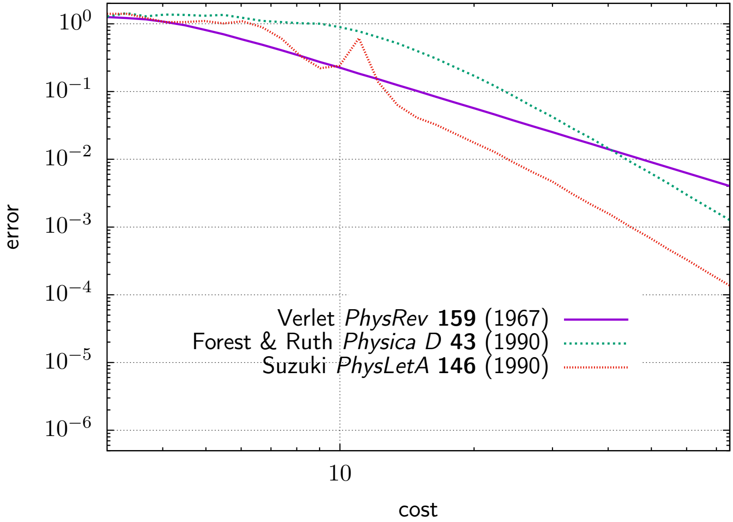
$$s' = \frac{1}{2} - 2s$$

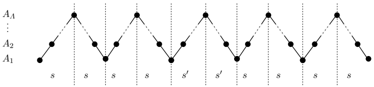
$$\text{order} = 4\,,$$

$$\text{cycles} = 3\,,$$

$$\text{Eff}_4 = 0.315$$

Benchmarking the Heisenberg model





$$s = \frac{1}{2(4-\sqrt[3]{4})}$$

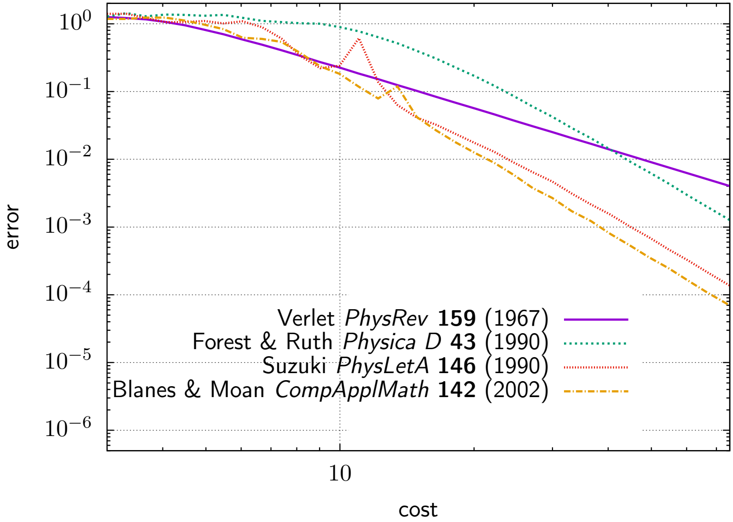
$$s' = \frac{1}{2} - 4s$$

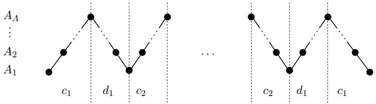
$$\text{order} = 4\,,$$

$$\text{cycles} = 5\,,$$

$$\mathrm{Eff}_4 = 1.10$$

Benchmarking the Heisenberg model

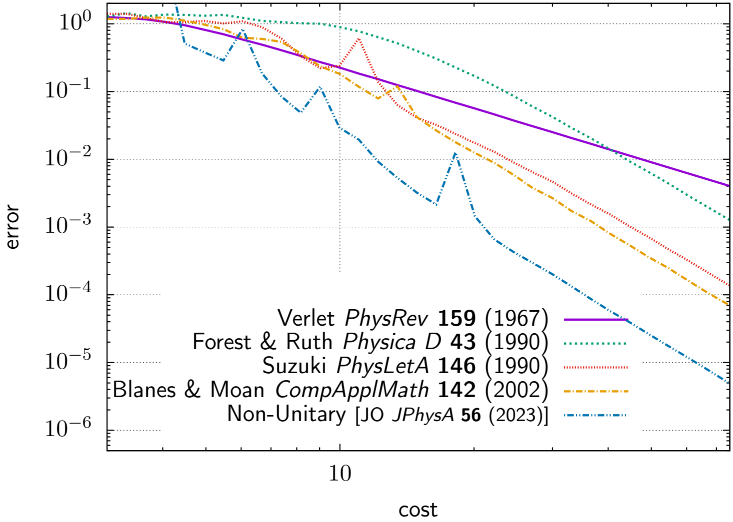


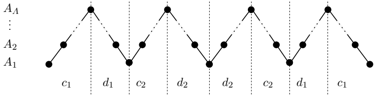


$$c_1 \approx 0.08 \quad d_1 \approx 0.13$$
$$c_2 \approx 0.22 \quad d_2 \approx -0.36$$
$$c_3 \approx 0.32 \quad d_3 \approx 0.11$$

$$\text{order} = 4\,,$$
$$\text{cycles} = 6\,,$$
$$\text{Eff}_4 = 10.2$$

Benchmarking the Heisenberg model





$$c_1 \approx 0.10 + 0.02\,\mathrm{i}$$

$$d_1 \approx 0.15 + 0.07\,\mathrm{i}$$

$$c_2 \approx 0.14 + 0.07\,\mathrm{i}$$

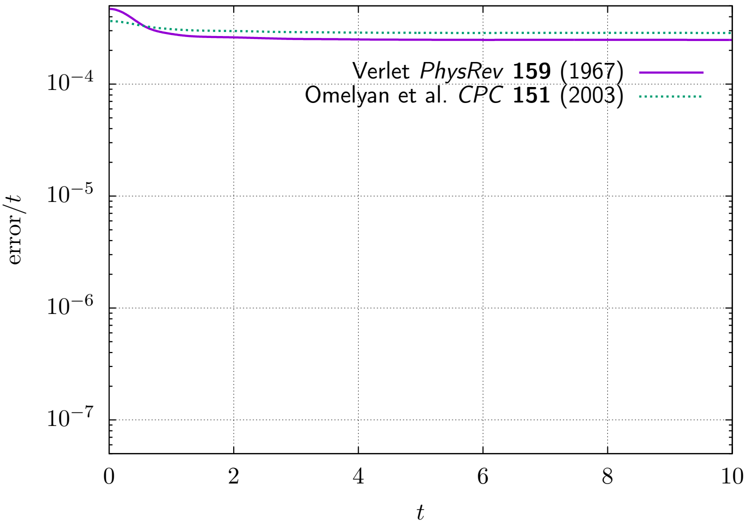
$$d_2 \approx 0.11 - 0.16\,\mathrm{i}$$

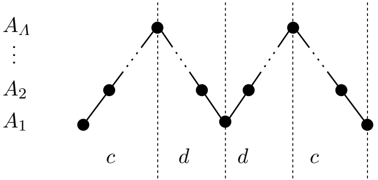
$$\text{order} = 4\,,$$

$$\text{cycles} = 4\,,$$

$$\mathrm{Eff}_4 = 29.9$$

Error accumulation





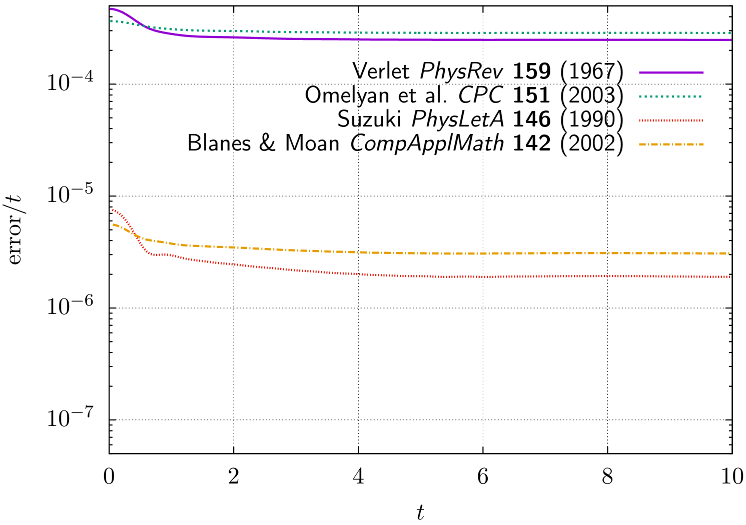
$$c \approx 0.193$$

$$d \approx 0.407$$

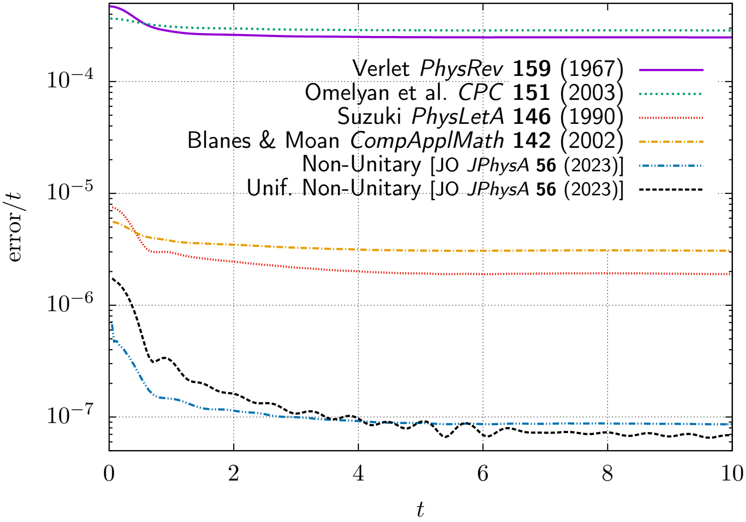
$$\text{order} = 2\,,$$

$$\text{cycles} = 2$$

Error accumulation



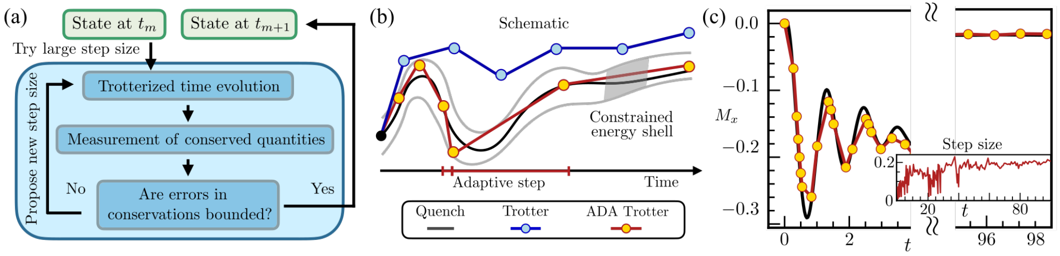
Error accumulation



$$c_1 = 0.1 + 0.025\,\mathrm{i}$$
$$d_1 = 0.1 + 0.025\,\mathrm{i}$$
$$c_2 = 0.1 - 0.066\,\mathrm{i}$$
$$d_2 = 0.1 - 0.066\,\mathrm{i}$$
$$c_3 = 0.1 + 0.082\,\mathrm{i}$$
$$\text{order} = 4\,,$$
$$\text{cycles} = 5\,,$$
$$\mathrm{Eff}_4 = 6.38$$

Adaptive step size [Blanes et al. *AplNumMat* **146** (2019); Zhao et al. *PRXQ* **4** (2023)]

ZHAO, BUKOV, HEYL, and MOESSNER PRX QUANTUM **4,** 030319 (2023)

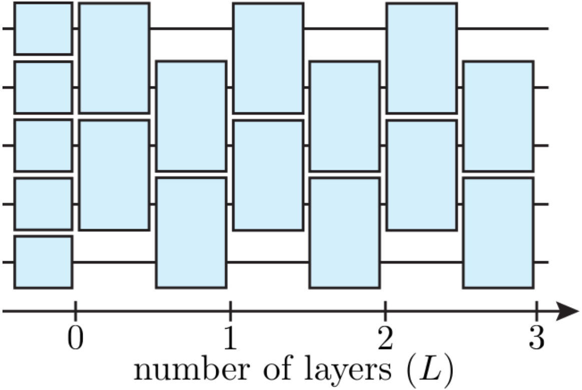


Quantum circuit optimisation

[Mansuroglu et al. *QuantSciTech* **8** (2023); Tepaske et al. *SciPostPhys* **14** (2023)]

[Mc Keever & Lubasch *PRR* **5** (2023)]

Ansatz: brickwall circuit

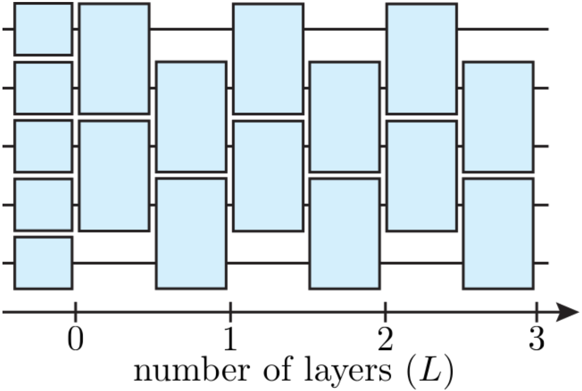


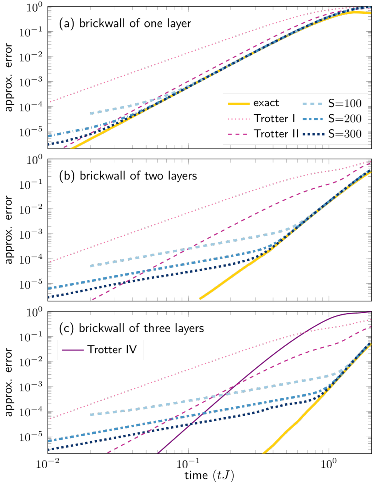
Quantum circuit optimisation

[Mansuroglu et al. *QuantSciTech* **8** (2023); Tepaske et al. *SciPostPhys* **14** (2023)]

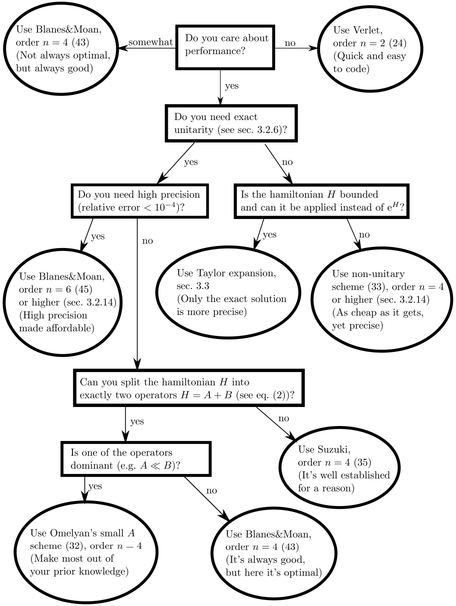
[Mc Keever & Lubasch *PRR* **5** (2023)]

Ansatz: brickwall circuit





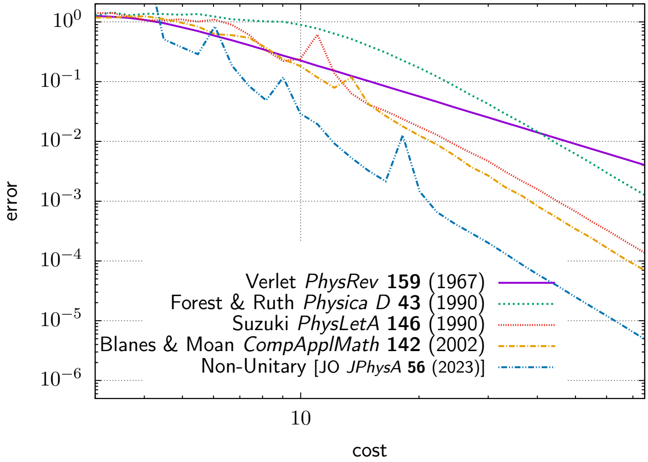
How to choose... [JO *JPhysA* **56** (2023)]



The A4 Project Plan

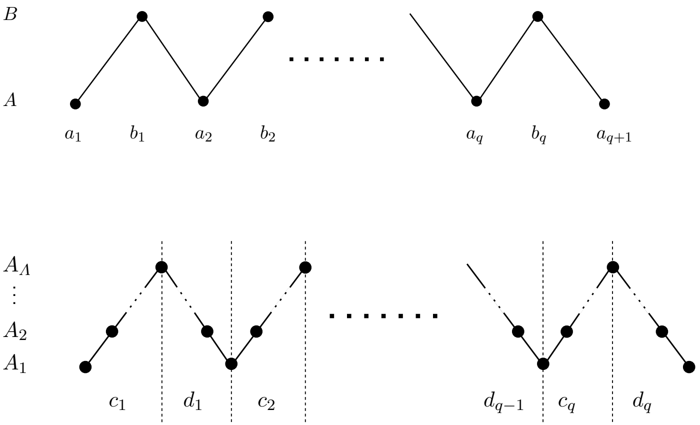
The A4 Project Plan

1. Optimise higher order schemes.



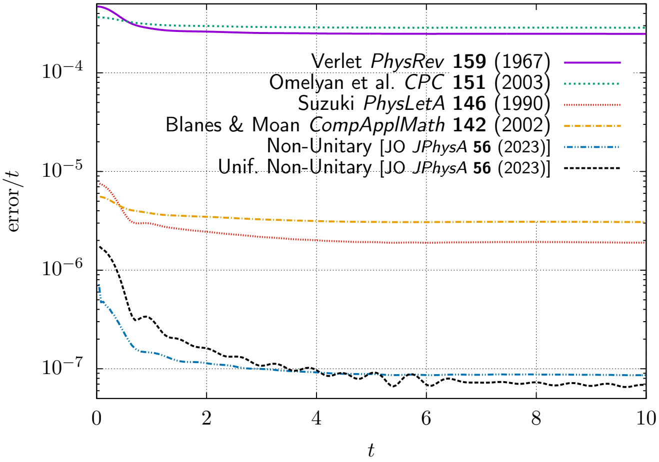
The A4 Project Plan

1. Optimise higher order schemes.
2. Generalise 2-operator efficiencies for Λ operators.



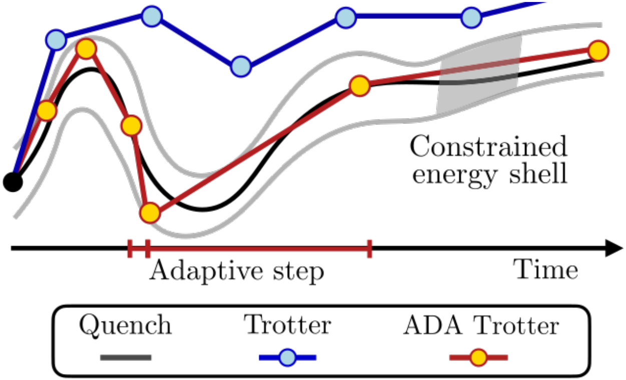
The A4 Project Plan

1. Optimise higher order schemes.
2. Generalise 2-operator efficiencies for Λ operators.
3. Include in-practice error accumulation.



The A4 Project Plan

1. Optimise higher order schemes.
2. Generalise 2-operator efficiencies for Λ operators.
3. Include in-practice error accumulation.
4. Combine with alternative approaches.



Bibliography I

1. Blanes & Moan, "Practical symplectic partitioned Runge–Kutta and Runge–Kutta–Nyström methods", Journal of Computational and Applied Mathematics **142**, 313–330 (*CompApplMath* **142** (2002)).
2. S. Blanes, F. Casas, M. Thalhammer, "Splitting and composition methods with embedded error estimators", Applied Numerical Mathematics **146**, 400–415 (*AplNumMat* **146** (2019)).
3. A. M. Childs, Y. Su, M. C. Tran, N. Wiebe, S. Zhu, "Theory of Trotter Error with Commutator Scaling", Phys. Rev. X **11**, 011020 (*PRX* **11** (2021)).
4. Forest & Ruth, "Fourth-order symplectic integration", Physica D: Nonlinear Phenomena **43**, 105–117 (*Physica D* **43** (1990)).
5. M. Heyl, P. Hauke, P. Zoller, "Quantum localization bounds Trotter errors in digital quantum simulation", Science Advances **5**, 10.1126/sciadv.aau8342 (*SciAdv* **5** (2019)).
6. JO, *j-ostmeyer/efficient-trotter: Optimised Trotter Decompositions*, version v1.0.0, Nov. 2022.
7. JO, "Optimised Trotter decompositions for classical and quantum computing", J. Phys. A **56**, 285303 (*JPhysA* **56** (2023)).

Bibliography II

[8] R. Mansuroglu, T. Eckstein, L. Nützel, S. A. Wilkinson, M. J. Hartmann, "Variational Hamiltonian simulation for translational invariant systems via classical pre-processing", Quantum Science and Technology **8**, 025006 (*QuantSciTech* **8** (2023)).

[9] C. Mc Keever, M. Lubasch, "Classically optimized hamiltonian simulation", Physical Review Research **5**, `10.1103/physrevresearch.5.023146` (*PRR* **5** (2023)).

[10] P. Molignini, "Analyzing the two dimensional ising model with conformal field theory", (Mar. 2013).

[11] I. Omelyan, I. Mryglod, R. Folk, "Optimized Forest–Ruth- and Suzuki-like algorithms for integration of motion in many-body systems", Computer Physics Communications **146**, 188–202 (*CPC* **146** (2002)).

[12] I. Omelyan, I. Mryglod, R. Folk, "Symplectic analytically integrable decomposition algorithms: classification, derivation, and application to molecular dynamics, quantum and celestial mechanics simulations", Computer Physics Communications **151**, 272–314 (*CPC* **151** (2003)).

Bibliography III

[13] S. Onoda, "Pushing bits through a spin wire", Physcs Online Journal **5**, 53– (2012).

[14] A. Schubert, C. B. Mendl, "Trotter error with commutator scaling for the fermi-hubbard model", Physical Review B **108**, `10.1103/physrevb.108.195105` (*PRB* **108** (2023)).

[15] M. Suzuki, "Generalized Trotter's Formula and Systematic Approximants of Exponential Operators and Inner Derivations with Applications to Many Body Problems", Commun. Math. Phys. **51**, 183–190 (*CommunMathPhys* **51** (1976)).

[16] M. Suzuki, "Decomposition formulas of exponential operators and Lie exponentials with some applications to quantum mechanics and statistical physics", Journal of Mathematical Physics **26**, 601–612 (*JMatPhys* **26** (1985)).

[17] M. Suzuki, "Fractal decomposition of exponential operators with applications to many-body theories and monte carlo simulations", Physics Letters A **146**, 319–323 (*PhysLetA* **146** (1990)).

Bibliography IV

[18]M. S. J. Tepaske, D. Hahn, D. J. Luitz, “Optimal compression of quantum many-body time evolution operators into brickwall circuits”, SciPost Physics **14**, 10.21468/scipostphys.14.4.073 (*SciPostPhys* **14** (2023)).

[19]H. F. Trotter, “On the Product of Semi-Groups of Operators”, Proceedings of the American Mathematical Society **10**, 545–551 (*ProcAMS* **4** (1959)).

[20]L. Verlet, “Computer "Experiments" on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Molecules”, Phys. Rev. **159**, 98–103 (*PhysRev* **159** (1967)).

[21]H. Yoshida, “Construction of higher order symplectic integrators”, Physics Letters A **150**, 262–268 (*PhysLetA* **150** (1990)).

[22]H. Zhao, M. Bukov, M. Heyl, R. Moessner, “Making Trotterization Adaptive and Energy-Self-Correcting for NISQ Devices and Beyond”, PRX Quantum **4**, 030319 (*PRXQ* **4** (2023)).

Proof of validity of Λ-operator decomposition I

For every $i \in \{1, \ldots, q\}$ (setting $d_0 = 0$)

$$\begin{aligned} c_i + d_{i-1} &= a_i - d_{i-1} + d_{i-1} \\ &= a_i \, , \\ d_i + c_i &= b_i - c_i + c_i \\ &= b_i \, , \end{aligned}$$

i.e. decomposition works trivially for $\Lambda = 2$.

Proof of validity of Λ-operator decomposition II

Use the Baker–Campbell–Hausdorff formula:

$$\left(\prod_{k=1}^{\Lambda} \mathrm{e}^{A_k c_i h}\right) = \mathrm{e}^{C_1 c_i h + C_2 (c_i h)^2 + C_3 (c_i h)^3 + \cdots}$$

$$\left(\prod_{k=\Lambda}^{1} \mathrm{e}^{A_k d_i h}\right) = \mathrm{e}^{D_1 d_i h + D_2 (d_i h)^2 + D_3 (d_i h)^3 + \cdots}$$

where $C_1 = D_1 = \sum_{k=1}^{\Lambda} A_k$ and the remaining operators C_l, D_l are some linear combinations of lth order commutators $[A_{k_1}, [A_{k_2}, \cdots [A_{k_{l-1}}, A_{k_l}] \cdots]]$.

Proof of validity of Λ-operator decomposition III

C_l, D_l are independent of i and for every $\Lambda \geq 2$ all the C_l (D_l) are mutually non-commuting and linearly independent in general. Thus, the right hand side is completely independent of Λ.
For $\Lambda = 2$:

$$\mathrm{e}^{h\sum\limits_{k=1}^{\Lambda} A_k + \mathcal{O}\left(h^{n+1}\right)} = \mathrm{e}^{C_1 c_1 h + C_2 (c_1 h)^2 + \cdots} \mathrm{e}^{D_1 d_1 h + D_2 (d_1 h)^2 + \cdots} \\ \ldots \mathrm{e}^{C_1 c_q h + C_2 (c_q h)^2 + \cdots} \mathrm{e}^{D_1 d_q h + D_2 (d_q h)^2 + \cdots}$$

Since the c_i, d_i fulfil this condition for every C_i, D_i (they solve the corresponding system of polynomial equations), they automatically fulfil it for every Λ.

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$H = \sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z + h_i \sigma_i^z \right) ,$$

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$H = \sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z + h_i \sigma_i^z \right) ,$$

$$\mathrm{e}^{\mathrm{i}\,Ht} \equiv U(t) = U(h)^{t/h}$$

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$
\begin{aligned}
H &= \sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z + h_i \sigma_i^z\right) \,, \\
\mathrm{e}^{\mathrm{i}\,Ht} &\equiv U(t) = U(h)^{t/h} \\
&= S(h)^{t/h} + \mathcal{O}\left(h^n\right) \,,
\end{aligned}
$$

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$
\begin{aligned}
H &= \sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z + h_i \sigma_i^z \right) \, , \\
\mathrm{e}^{\mathrm{i}\, H t} &\equiv U(t) = U(h)^{t/h} \\
&= S(h)^{t/h} + \mathcal{O}\left(h^n\right) \, , \\
S(h) &= \mathrm{e}^{\mathrm{i}\, H_1^x c_1 h} \mathrm{e}^{\mathrm{i}\, H_1^y c_1 h} \mathrm{e}^{\mathrm{i}\, H_1^z c_1 h}
\end{aligned}
$$

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$H = \sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z + h_i \sigma_i^z\right) \,,$$

$$\begin{aligned} \mathrm{e}^{\mathrm{i}\,Ht} &\equiv U(t) = U(h)^{t/h} \\ &= S(h)^{t/h} + \mathcal{O}\left(h^n\right) \,, \end{aligned}$$

$$S(h) = \mathrm{e}^{\mathrm{i}\,H_1^x c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^y c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^z c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^x c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^y c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^z c_1 h}$$

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$
\begin{aligned}
H &= \sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z + h_i \sigma_i^z \right) \, , \\
\mathrm{e}^{\mathrm{i}\,Ht} &\equiv U(t) = U(h)^{t/h} \\
&= S(h)^{t/h} + \mathcal{O}\left(h^n\right) \, , \\
S(h) &= \mathrm{e}^{\mathrm{i}\,H_1^x c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^y c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^z c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^x c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^y c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^z c_1 h} \dots \mathrm{e}^{\mathrm{i}\,H_1^z d_q h} \mathrm{e}^{\mathrm{i}\,H_1^y d_q h} \mathrm{e}^{\mathrm{i}\,H_1^x d_q h} \, ,
\end{aligned}
$$

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$H = \sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z + h_i \sigma_i^z\right) ,$$

$$\mathrm{e}^{\mathrm{i}\,Ht} \equiv U(t) = U(h)^{t/h}$$

$$= S(h)^{t/h} + \mathcal{O}\left(h^n\right) ,$$

$$S(h) = \mathrm{e}^{\mathrm{i}\,H_1^x c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^y c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^z c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^x c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^y c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^z c_1 h} \dots \mathrm{e}^{\mathrm{i}\,H_1^z d_q h} \mathrm{e}^{\mathrm{i}\,H_1^y d_q h} \mathrm{e}^{\mathrm{i}\,H_1^x d_q h} ,$$

$$\mathrm{error} = \frac{1}{\sqrt{N}} \left\| U(t) - S(h)^{t/h} \right\|_{\mathsf{F}}$$

Heisenberg model and error estimation

[Childs et al. *PRX* **11** (2021); Heyl et al. *SciAdv* **5** (2019); Schubert & Mendl *PRB* **108** (2023)]

$$H = \sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z + h_i \sigma_i^z \right) ,$$

$$\mathrm{e}^{\mathrm{i}\,Ht} \equiv U(t) = U(h)^{t/h}$$

$$= S(h)^{t/h} + \mathcal{O}\left(h^n\right) ,$$

$$S(h) = \mathrm{e}^{\mathrm{i}\,H_1^x c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^y c_1 h} \mathrm{e}^{\mathrm{i}\,H_1^z c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^x c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^y c_1 h} \mathrm{e}^{\mathrm{i}\,H_2^z c_1 h} \cdots \mathrm{e}^{\mathrm{i}\,H_1^z d_q h} \mathrm{e}^{\mathrm{i}\,H_1^y d_q h} \mathrm{e}^{\mathrm{i}\,H_1^x d_q h} ,$$

$$\text{error} = \frac{1}{\sqrt{N}} \left\| U(t) - S(h)^{t/h} \right\|_{\mathsf{F}}$$

$$= \frac{1}{\sqrt{N}} \sqrt{\sum_v \left| U(t) \cdot v - S(h)^{t/h} \cdot v \right|^2}$$

Symplectic integrators [Omelyan et al. *CPC* **151** (2003)]

- Numerically solve equations of motion

$$\dot{x} = p$$
$$\dot{p} = -V'(x)$$

Symplectic integrators [Omelyan et al. *CPC* **151** (2003)]

- Numerically solve equations of motion

$$\dot{x} = p$$
$$\dot{p} = -V'(x)$$

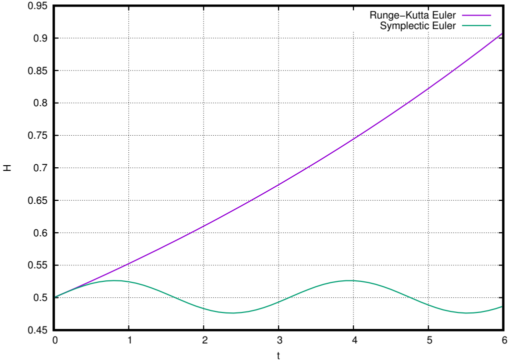
- Preserve phase space $\Rightarrow$ error of $H = \frac{1}{2}p^2 + V(x)$ bounded.

Symplectic integrators [Omelyan et al. *CPC* **151** (2003)]

- Numerically solve equations of motion

$$\dot{x} = p$$
$$\dot{p} = -V'(x)$$

- Preserve phase space $\Rightarrow$ error of $H = \frac{1}{2}p^2 + V(x)$ bounded.

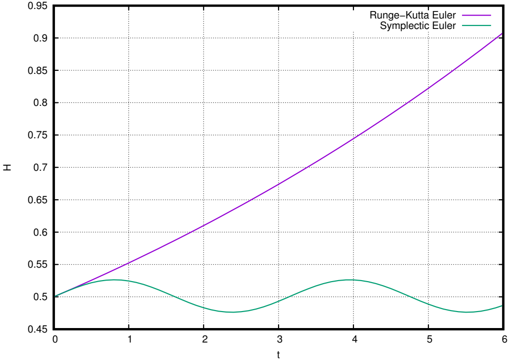


Symplectic integrators [Omelyan et al. *CPC* **151** (2003)]

- Numerically solve equations of motion

$$\dot{x} = p$$
$$\dot{p} = -V'(x)$$

- Preserve phase space $\Rightarrow$ error of $H = \frac{1}{2}p^2 + V(x)$ bounded.



$$x_1 = x_0 + a_1 h p_0$$
$$p_1 = p_0 - b_1 h V'(x_1)$$
$$x_2 = x_1 + a_2 h p_1$$
$$\vdots$$

Special case of Trotterization [Omelyan et al. *CPC* **151** (2003)]

$$\begin{pmatrix} x(t) \\ p(t) \end{pmatrix} = \mathrm{e}^{t\left(p\frac{\partial}{\partial x} - V'(x)\frac{\partial}{\partial p}\right)} \begin{pmatrix} x(0) \\ p(0) \end{pmatrix}$$

Special case of Trotterization [Omelyan et al. *CPC* **151** (2003)]

$$\begin{pmatrix} x(t) \\ p(t) \end{pmatrix} = \mathrm{e}^{t\left(p\frac{\partial}{\partial x} - V'(x)\frac{\partial}{\partial p}\right)} \begin{pmatrix} x(0) \\ p(0) \end{pmatrix}$$

$$=: \mathrm{e}^{t(A+B)} \begin{pmatrix} x(0) \\ p(0) \end{pmatrix}$$

Special case of Trotterization [Omelyan et al. *CPC* **151** (2003)]

$$\begin{pmatrix} x(t) \\ p(t) \end{pmatrix} = \mathrm{e}^{t\left(p\frac{\partial}{\partial x} - V'(x)\frac{\partial}{\partial p}\right)} \begin{pmatrix} x(0) \\ p(0) \end{pmatrix}$$

$$=: \mathrm{e}^{t(A+B)} \begin{pmatrix} x(0) \\ p(0) \end{pmatrix}$$

$$\Rightarrow [B,[B,[A,B]]] = 0$$

Special case of Trotterization [Omelyan et al. *CPC* **151** (2003)]

$$\begin{pmatrix} x(t) \\ p(t) \end{pmatrix} = \mathrm{e}^{t\left(p\frac{\partial}{\partial x} - V'(x)\frac{\partial}{\partial p}\right)} \begin{pmatrix} x(0) \\ p(0) \end{pmatrix}$$

$$=: \mathrm{e}^{t(A+B)} \begin{pmatrix} x(0) \\ p(0) \end{pmatrix}$$

$$\Rightarrow [B,[B,[A,B]]] = 0$$

$$\mathcal{O}_3 = \alpha[A,[A,B]] + \beta[B,[A,B]]$$

Special case of Trotterization [Omelyan et al. *CPC* **151** (2003)]

$$\begin{pmatrix} x(t) \\ p(t) \end{pmatrix} = \mathrm{e}^{t\left(p\frac{\partial}{\partial x} - V'(x)\frac{\partial}{\partial p}\right)} \begin{pmatrix} x(0) \\ p(0) \end{pmatrix}$$

$$=: \mathrm{e}^{t(A+B)} \begin{pmatrix} x(0) \\ p(0) \end{pmatrix}$$

$$\Rightarrow [B,[B,[A,B]]] = 0$$

$$\mathcal{O}_3 = \alpha[A,[A,B]] + \beta[B,[A,B]]$$

$$\Rightarrow \mathcal{O}_5 = \gamma_1[A,[A,[A,[A,B]]]] + \gamma_2[A,[A,[B,[A,B]]]]$$

$$+ \gamma_3[B,[A,[A,[A,B]]]] + \cancel{\gamma_4[B,[B,[B,[A,B]]]]}$$

$$+ \gamma_5[B,[B,[A,[A,B]]]] + \cancel{\gamma_6[A,[B,[B,[A,B]]]]}$$

Suzuki's recursive method [Suzuki *JMatPhys* **26** (1985)]

1. Choose a symmetric decomposition $S_n(h)$ of order $\mathcal{O}(h^n)$.

Suzuki's recursive method [Suzuki *JMatPhys* **26** (1985)]

1. Choose a symmetric decomposition $S_n(h)$ of order $\mathcal{O}\left(h^n\right)$.

2. Choose $p \in \mathbb{N}$, best $p = 2$.

Suzuki's recursive method [Suzuki *JMatPhys* **26** (1985)]

1. Choose a symmetric decomposition $S_n(h)$ of order $\mathcal{O}\left(h^n\right)$.
2. Choose $p \in \mathbb{N}$, best $p = 2$.
3. Calculate coefficient $s_n = \frac{1}{2p-(2p)^{\frac{1}{n+1}}}$.

Suzuki's recursive method [Suzuki *JMatPhys* **26** (1985)]

1. Choose a symmetric decomposition $S_n(h)$ of order $\mathcal{O}\left(h^n\right)$.
2. Choose $p \in \mathbb{N}$, best $p = 2$.
3. Calculate coefficient $s_n = \frac{1}{2p-(2p)^{\frac{1}{n+1}}}$.
4. Construct $\mathcal{O}\left(h^{n+2}\right)$ method:

$$S_{n+2}(h) = S_n(s_n h)^p \, S_n\left((1 - 2ps_n)h\right) \, S_n(s_n h)^p$$

Yoshida's optimisation method [Yoshida *PhysLetA* **150** (1990)]

1. Use 2nd order building blocks $S_2(h)$.

Yoshida's optimisation method [Yoshida *PhysLetA* **150** (1990)]

1. Use 2nd order building blocks $S_2(h)$.
2. Choose target order n and parameter m.

Yoshida's optimisation method [Yoshida *PhysLetA* **150** (1990)]

1. Use 2nd order building blocks $S_2(h)$.
2. Choose target order n and parameter m.
3. Ansatz:

$$S_n(h) = S_2(w_m h) \cdots S_2(w_2 h) S_2(w_1 h)\, S_2(w_0 h)\, S_2(w_1 h) \cdots S_2(w_m h)\,,$$

$$w_0 = 1 - 2\sum_{i=1}^{m} w_m$$

Yoshida's optimisation method [Yoshida *PhysLetA* **150** (1990)]

1. Use 2nd order building blocks $S_2(h)$.
2. Choose target order n and parameter m.
3. Ansatz:

$$S_n(h) = S_2(w_m h) \cdots S_2(w_2 h) S_2(w_1 h)\, S_2(w_0 h)\, S_2(w_1 h) \cdots S_2(w_m h)\,,$$

$$w_0 = 1 - 2 \sum_{i=1}^{m} w_m$$

4. Find weights w_i so that $S_n(h)$ has order $\mathcal{O}\left(h^n\right)$.