State-dependent Trotter bounds

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Burgarth, Facchi, Hahn, Johnsson, Yuasa, in preparation (2023)

MPQT 2023 workshop at ICMS, 25/05/2023 in Edinburgh

Agenda

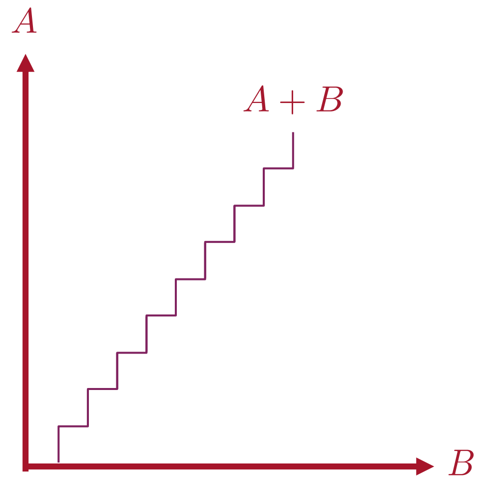
1. The Trotter product formula in Quantum Control and Dynamical Decoupling
2. State-dependent error bounds for finite-dimensional quantum systems
3. Lifting to infinite dimensions
4. Direct infinite-dimensional bounds and application in quantum chemistry

Quantum Control

Implement a target dynamics by only using some accessible dynamics

Given operators A, B, implement the dynamics under the sum $A+B$

Trotter product formula: $\left(\mathrm{e}^{-\mathrm{i}\frac{t}{N}A}\mathrm{e}^{-\mathrm{i}\frac{t}{N}B}\right)^N = \mathrm{e}^{-\mathrm{i}t(A+B)} + \mathcal{O}\left(\frac{t^2}{N}\right)$



Dynamical Decoupling

Decouple system dynamics from bath dynamics

$\mathscr{H} = \mathscr{H}_{\mathrm{s}} \otimes \mathscr{H}_{\mathrm{b}}$ $\qquad$ $H = H_{\mathrm{s}} \otimes \mathbb{1}_{\mathrm{b}} + \mathbb{1}_{\mathrm{s}} \otimes H_{\mathrm{b}} + \sum_i h_{\mathrm{s}}^{(i)} \otimes h_{\mathrm{b}}^{(i)}$

Intersperse Hamiltonian dynamics with action of finite unitary group V that acts irreducibly, i.e., via

$\mathrm{Ad}_g(A) = gAg^{\dagger}, g \in V, A \in \mathscr{H}_{\mathrm{s}}$

$$\left(Z\mathrm{e}^{-\mathrm{i}\frac{t}{4N}H}ZY\mathrm{e}^{-\mathrm{i}\frac{t}{4N}H}YX\mathrm{e}^{-\mathrm{i}\frac{t}{4N}H}X\mathbb{1}\mathrm{e}^{-\mathrm{i}\frac{t}{4N}H}\mathbb{1}\right)^N$$

$$\begin{aligned}\tilde{H} &= \frac{1}{4}(ZHZ + YHY + XHX + H)\\ &= \mathbb{1}_{\mathrm{s}} \otimes H_{\mathrm{b}}\end{aligned}$$

J. Math. Phys. 59 032203 (2018)

Standard way

$$\left\|\left(\mathrm{e}^{-\mathrm{i}\frac{t}{N}A}\mathrm{e}^{-\mathrm{i}\frac{t}{N}B}\right)^N - \mathrm{e}^{-\mathrm{i}t(A+B)}\right\|_\infty \leq \frac{t^2}{2N}\,\|[A,B]\|_\infty$$

$$\|A\|_\infty = \sup_{\|\psi\|=1} \|A\psi\|$$

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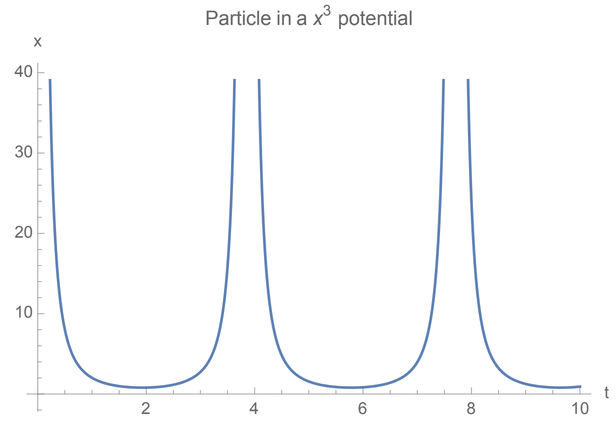
Example 1



- $A = p^2, B = x^3$
- $p^2 + x^3$ is not self-adjoint
- Trotter does not converge

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Example 2

$$\left\|\left(\mathrm{e}^{-\mathrm{i}\frac{t}{N}A}\mathrm{e}^{-\mathrm{i}\frac{t}{N}B}\right)^N - \mathrm{e}^{-\mathrm{i}t(A+B)}\right\|_\infty = 2$$

- $A = p, B = x^k, k \geq 2$
- Norm difference becomes maximal
- Trotter does not converge

Phys. Rev. X **11**, 011020 (2021), Amer. J. Phys. 61, 605-611 (1993), Lett. Math. Phys. **70**, 65-81 (2004)

Strong convergence

$$\left\| \left(e^{-i\frac{t}{N}A} e^{-i\frac{t}{N}B} \right)^N \psi - e^{-it(A+B)}\psi \right\|$$

Strong error bounds in finite dimensions

$\dim(\mathscr{H}) < \infty$

$A = A^\dagger, B = B^\dagger$

$(A + B)\varphi = h\varphi$

$$\left\| \left(\mathrm{e}^{-\mathrm{i}\frac{t}{N}A} \mathrm{e}^{-\mathrm{i}\frac{t}{N}B} \right)^N \varphi - \mathrm{e}^{-\mathrm{i}t(A+B)}\varphi \right\| \le \frac{t^2}{2N} \left(\left\| \left[A - \frac{h}{2} \right]^2 \varphi \right\| + \left\| \left[B - \frac{h}{2} \right]^2 \varphi \right\| \right)$$

Proof sketch of strong error bounds

Generator of Trotterized evolution: $H_1(s) = \begin{cases} A, & s \in \left[0, \frac{t}{N}\right) \\ B, & s \in \left[\frac{t}{N}, \frac{2t}{N}\right) \end{cases}$ extended periodically $H_1\left(s + \frac{2t}{N}\right) = H_1(s)$

Generator of target evolution: $H_2(s) = \frac{A+B}{2}$ (time-independent average Hamiltonian)

Lemma 1 of Quantum 6, 737 (2022)

$$U_2(2t) - U_1(2t) = \cancel{-\mathrm{i}S_{21}(2t)U_2(2t)} - \int_0^{2t} U_1(2t)U_1(s)^\dagger \left[H_1(s)S_{21}(s) - S_{21}(s)H_2(s)\right] U_2(s)\mathrm{d}s$$

where $$S_{21}(t) = \int_0^t \left[H_2(s) - H_1(s)\right] \mathrm{d}s$$ (integral action)

The integral action vanishes after a full Trotter cycle, so that the first summand is zero. It follows:

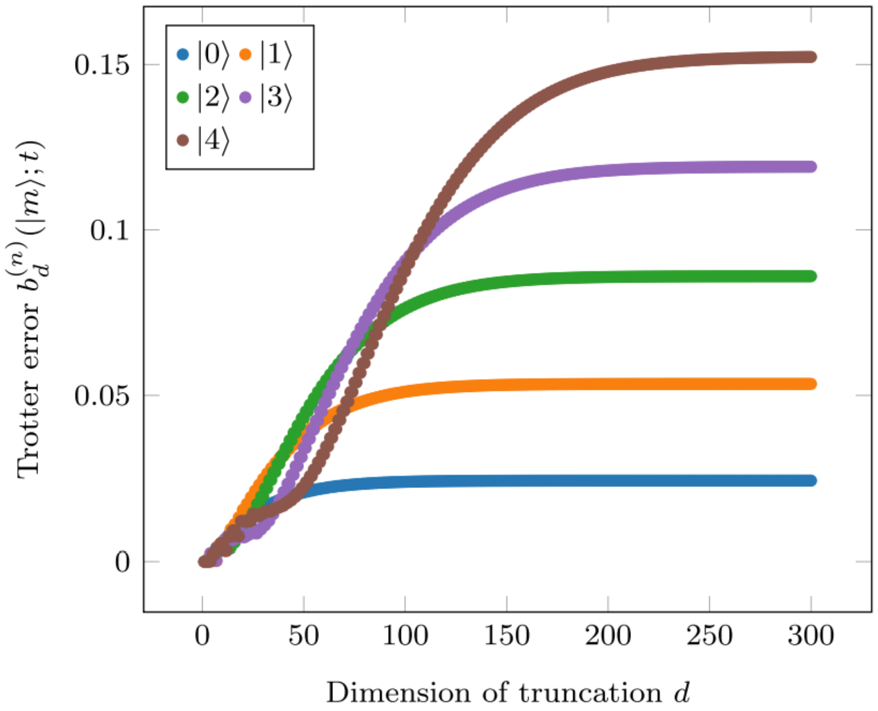
$$\|\left[U_2(2t) - U_1(2t)\right]\varphi\| \leq \int_0^{2t} \left\| \left[H_1(s) - \frac{h}{2}\right] S_{21}(s)\varphi \right\| \mathrm{d}s$$

Computing the integral gives the bound

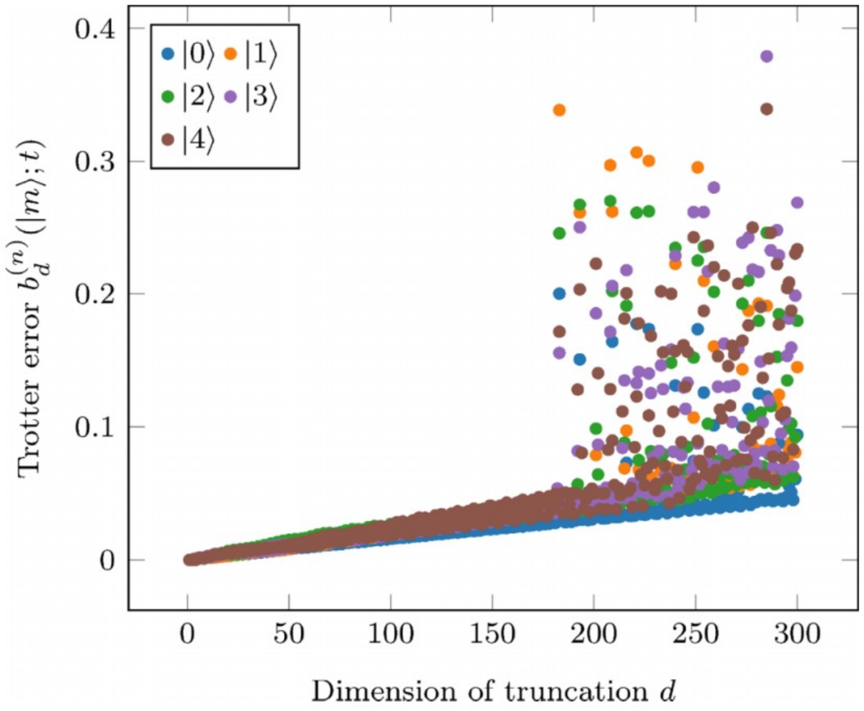
Lifting to infinite dimensions

Truncate Hilbert space at finite level d and project all operators and states onto the finite-dimensional subspace

$V_d = \mathrm{span}(|0\rangle, \dots, |d-1\rangle)$ with $P = \sum_{i=1}^{d} |i\rangle \langle i|$



$$A = \frac{1}{2}(q^2 + p^2), B = \frac{1}{2}(qp + pq)$$



$$A = p^2, B = q^3$$

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Lifting to infinite dimensions

Define $$b_d^{(N)}(\psi;t) \equiv \left\| \left(\mathrm{e}^{-\mathrm{i}\frac{t}{N}A_d}\mathrm{e}^{-\mathrm{i}\frac{t}{N}B_d}\right)^N \psi_d - \mathrm{e}^{-\mathrm{i}t(A_d+B_d)}\psi_d \right\|$$

$$b^{(N)}(\psi;t) \equiv \limsup_{d\to\infty} b_d^{(N)}(\psi;t)$$

Theorem:

$$\operatorname*{s-lim}_{N\to\infty} \left(\mathrm{e}^{-\mathrm{i}\frac{t}{N}A}\mathrm{e}^{-\mathrm{i}\frac{t}{N}B}\right)^N = \mathrm{e}^{-\mathrm{i}t(A+B)}$$

if (i) A and B can be simultaneously approximated by the same truncation scheme, i.e. $\mathcal{V} = \bigcup_d V_d$ is a common core,

(ii) for all $t \in \mathbb{R}$, $\lim_{N\to\infty} b^{(N)}(\psi;t) = 0$.

Proof sketch of truncation result

Show that $\mathrm{e}^{-\mathrm{i}t(A_d+B_d)}\psi$ has a well-defined limit $\phi(t)$ as $d \to \infty$

Trotter-Kato approximation theorems I & II

$$\lim_{N\to\infty} \left(\mathrm{e}^{-\mathrm{i}\frac{t}{N}A_d}\mathrm{e}^{-\mathrm{i}\frac{t}{N}B_d}\right)^N \psi = \mathrm{e}^{-\mathrm{i}t(A_d+B_d)}\psi$$

Finite-dimensional Trotter product

$$\lim_{N\to\infty} \left(\mathrm{e}^{-\mathrm{i}\frac{t}{N}A}\mathrm{e}^{-\mathrm{i}\frac{t}{N}B}\right)^N \psi = \phi(t)$$

assumption $\lim_{N\to\infty} b^{(N)}(\psi;t) = 0$

$\phi(t) = U(t)\psi$ and the generator of the unitary $U(t)$ agrees with $A+B$ wherever both are defined

Properties of one-parameter semigroups, see Engel & Nagel

Practicality

In practice, we only need to consider basis vectors:

If $\psi \in \mathcal{V}$, there exists a truncation dimension d, such that $\psi = \sum_{i=0}^{d-1} \langle i|\psi\rangle |i\rangle$

Thus, by triangle inequality

$$b^{(N)}(\psi;t) \leq \left(\sum_{i=0}^{d-1} |\langle i|\psi\rangle|^2 b^{(N)}(|i\rangle;t)^2 \right)^{1/2}$$

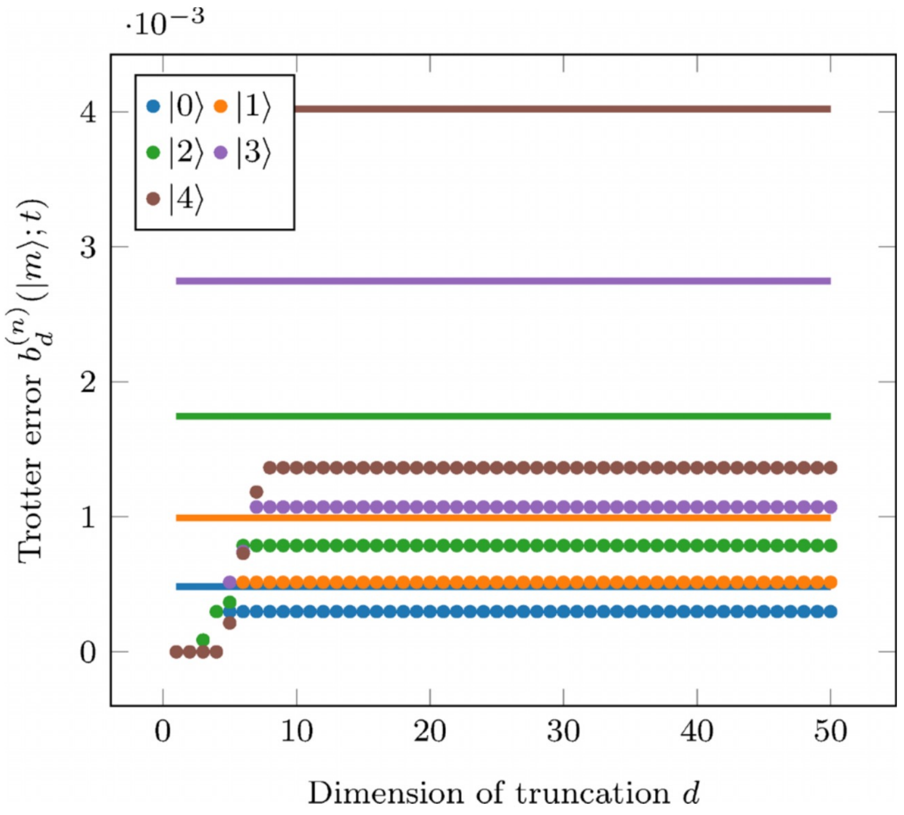
Immediately obtain Trotter bound for infinite-dimensional case

Naturally generalizes to more than two operators

Example

Harmonic oscillator: $A = \frac{1}{2}q^2, B = \frac{1}{2}p^2$

$$b_d^{(N)}(|m\rangle\,;t) \leq \frac{t^2}{4N}\sqrt{\frac{3}{8}[m(m+1)(m^2+m+14)+10]}$$



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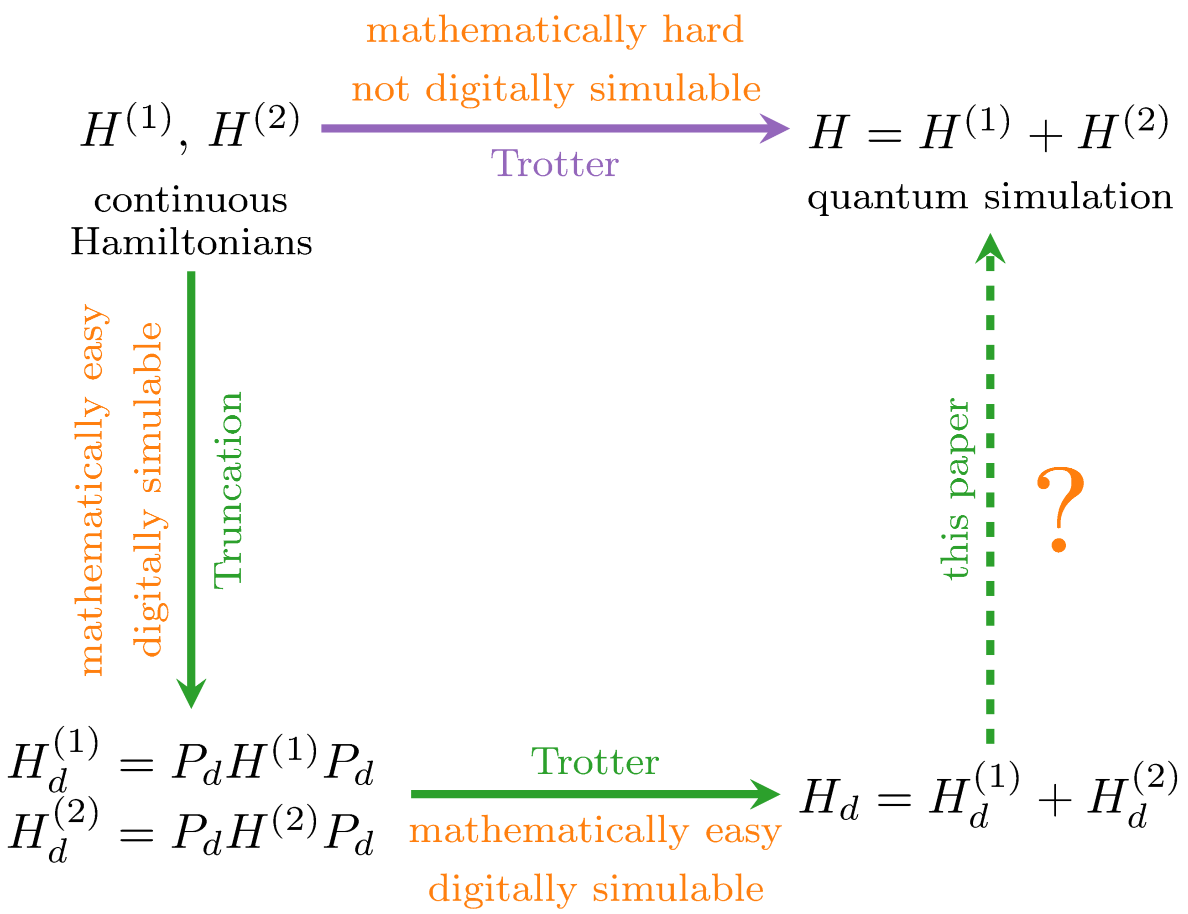
Applications



Direct infinite-dimensional bounds

A self-adjoint on $\mathcal{D}(A)$ and B self-adjoint on $\mathcal{D}(B)$

$\varphi \in \mathcal{D}(A^2) \cap \mathcal{D}(B^2)$

$(A+B)\varphi = h\varphi$

Then for all $g \in \mathbb{R}$

$$\xi_N(t;\varphi) \equiv \left\| \left(\mathrm{e}^{-\mathrm{i}\frac{t}{N}A} \mathrm{e}^{-\mathrm{i}\frac{t}{N}B} \right)^N \varphi - \mathrm{e}^{-\mathrm{i}th}\varphi \right\| \leq \frac{t^2}{2N} \left(\left\| \left[A-g\right]^2 \varphi \right\| + \left\| \left[B-h+g\right]^2 \varphi \right\| \right)$$

In particular, the Trotter product formula converges on φ

(Notice difference $\xi_N(t;\varphi) \neq b^{(N)}(\varphi;t)$)

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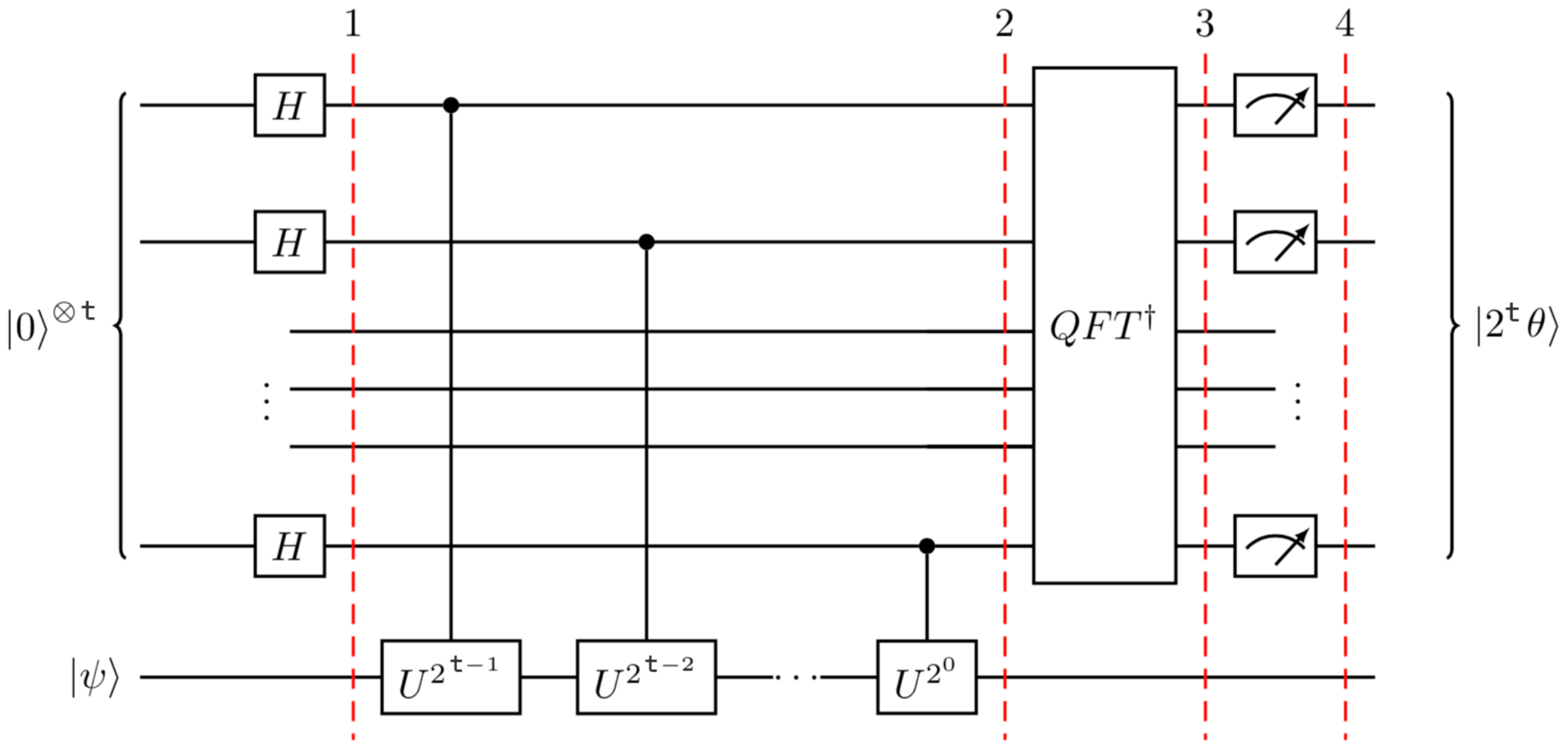
Quantum Phase Estimation



Source: https://learn.qiskit.org/course/ch-algorithms/quantum-phase-estimation

Superposition states

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For superposition states

$$\psi = \sum_i c_i \varphi_i$$

$$\xi_N(t;\psi) \leq \sum_i \frac{t^2}{2N} |c_i| \left(\left\| \left[A - g\right]^2 \varphi_i \right\| + \left\| \left[B - h + g\right]^2 \varphi_i \right\| \right)$$

(RHS defined as ∞ if not converging)

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The hydrogen atom

Split-step method: Trotterize between kinetic and potential energy

$$A = -\frac{\hbar^2}{2m_\mathrm{e}}\Delta \qquad\qquad B = -\frac{\hbar^2}{m_\mathrm{e}a_0}\frac{1}{r}$$

$H^{\mathrm{hydro}} = A + B$ has eigenvalues $E_n = -\frac{\hbar^2}{m_\mathrm{e}a_0^2}\frac{1}{2n^2}$ corresponding to its radial eigenfunctions

$$R_{n\ell}(r) = \left(\frac{2}{a_0 n}\right)^{3/2}\sqrt{\frac{(n-\ell-1)!}{2n(n+\ell)!}}\mathrm{e}^{-r/a_0 n}(2r/a_0 n)^\ell L_{n-\ell-1}^{(2\ell+1)}(2r/a_0 n)$$

where

$$L_n^{(\alpha)}(x) = \sum_{i=0}^{n}\frac{(-1)^i}{i!}\binom{n+\alpha}{n-i}x^i$$

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Azimuthal quantum number ℓ	**Scaling of bound for Trotter error $\xi_N(t; R_{n\ell})$**
$\ell = 0$ (s-orbitals)	$\mathcal{O}\left(\frac{t^2}{n^{3/2}}\frac{1}{N^{1/4}}\right)$
$\ell = 1$ (p-orbitals)	$\mathcal{O}\left(\frac{t^2}{n^{3/2}}\frac{1}{N^{3/4}}\right)$
$\ell \geq 2$ (d-orbitals and higher)	$\mathcal{O}\left(\frac{t^2}{n^{3/2}}\frac{1}{N}\right)$

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Trotter theorem applied to the hydrogen atom

If only $\varphi \in \mathcal{D}(A) \cap \mathcal{D}(B)$, then

$$\xi_N(t;\varphi) \leq N \left\| \left(\mathrm{e}^{-\mathrm{i}\frac{t}{N}A} - 1 + \mathrm{i}\frac{t}{N}A \right) \varphi \right\| + N \left\| \left(\mathrm{e}^{-\mathrm{i}\frac{t}{N}B} - 1 + \mathrm{i}\frac{t}{N}B \right) \varphi \right\|$$

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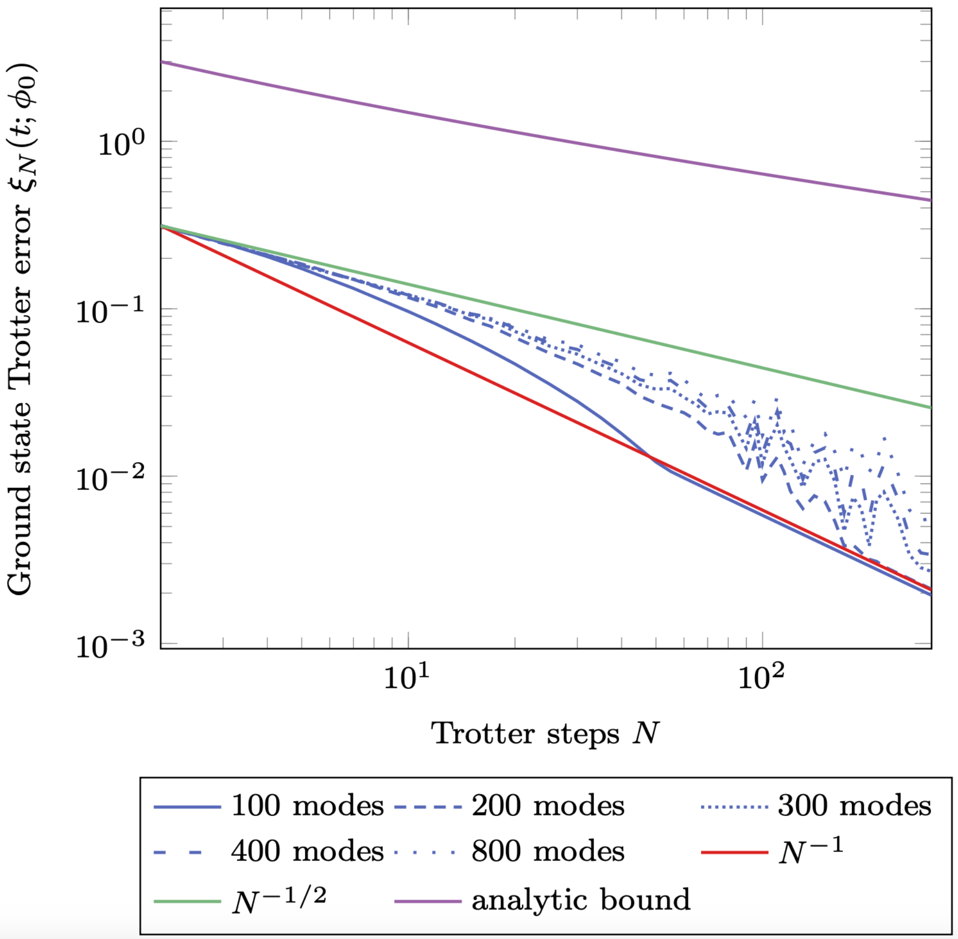

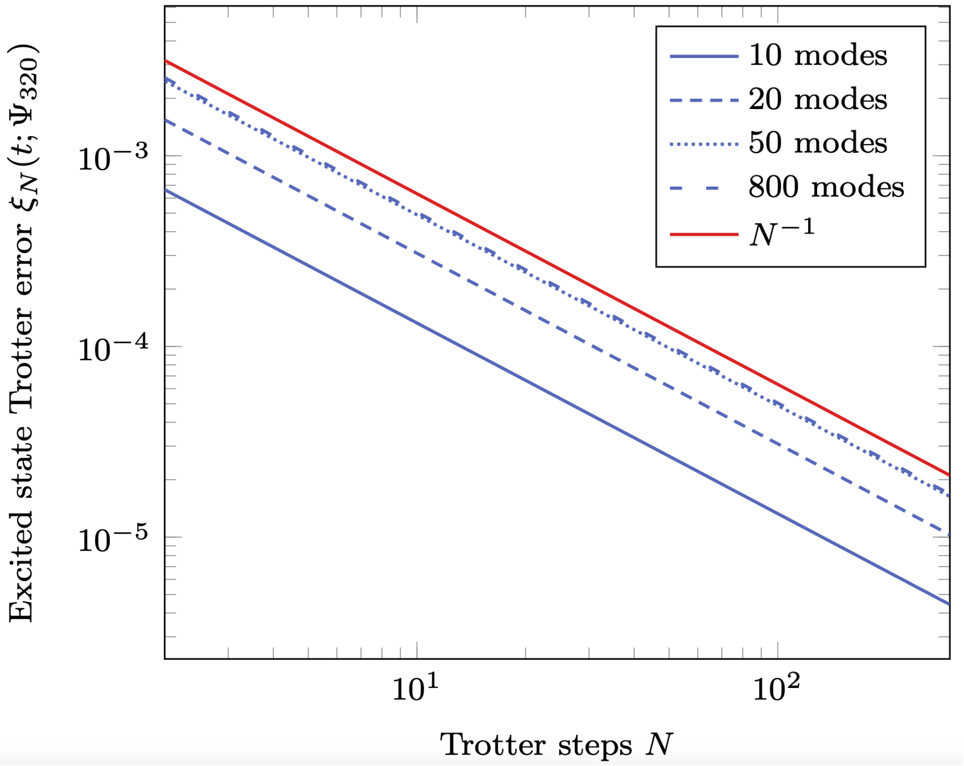

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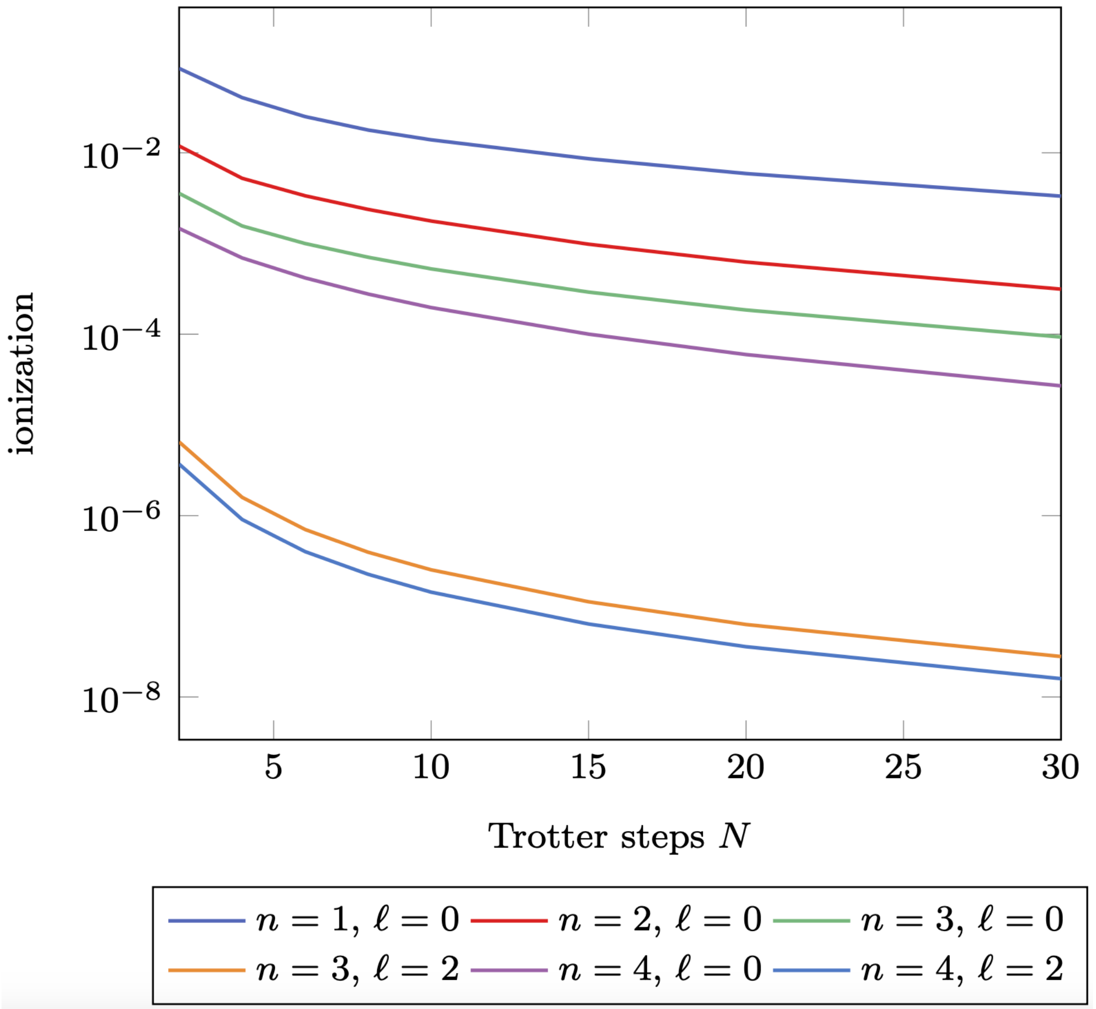

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Higher order Trotterization

$$\mathcal{S}_2(t,N) = \left(\mathrm{e}^{-\mathrm{i}\frac{t}{2N}A}\mathrm{e}^{-\mathrm{i}\frac{t}{N}B}\mathrm{e}^{-\mathrm{i}\frac{t}{2N}A}\right)^N$$

$$\mathcal{S}_4(t,N) = [\mathcal{S}_2(s_2t,N)]^2\mathcal{S}_2([1-4s_2]t,N)[\mathcal{S}_2(s_2t,N)]^2, \quad s_2 = 1/(4-4^{1/3})$$

$$\left\|\mathcal{S}_p(t,N) - \mathrm{e}^{-\mathrm{i}t(A+B)}\right\|_\infty = \mathcal{O}\left(\frac{t^{p+1}}{N^p}\right)$$

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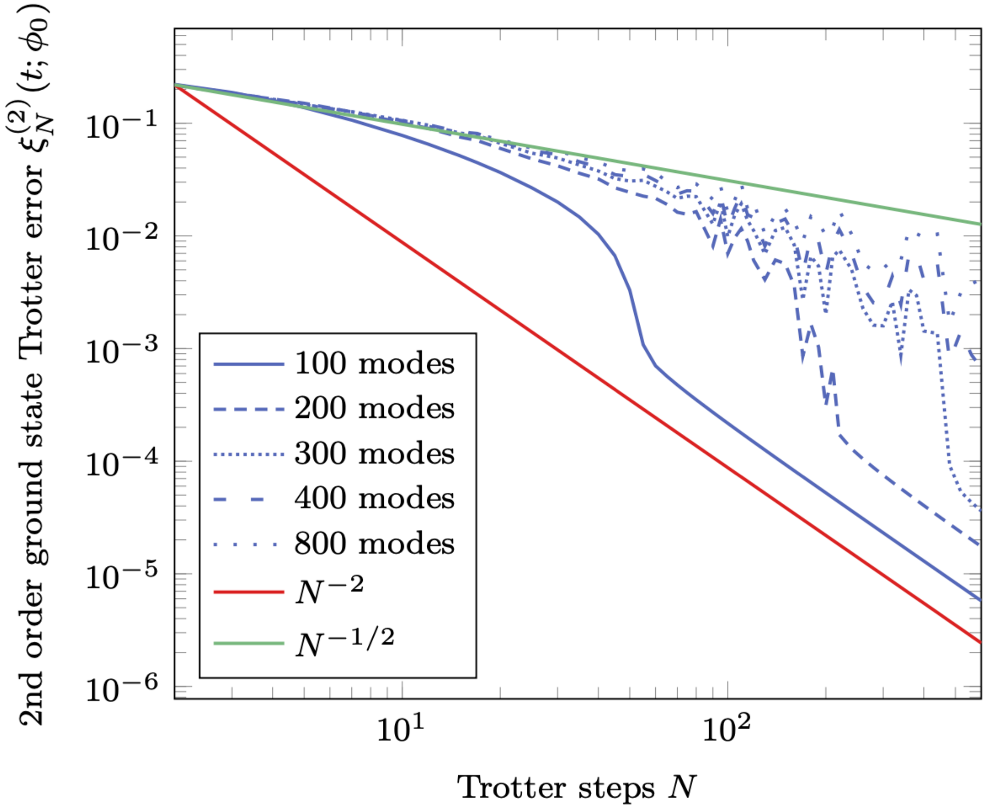
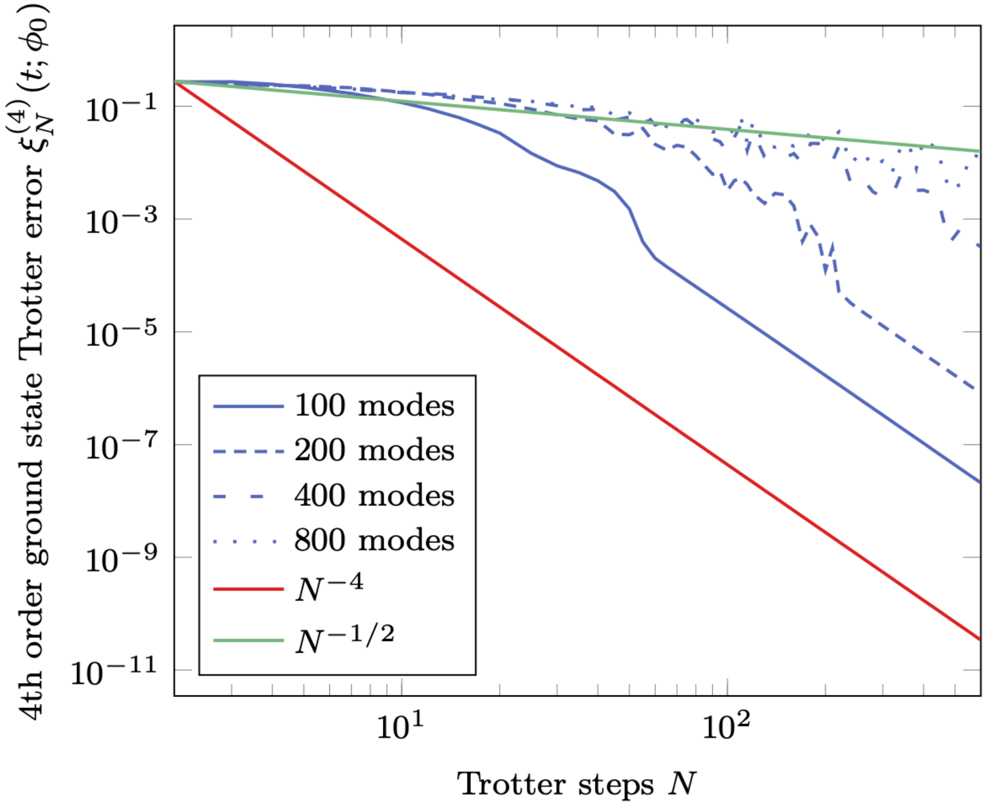
Higher order Trotterization hydrogen atom





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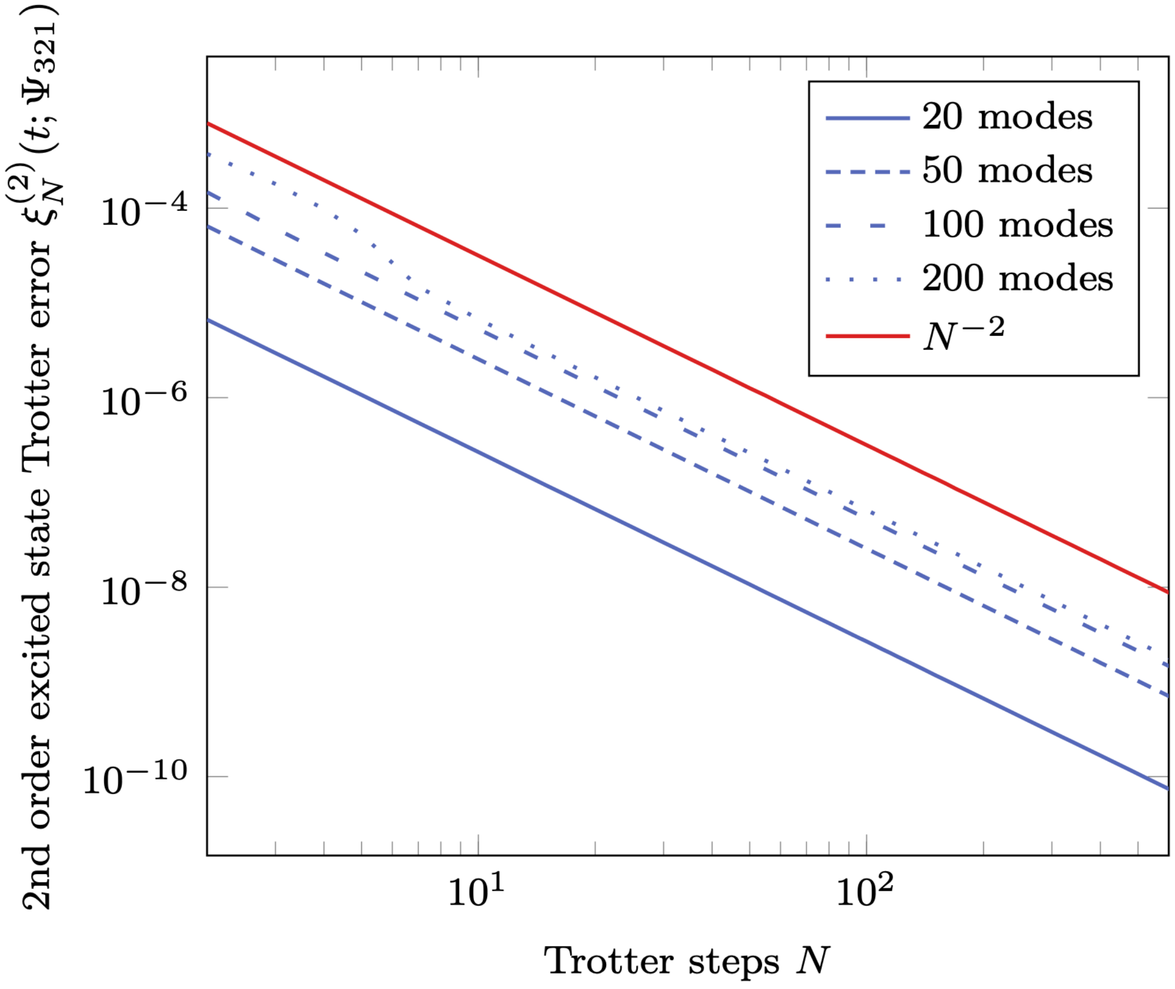
Higher order Trotterization hydrogen atom



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Summary

State-dependent Trotter error bound for finite-dimensional systems

Lifting this bound to infinite-dimensions and show Trotter convergence

Trotter error for low energy input states in quantum chemistry scales slower

Higher order Trotter hierarchy seems to break down for low energy input states in quantum chemistry

Open Research Questions

Bounds for generic states (not only eigenstates) → even finite-dimensional

Generalized eigenfunctions (rigged Hilbert space)

Case study of more complicated atoms and molecules (bounds for generic states needed)