Time-dependent Hamiltonian Simulation of Highly Oscillatory Dynamics

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Based on joint work with Dong An (U Maryland) and Lin Lin (UC Berkeley)

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Outline

1. Highly Oscillatory Dynamics
   - First source of oscillations
   - Second source of oscillations
2. Major Question
3. Our work (qHOP)
   - Idea of the algorithm
   - Interaction Picture and Superconvergence
4. Conclusion and Remarks

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$$H(t) \equiv H, \quad \left\|\mathcal{U}_{\text{app}} - e^{-\mathrm{i}Ht}\right\| \leq \epsilon.$$

$$\left\|\mathcal{U}_{\text{app}} - \mathcal{T}e^{-\mathrm{i}\int_0^t H(s)\,ds}\right\| \leq \epsilon.$$

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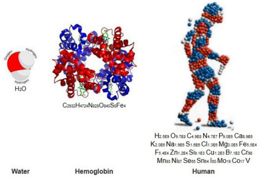
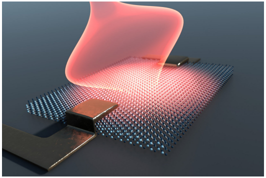
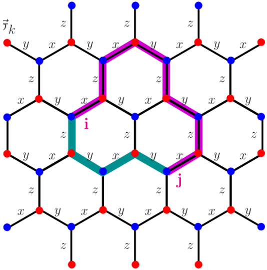
- 1st source: $\|H\|$ is large.
- 2nd source: $H(t)$ oscillates itself!

Highly Oscillatory Dynamics are Ubiquitous!







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Time-independent Ham. Sim.

- Trotterization:
  1st-order Trotter formula
  $$e^{-\mathrm{i}Ht} = \left(e^{-\mathrm{i}H_1 t/L} e^{-\mathrm{i}H_2 t/L}\right)^L + \mathcal{O}(\|[H_1, H_2]\| t^2/L)$$
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- LCU, e.g. Truncated Taylor series:
  $$\mathcal{O}\left(\|H\| t \frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right).$$
- Qubitization/QSP/QSVT: $\mathcal{O}(\|H\| t + \log(1/\epsilon))$
- Randomized algorithms e.g., qDRIFT: *Weak Convergence* wrt the diamond norm of Quantum channels
  $$\mathcal{O}\left(\|H\| t^2/\epsilon\right).$$

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Commutator scaling gives great cancellation. [Childs-Su-et al. 2021]

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e.g. interaction picture $e^{\mathrm{i}As}Be^{-\mathrm{i}As}$ with $\|A\| \gg 1$.

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- Trotterization: $H = H_1(t) + H_2(t)$

$$\mathcal{T} e^{-\mathrm{i} \int_{t_j}^{t_{j+1}} H(s)\, ds} \approx e^{-\mathrm{i} h H_2(\tau_j)} e^{-\mathrm{i} h H_1(\tau_j)},$$

where $\tau_j \in [t_j, t_{j+1}]$ are chosen according to Suzuki construction. The number of unitaries depends on $\|\partial_t H(t)\|$.

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Applying to interaction picture (IP)?

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  Interaction Picture: Best asymptotic scaling. The circuit requires complicated quantum control logic for time clocking, which can lead to undesirable constant factor. [2]

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  Interaction Picture: hybridized methods (first order) [2]

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Major Question

- Two challenges: $\|H\|$ large; rapid change of H.
- Two desirable features:
  commutator scaling (like Trotter for time-independent);
  weak dependence on derivatives (e.g. randomized/ Dyson-based methods).
- Question: Can we get both?

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- remaining insensitive to the rapid change of the Hamiltonian
  ✓**(log dependence on derivative)**
- is high-order (in accuracy).
- achieves **superconvergence** in the digital simulation of Schrödinger equation, yielding a surprising second order convergence rate.

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A naive (but insufficient) attempt for commutator bound

- Standard Trotter: As an example, take the special controlled form

$$H(t) = f_1(t)H_1 + f_2(t)H_2$$

with f_1 and f_2 smooth and scalar, and the second order time discretization. (step size: h) [Lloyd 1996]

$$U_s(t+h,t) = e^{-\frac{ih}{2}f_1(t+\frac{h}{2})H_1} e^{-ihf_2(t+\frac{h}{2})H_2} e^{-\frac{ih}{2}f_1(t+\frac{h}{2})H_1}.$$

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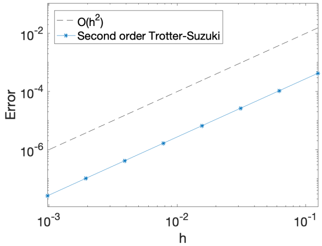

Take the case $[H_1, H_2] = 0$.

Error is not machine precision!
$\Rightarrow$ No commutator scaling.

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- Generalized Trotter [Huyghebaert–De Raedt 1990]
For general $H_1(t) + H_2(t)$,

$$\mathcal{T}e^{-\mathrm{i}\int_{t_j}^{t_{j+1}} H(s)\,ds} = \mathcal{T}e^{-\mathrm{i}\int_{t_j}^{t_{j+1}} H_1(s)\,ds}\mathcal{T}e^{-\mathrm{i}\int_{t_j}^{t_{j+1}} H_2(s)\,ds} + \mathcal{O}\Big(\max_{s,\tau\in[t_j,t_{j+1}]}\|[H_1(s),H_2(\tau)]\|\,h^2\Big).$$

NOT an algorithm yet! Two time-dependent Ham. sim. problems still need to implement!

Idea of qHOP

$$U(t_{n+1}, t_n) = \mathcal{T} e^{-\mathrm{i} \int_{t_n}^{t_{n+1}} H(s) ds} \approx e^{-\mathrm{i} \int_{t_n}^{t_{n+1}} H(s) ds} \quad [4]$$

[4] widely used in Trotter for time-dependent Ham., randomized product formula, e.g. [Poulin-Qarry-Somma-Verstraete 2011], classical Magnus integrator, etc

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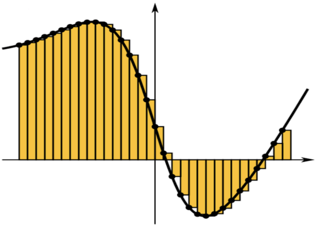

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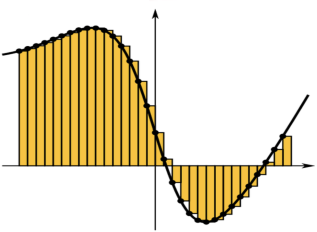

- Rectangular quadrature (*aka* Riemann sum with M quadrature points).

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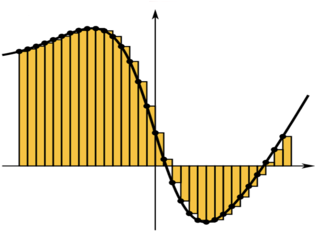

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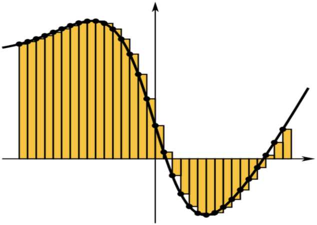

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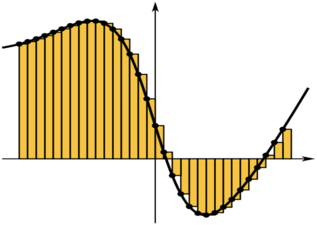

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- Time-dependent Ham. Sim $\Rightarrow$ Time-independent! can use QSVT and OAA.

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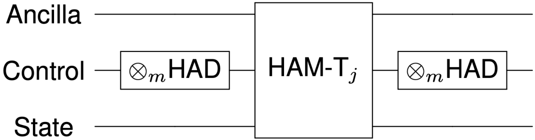
Answer to Q1:



[4] widely used in Trotter for time-dependent Ham., randomized product formula, e.g. [Poulin-Qarry-Somma-Verstraete 2011], classical Magnus integrator, etc

Idea of qHOP

$$U(t_{n+1},t_n) = \mathcal{T}e^{-\mathrm{i}\int_{t_n}^{t_{n+1}} H(s)ds} \approx e^{-\mathrm{i}\int_{t_n}^{t_{n+1}} H(s)ds}$$ [4]

$$\approx e^{-\mathrm{i}h\frac{1}{M}\sum_{k=0}^{M-1} H(jh+kh/M)}$$

Questions:

1. How to implement?
2. What are the approximation errors?

Answer to Q2: (h: step size)

$$\|U_{\text{exact}}(t_{j+1},t_j) - U_{\text{num}}(t_{j+1},t_j)\|$$
$$\leq h^2\Big(\underbrace{\frac{1}{2}\max_{s,\tau\in[jh,(j+1)h]}\|[H(\tau),H(s)]\|}_{\text{Dropping time-ordering}} + \underbrace{\frac{1}{M}\max_{s\in[jh,(j+1)h]}\|H'(s)\|}_{\text{numerical quadrature error}\Rightarrow\log\ \text{(LCU)}}\Big).$$

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$$\widetilde{\mathcal{O}}\left(\max_{s,t\in[0,T]} \|[H(s),H(t)]\|\frac{T^2}{\epsilon} + \max_{s\in[0,T]} \|H(s)\|T\right)$$

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Application to Interaction Picture

$H = A + B$ and A has a much larger norm but fast-forwardable.

$\mathrm{i}\partial_t \psi = H\psi = (A + B)\psi$

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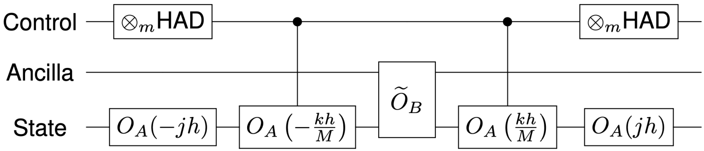
Challenges? highly oscillatory time-dependent problem

Interaction Picture $A + B(t)$

Take $A + B$ for simplicity. It also works for $A + B(t)$ (and even $f(t)A + B(t)$) given $O_A(s) := e^{-\mathrm{i}As}$ fast-forwardable.

$$H_I(s) = e^{\mathrm{i}As} B e^{-\mathrm{i}As}$$



$$\|U_{\text{exact}}(T,0) - U_{\text{num}}(T,0)\|$$
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Superconvergence for the Schrödinger equation

Schrödinger equation (Unbounded/Real-space Ham. Sim.)

$$H = -\Delta + V(x)$$

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Take one-spatial dimension with domain $[0, 1]$ for simplicity. Using N spatial grids,

$$\Delta_h^{\text{per}} := N^2 \begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ 1 & & & 1 & -2 \end{pmatrix},$$

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After discretization using N spatial grids, $\|A\| = \|-\Delta_h\| = \mathcal{O}(N^2)$!
But gate $\sim \mathcal{O}(\|H\| n^k)$, where n is the number of qubits and $2^n = N$.

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Superconvergence for the Schrödinger equation

Commutator reductions?

$$\|[A,B]\| \sim N, \quad \|[B,[A,B]]\| \sim N, \quad \|[A,[A,B]]\| \sim N^2$$

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N-independent operator norm scaling? $\Rightarrow$ Interaction Picture!

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Superconvergence for the Schrödinger equation

$$h \max_{s\in[-h,h]} \left\| [B, e^{\mathrm{i}As} B e^{-\mathrm{i}As}] \right\| \leq 2h \left\| B \right\|^2$$

$\Rightarrow$ First order scheme with N independent error preconstant.

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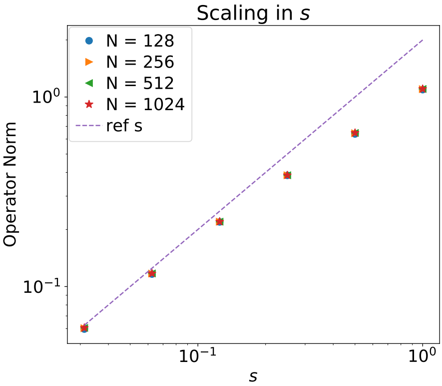
Theorem (An-Fang-Lin arXiv:2111.03103)

For a smooth function V bounded together with all of its derivatives and $0 < h \le 1$, we have

$$\max_{s\in[-h,h]} \left\|[V(x), e^{\mathrm{i}s\Delta} V(x) e^{-\mathrm{i}s\Delta}]\right\|_{\mathcal{L}(L^2)} \le C_V h,$$

where C_V depending only on V and its the derivatives (and independent of the number of spatial grids N!).

Numerical Evidence of Superconvergence



High Level Idea of the Proof of Superconvergence

$$[B, e^{\mathrm{i}As} B e^{-\mathrm{i}As}].$$

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Imagine Taylor expand $e^{\mathrm{i}As} = I + \mathrm{i}As + \cdots$ and $e^{-\mathrm{i}As}$.

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- But this still depend on A which depends on the number of spatial grids N!
- Note this indeed resembles Trotter, where second order Trotter depends on $[B, [A, B]] \sim N$ and $[A, [A, B]] \sim N^2$.

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No truncations! Borrow from pseudo-differential calculus.

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op$(a(x,p))$ is a so-called quantization:

$$\mathrm{op}(x) = x, \quad \mathrm{op}(p) = -i\partial_x$$

$$e^{i\Delta s} V(x) e^{-i\Delta s} = \mathrm{op}(V(x - 2ps))$$

Exact! No truncation of series!

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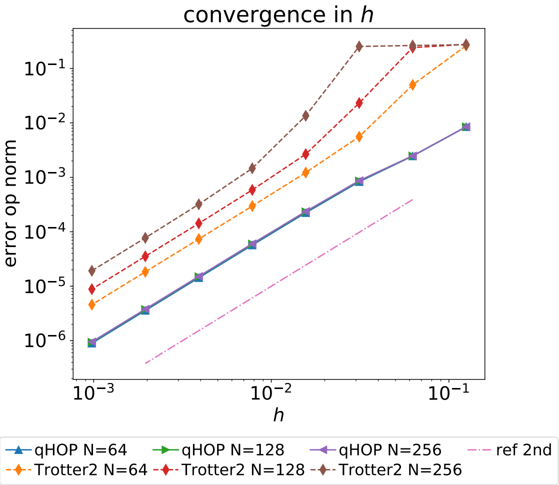
$$\sim \{V(x), V(x - 2ps)\} \sim \nabla_x V(x) \cdot \nabla_x V(x - 2ps) s$$

Numerical results: superconvergence



Connection with Trotterization

qHOP can be viewed as a generalization of the first and second order Trotter formulae.

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(Similarly, end-point quadrature rule gives the first order Trotter.)

Conclusion and Remark

We propose a simple algorithm, called quantum Highly Oscillatory Protocol (qHOP), which does not require complicated quantum control logic for handling time-ordering operators.

This new algorithm:

- to our knowledge, is the **first** quantum algorithm that is proved to simultaneously exhibit commutator scaling (in high precision limit) and remain insensitive to fast oscillations of $H(t)$.
- when applying to the interaction picture, can be viewed as a generalization of the first and second order Trotter formulae.
- achieves **superconvergence** for the digital simulation of the Schrödinger equation, achieving a surprising second order convergence *independent* of the number of spatial grids N.

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4. Problem set-up with physical/chemical applications.
5. Explicit dimension dependence.

References

1. Time-dependent Hamiltonian Simulation of Highly Oscillatory Dynamics, (with Dong An and Lin Lin) [arXiv:2111.03103].

2. Time-dependent unbounded Hamiltonian simulation with vector norm scaling, (with Dong An and Lin Lin), Quantum, 2021 [arXiv 2012.13105].

Thank you for your attention! (and ...)

IPAM long program “Mathematical and Computational Challenges in Quantum Computing”, Fall 2023

Workshop 1: Quantum algorithms for scientific computation

Workshop 2: Mathematical aspects of quantum learning

Workshop 3: Many-body quantum systems via classical and quantum computation

Workshop 4: Topology, quantum error correction and quantum gravity

Lecture Notes on “Quantum Algorithms for Scientific Computation” by Lin Lin [arXiv:2201.08309]

Di