Time-evolution with quantum computers (continued)

Previously we derived the LO Trotter expansion of the evolution operator $U(t) = e^{-iHt}$:

if $H = \sum_{k=1}^{L} H_k$, the LO Trotter approx is

$$U(t)_{LO} = \left(\prod_{k=1}^{L} U_k(\Delta_t) \right)^{N_S} \qquad (*)$$

where $\begin{cases} \Delta_t = \dfrac{t}{N_S} = \text{time step.} \\ N_S = \text{number of "Trotter steps".} \end{cases}$

The error associated with this approximation is $O\left(\frac{t^2}{N_S} * L\right) = O\left(\Delta_t^2 \; N_S * L\right)$

where L = # of commutators $[H_k, H_{k'}]$
$= O(n^c)$ when H is c-local
$= O(n)$ when H is also spatially local.

Examples

① Time-Evolution of a one-qubit system.

Consider a single spin in magnetic fields along x (transverse) and z (direction)

$$H = -\frac{\Gamma}{2} X - \frac{h}{2} Z .$$

$$U(t) = e^{-iHt}$$

$$\underset{\text{LO Trotter}}{\approx} \left(e^{+i\frac{\Gamma}{2} X \Delta_t} \; e^{+i\frac{h}{2} Z \Delta_t} \right)^{N_s}$$

In general, if the Hamiltonian has small dimensions, the exact exponentiation can be done numerically (classically) (e.g. Mathematica, Python etc).

This allows to study the impact of Trotterizing time evolution.

In the one-qubit case, one can also do that analytically since any one-qubit unitary can be written in terms of Euler rotations:

$$U(t) = e^{-iHt} = e^{i\phi} \, e^{i\theta_3 Z} \, e^{i\theta_2 Y} \, e^{i\theta_1 Z}$$

where the angles $\phi, \theta_3, \theta_2, \theta_1$ are related to Γ and h.

These relations can be found by direct matrix comparison -

Again numerically or analytically using e.g.:

$$U(t) = e^{-iHt} = e^{+\frac{i}{2}[\Gamma X + hZ]t}$$

$$= e^{i\frac{\alpha}{2}\hat{n}.\vec{\sigma}} = \cos\left(\frac{\alpha}{2}\right)\mathbb{1} - i\sin\left(\frac{\alpha}{2}\right)\hat{n}.\vec{\sigma}$$

with $\vec{n} = (\Gamma X + hZ)$

$$\Rightarrow \hat{n} = \frac{\vec{n}}{\|\vec{n}\|} = \frac{\Gamma X + hZ}{\sqrt{\Gamma^2 + h^2}}$$

$$\Rightarrow \alpha = \|\vec{n}\| \times t.$$

In the end this gives :

$$\begin{cases} \sin\theta_2 = \dfrac{\Gamma}{\eta}\sin\left(\dfrac{\eta t}{2}\right) \\ \tan(2\theta_1) = -\dfrac{\eta}{h(\tan \eta t/2)} \\ \theta_3 = \theta_1 + \pi/2 \end{cases}$$

where $\eta = \|\vec{n}\| = \sqrt{\Gamma^2 + h^2}$

One can then compare the exact and Trotterized evolution of various quantities.

(Energy, survival probability ...)

$\downarrow$ $\langle \psi(t) | \hat{H} | \psi(t) \rangle$ (in class)

$\downarrow$ $|\langle \psi(0) | \psi(t) \rangle|^2$ (tutorial)

(see results in class)

(2) Time Evolution of a 2-qubit system :

$$\mathcal{H} = a\,\vec{\sigma}\cdot\vec{\sigma} = a\,(X\otimes X + Y\otimes Y + Z\otimes Z)$$

(this was the Hami of the Hydrogen atom
e^- + proton (with only spin degrees of freedom))

At LO Trotter :

$$U_{LO}(t) = \left[U_{LO}(\Delta_t)\right]^{N_S}$$

with $U_{LO}(\Delta_t) = e^{-iaXX\Delta_t}\, e^{-iaYY\Delta_t}\, e^{-iaZZ\Delta_t}$

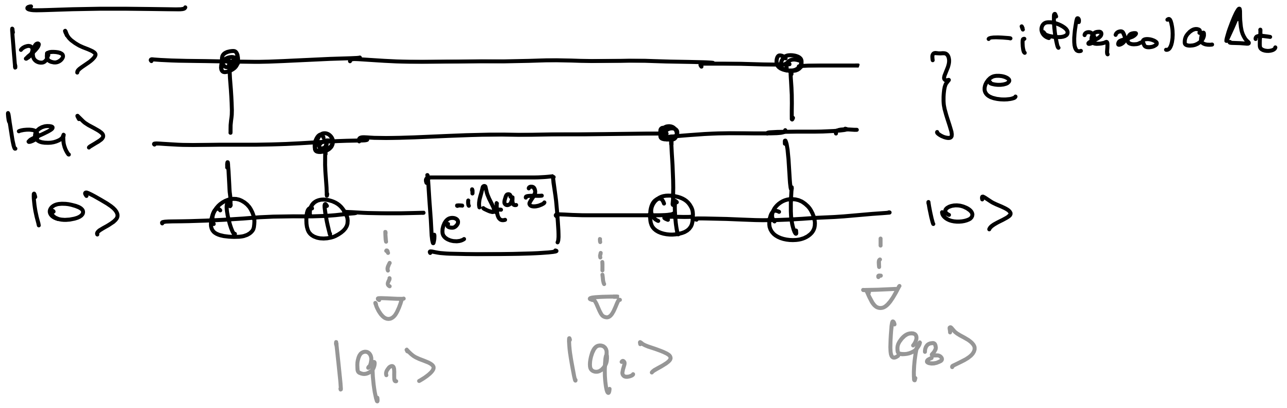
* Consider $U_{LO}^{ZZ}(\Delta_t) = e^{-iaZZ\Delta_t}$

Action on computational basis states :

$$e^{-iaZ_1Z_0\Delta_t}\,|x_1\,x_0\rangle = e^{-ia\phi(x_1,x_0)\Delta_t}\,|x_1\,x_0\rangle$$

$\Rightarrow$ phase which can be obtained using 1 ancilla qubit & CNOT gates to count how many qubits are in state $|1\rangle$, and rotating the ancilla qubit.

Circuit :



state of ancilla qubit

$$|q_1\rangle = |x_1 \oplus x_0\rangle$$

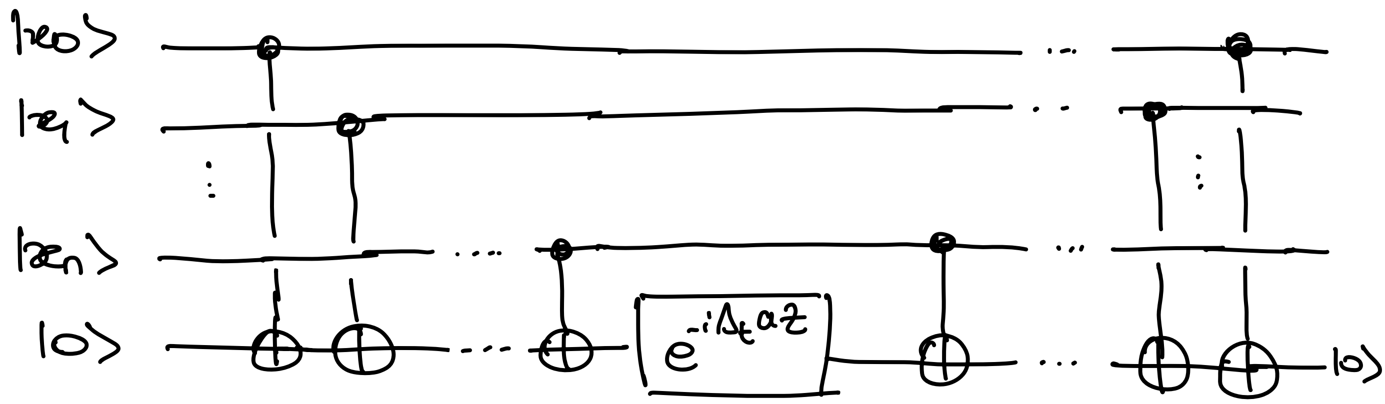
$$|q_2\rangle = e^{-i\Delta_t a (-)^{x_1 \oplus x_0}} \quad |x_1 \oplus x_0\rangle$$

$$|q_3\rangle = e^{-i\Delta_t a (-)^{x_1 \oplus x_0}} \quad |0\rangle$$

In the end the ancilla qubit is put back in its orignal state $|0\rangle$ while the phase has been kick-backed to the $|x_1 x_0\rangle$ register.

When the top qubits are entangled this will create a relative phase.

Generalization to n qubits:



" stair case algorithm "

* The same can be done for $U_\omega^{(xx)}(t)$ and $U_\omega^{(yy)}(t)$ using:

$$\begin{cases} X = HZH \\ Y = (SH)\,Z\,(SH)^\dagger \end{cases}$$

The trick is to see that

$$e^{OZO^{-1}} = O\, e^{Z}\, O^{-1}$$ (for O arbitrary invertible op.)

proof :

$$e^{OZO^{-1}} = \sum_{n=0}^{\infty} \frac{1}{n!} (OZO^{-1})$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \underbrace{\left(OZ\underbrace{O^{-1}O}_{\mathbb{1}}Z\underbrace{O^{-1}O}_{\mathbb{1}} \dots \underbrace{O^{-1}O}_{\mathbb{1}}ZO^{-1} \right)}_{OZ^nO^{-1}}$$

$$= O \left(\sum_{n=0}^{\infty} \frac{1}{n!} Z^n \right) O^{-1}$$

$$= O\, e^{Z}\, O^{-1} \quad ✓$$

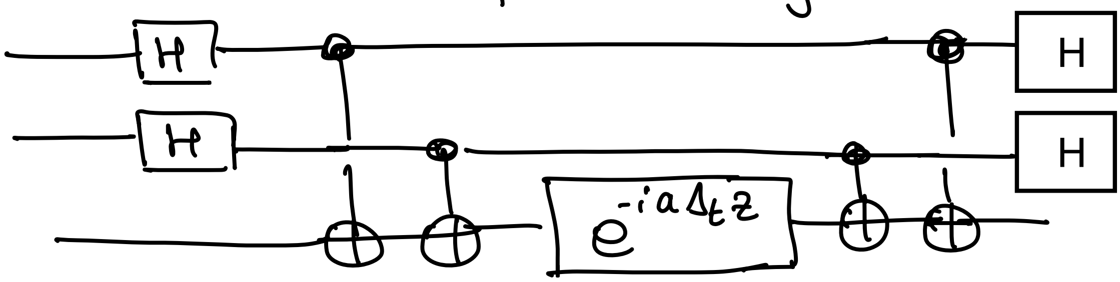
$$\Rightarrow U_{LO}^{(XX)}(\Delta_t) = e^{-ia X_1 X_0 \Delta_t}$$

$$= e^{-ia H_1 Z_1 H_1 H_0 Z_0 H_0 \Delta_t}$$

$$= e^{-ia (H_1 H_0) Z_1 Z_0 (H_0 H_1) \Delta_t}$$

$$= (H_1 H_0)\, e^{-ia Z_1 Z_0 \Delta_t} \underbrace{(H_0 H_1)}_{=(H_1 H_0)^{\dagger}}$$

$\Rightarrow$ simply need to apply Hadamard gates before and after the staircase :



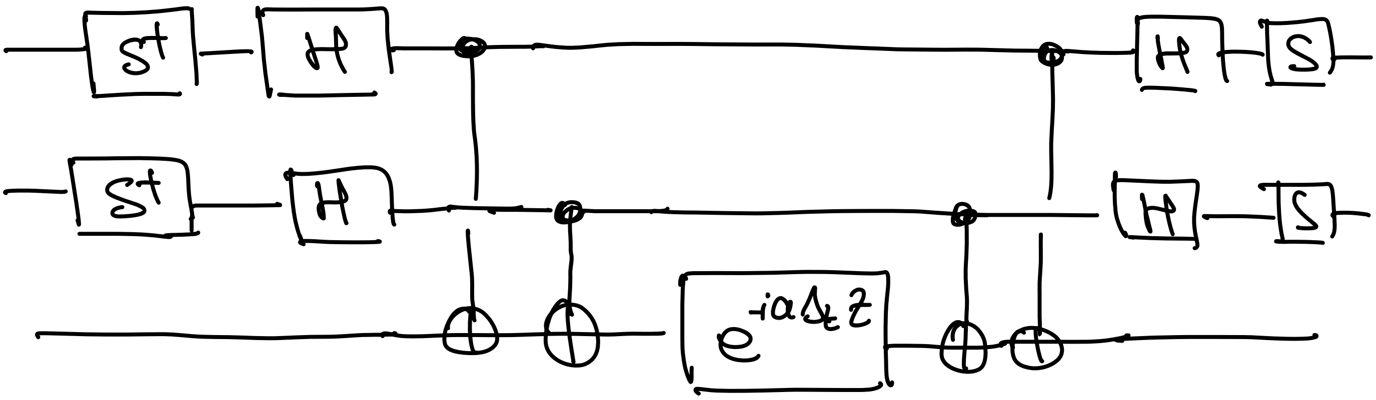
similarly

$$U^{(YY)}_{10}(\Delta_t) = e^{-ia\Delta_t Y_1 Y_0}$$

$$= e^{-ia\Delta_t (SH)_1 Z_1 (SH)_1^\dagger (SH)_0 Z_0 (SH_0)^\dagger}$$

$$= e^{-ia\Delta_t (SH)_1 (SH)_0 (Z_1 Z_0) (SH)_1^\dagger (SH)_0^\dagger}$$

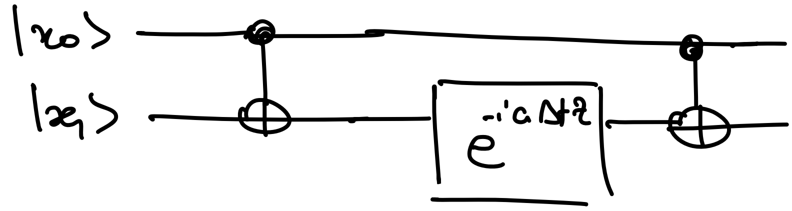
$$= S_1 H_1 S_0 H_0 \; e^{-ia\Delta_t Z_1 Z_0} \; H_1 S_1^\dagger H_0 S_0^\dagger$$



→ these is the text book approach

but these circuits can be optimized :

* ancilla qubit not needed :

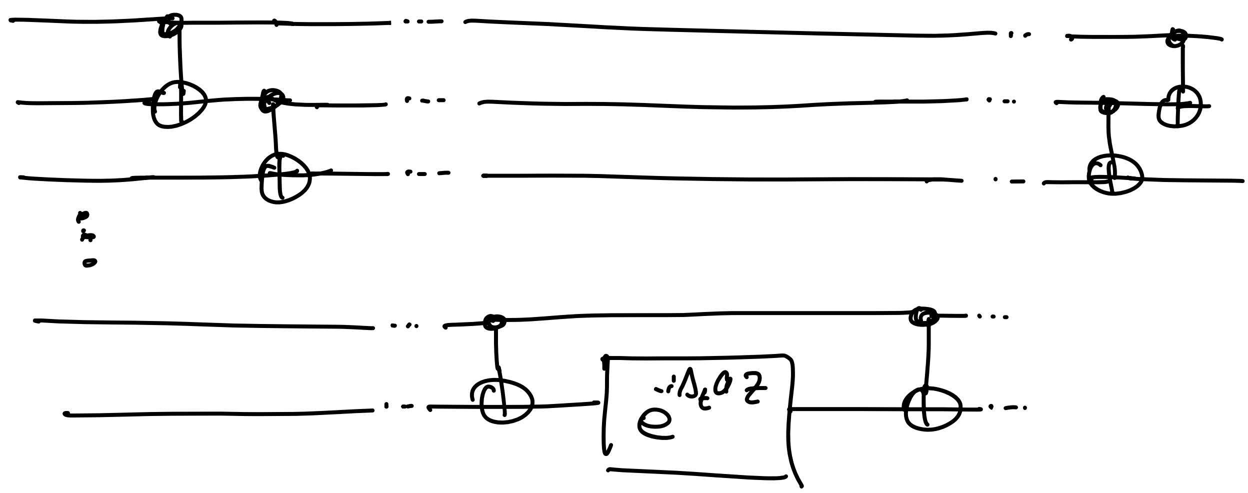


$$|x_1, x_0\rangle \xmapsto{\text{CNOT}} |x_1 \oplus x_0 \;\; x_0\rangle$$

$$\longmapsto e^{-i a \Delta t (-)^{x_1 \oplus x_0}} |x_1 \oplus x_0 \;\; x_0\rangle$$

$$\longmapsto e^{-i a \Delta_t (-)^{x_1 \oplus x_0}} |x_1 \, x_0\rangle$$

in general :

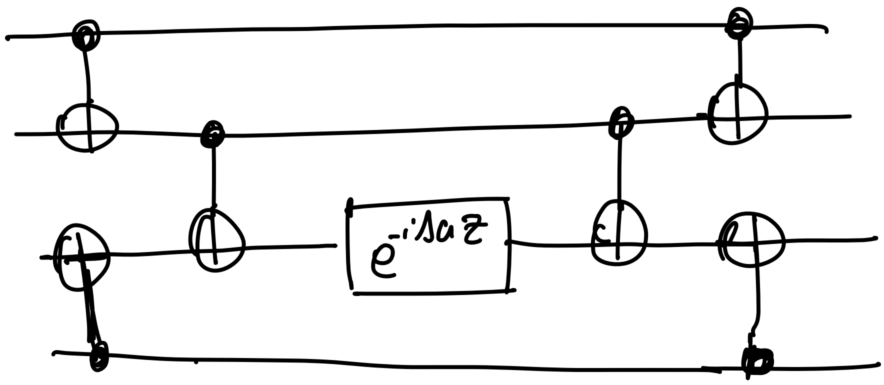


this allows to act with CNOT gates only btw adjacent qubits

(for ex IBM quantum computer only have nearest - neighbour connectivity)

* can also reorganize into an $\mathbb{X}$ shape to decrease the depth:

ex with $n=4$:



here the # of CNOT is the same as before but the circuit depth has been decreased, leading to smaller run time of the algorithm (and thus less noise)

How to go beyond leading order Trotter ?

1) include the commutator :

At LO the main source of error is the commutators btw terms of the Hamiltonian:

$$e^{-i(H_1+H_2)\Delta t - [H_1,H_2]\Delta t^2/2 + \mathcal{O}(\Delta t^3)} = e^{-iH_1\Delta t} e^{-iH_2\Delta t}$$

one possible solution is to include the commutator :

$$e^{-i(H_1+H_2)\Delta t} \simeq e^{-iH_1\Delta t} e^{-iH_2\Delta t} e^{+[H_1,H_2]\frac{\Delta t^2}{2}}$$

see ex in class for the 1-q system.

But in general finding circuits for such commutators is difficult & becomes untractable when H has many terms the -

2) Higher-order Trotterization :

We saw that at LO :

$$\boxed{e^{-i(H_1+H_2)\Delta_t + O(\Delta_t^2)} = e^{-iH_1\Delta_t}\, e^{-iH_2\Delta_t}}$$

The idea is to keep approx the evolution op as a product of exp op (because these we know how to compute) but we will increase the # of terms in order to kill the higher order corrections in the l.hs :

We want :

$$\left[e^{-i(H_1+H_2)\Delta_t + O(\Delta_t^{P+1})} = \prod_{m=1}^{P} e^{-iH_1\Delta_t a_m}\, e^{-iH_2\Delta_t b_m} \right]$$

P = order of the expansion

ex : P = 2 (next to leading order NLO)

$$e^{-i(H_1+H_2)\Delta_t + \alpha[H_1,H_2]\Delta_t^2 + O(\Delta_t^3)} = e^{-iH_1\Delta_t a_1}\, e^{-iH_2\Delta_t b_1}\, e^{-iH_1\Delta_t a_2}\, e^{-iH_2\Delta_t b_2} \qquad (*)$$

we want to find a_1, a_2, b_1, b_2 such that $\alpha = 0$.

Taking $\begin{cases} a_1 \equiv a, & a_2 \equiv 1-a \\ b_1 \equiv b, & b_2 \equiv 1-b. \end{cases}$

Baker - Campbell - Hausdorff formula (BCH)

$$e^X e^Y = e^Z \quad \text{with} \quad Z = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}[[X,Y],Y] - \frac{1}{12}[Y,[X,Y]] + \dots$$

$$\underset{\substack{\text{BCH}\\\text{NLO}}}{\Rightarrow} e^{-iH_1\Delta_t a} e^{-iH_2\Delta_t b} = \exp\left\{-i\Delta_t (H_1 a + H_2 b) - \frac{1}{2}\Delta_t^2 ab [H_1, H_2]\right\}$$

and similarly for $e^{-iH_1\Delta_t(1-a)} e^{-iH_2\Delta_t(1-b)}$

$$\Rightarrow (*) = e^{\overbrace{-i\Delta_t(H_1 a + H_2 b) - \frac{1}{2}\Delta_t^2 ab [H_1, H_2]}^{X}} \times e^{\overbrace{-i\Delta_t(H_1(1-a) + H_2(1-b)) - \frac{1}{2}\Delta_t^2 (1-a)(1-b)[H_1, H_2]}^{Y}}$$

use NLO BCH again:

$$[X,Y] = \frac{-1}{2}\Delta_t^2 \Big([H_1 a, H_2(1-b)] + [H_2 b, H_1(1-a)]\Big) + O(\Delta_t^3)$$

$$= \frac{-1}{2}\Delta_t^2 [H_1, H_2] \Big(a(1-b) - b(1-a)\Big) + O(\Delta_t^3)$$

$$\Rightarrow (*) = \exp\Big\{ -i\Delta_t \Big(H_1 (a+1-a) + H_2 (b+1-b) \Big) - \frac{1}{2}\Delta_t^2 [H_1, H_2] \Big(ab + (1-a)(1-b) + a(1-b) - b(1-a) \Big) \Big\} + O(\Delta_t^3)$$

$$= \exp\Big\{ -i\Delta_t (H_1 + H_2) - \frac{1}{2}\Delta_t^2 [H_1, H_2] \big(1 - 2b(1-a) \big) \Big\}.$$

$\Rightarrow$ the r.h.s in Eq $(*)$ above

$$e^{-iH_1\Delta_t a_1} e^{-iH_2\Delta_t b_1} e^{-iH_1\Delta_t a_2} e^{-iH_2\Delta_t b_2}$$

$$= e^{-i\Delta_t (H_1+H_2) - \frac{1}{2}\Delta_t^2 [H_1, H_2] (1-2b(1-a)) + O(\Delta_t^3)}$$

if we choose $b = 1$ and $a = 1/2$ the term of order Δ_t^2 cancels.

$$\Rightarrow \boxed{e^{-i(H_1+H_2)\Delta_t + O(\Delta_t^3)} = e^{-iH_1\Delta t/2} e^{-iH_2\Delta_t} e^{-iH_1\Delta_t/2}}$$

Suzuki-Trotter at NLO.

$\Rightarrow$ the (systematic) error from Trotter expansion has been reduced by splitting one of the unitary.

$\underset{\sim\sim\sim}{P=1 \text{ (LO)}}$: we had error $O\left(\Delta_t^2 N_S\right) =$
$O\left(t^2/N_S\right)$

$\underset{\sim\sim\sim}{P=2 \text{ (NLO)}}$: error $O\left(\Delta_t^3 \times N_S\right)$

$$= O\left(t^3/N_S^2\right)$$

Generally, if $H = \sum_k^L H_k$

$$\boxed{\begin{aligned} U_{NLO}(t) &= \Big[e^{-iH_L \Delta_t/2} \, e^{-iH_{L-1}\Delta_t/2} \cdots e^{-iH_2 \Delta_t/2} \, e^{-iH_1 \Delta_t} \\ &\quad \times e^{-iH_2 \Delta_t/2} \cdots e^{-iH_{L-1}\Delta_t/2} \, e^{-iH_L \Delta_t/2} \Big]^{N_S} \\ &= \left[\left(\prod_{k=L}^{1} e^{-iH_k \Delta_t/2} \right) \left(\prod_{k=1}^{L} e^{-iH_k \Delta_t/2} \right) \right]^{N_S} \end{aligned}}$$

Can continue and use this to derive the 4th order :

$$U_2(\Delta_t) \equiv e^{-iH_1 \Delta_t/2} \, e^{-iH_2 \Delta_t} \, e^{-iH_1 \Delta_t/2}$$

consider

$$U_{4,s}(\Delta_t) = \left[U_2(s\Delta_t)\right]^2 U_2\left((1-4s)\Delta_t\right) \left[U_2(s\Delta_t)\right]^2$$

$$= e^{-i(H_1+H_2)\Delta_t + R_3 \Delta_t^3 \left(4s^3 + (1-4s)^3\right) + O(\Delta_t^5)}$$

choosing $s = \bar{s} = \dfrac{1}{4 - 4^{1/3}} \simeq 0.415$ allows to eliminate the term of order Δ_t^3 so that

$$e^{-i(H_1+H_2)\Delta_t + O(\Delta_t^5)} = \mathcal{U}_{4,\bar{s}}(\Delta_t)$$

In general:

$$e^{-i(H_1+H_2)\Delta_t + O(\Delta_t^{2p+1})} =$$

$$[\mathcal{U}_{2p-2}(s_p\Delta_t)]^2 \, \mathcal{U}_{2p-2}((1-4s_p)\Delta_t) \, [\mathcal{U}_{2p-2}(s_p\Delta_t)]^2$$

$$s_p = \frac{1}{4 - 4^{1/(2p-1)}}$$

One can continue this expansion to systematic. decrease the error associated to Trotterizat° – i.e. the time steps can be larger but the price to pay is a larger circuit for each time step:

the circuit ~ doubles at NLO
then $\times 5$ for each new order

(see example in class for the
one - qubit system)

Such higher order Trotter expansion will be useful for next - generation quantum computers (resilient to noise) but with the current ones , leading order Trotter is usually the best working approach.

How to mitigate Trotter errors ?

In real quantum computing, we saw that one cannot use too many Trotter steps N_s because the error due to noise and faulty gates become larger than Trotter errors as the circuit size increases.

Similarly if keep a fixed N_s but expand the Trotter expansion to higher orders beyond LO , the circuit size also increase considerably , leading to the same issues.

$\Rightarrow$ is there a way to mitigate the Trotter error without introducing larger circuits ?

there has been a lot of work exploring how this can be done using classical averaging

For example :

1) The ordering of operators in the right-hand side of the formulas above is arbitrary. We could have also chosen

$$e^{-i(H_1+H_2)t} \simeq e^{-i\underline{\underline{H_2}}\Delta t} e^{-i\underline{\underline{H_1}}\Delta t} + O(\underline{\underline{-}}\Delta t^2/2 \, [H_1, H_2])$$

One could imagine performing measurement statistics with half of the circuits with the 1st ordering and the second half with the 2nd ordering

The expectation values of observables would then be

$${}_{LO}\langle \psi(t) | \hat{A} | \psi(t) \rangle_{LO}$$

$$= \frac{1}{2} \Big[{}_{ex}\langle \psi(t) | \hat{A} \left(1 + O\left(\frac{\Delta t^2}{2} [H_1, H_2] \right) \right) | \psi(t) \rangle_{ex}$$
$$+ {}_{ex}\langle \psi(t) | \hat{A} \left(1 - O\left(\quad \text{———} \quad \right) \right) | \psi(t) \rangle_{ex}$$

$$= \langle \psi(t) | \hat{A} | \psi(t) \rangle_{ex} + \dots$$

the LO error in Δt^2 associated to commutator would cancel.

However this now relies on statistical averaging over all members of the ensemble (which becomes large when have many terms in $H = \Sigma H_k$).

If the distributions of results are too wide then the averaging slowly converges. or even worse could completely fail (if the evolution op completely wraps around the circle)

2) Another possibility could be to use sampling techniques to correct each member of the ensemble

For instance at each Trotter step,
pick a random ordering of the operators

For $H = \sum_{k=1}^{L} H_k$

At Trotter step $i = 1, \dots, N_S$:

$$U_{LO}^{i}(\Delta_t) = U_{i_1}(\Delta_t) U_{i_2}(\Delta_t) \dots U_{i_L}(\Delta_t)$$

$$i_j \in \{1 \dots L\}.$$

Ideally this would be repeated $L!$ time per Trotter step, to sample all possible $L!$ orderings.

However when the time step is not small we have again a sign pb.
(as the samples wrap around the circle)
(if the step size decreases $\rightarrow$ they are brought to an arc circle which allows for meaningful results.)

(in class example)

→ What we are trying to do here is to "trade off" the circuit depth for the ensemble size, to min error due to Trotterization.

However when doing this we go back toward classical statistical Monte Carlo sampling to evaluate observables and the pathologies (sgn pb) that we were initially trying to avoid with quantum computer come back.