

A. III. ⑤ Simulations of quantum systems

* Feynman (1981)

→ use QC to simulate the structure and dynamics of quantum many-body systems:

many-e⁻ pb → quantum chemistry

many-nucleon pb → nuclear phys.

etc... (condensed matter -
high-energy physics -)

→ hard to do classically because the size of the Hilbert space grows exponentially with the number of particles.

↳ n

$$|4\rangle = \sum_{x=0}^{2^n-1} c_x |x\rangle$$

↳ 2^n terms in the expansion.

Will discuss two aspects :

→ how to estimate energy eigenvalues
(of the Hamiltonian) (structure)

→ how to simulate dynamics
(time evolution) of these systems.

① Notion of "local" Hamiltonians

The quantum simulation of physical systems can be efficient if the system is governed by a local Hamiltonian -

A Hamiltonian H is local if it can be written as :

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

where each H_k acts non-trivially on a constant number of qubits (c) independent of the total size of the system:

$$H_k = \tilde{H}_k^{(c)} \otimes I^{(n-c)}$$

⇒ H is "c-local".

ex : * interacting e^- : (Coulomb)

the interaction involves (at most)
2 e^- at a time
 \Rightarrow "2-local".

* interacting nucleons :

can have 2-body, 3-body, 4-body ...
interactions. (because of the internal structure
of nucleons)

but $2N \text{ int} > 3N \text{ int} > \cancel{4N \text{ int}} \dots$

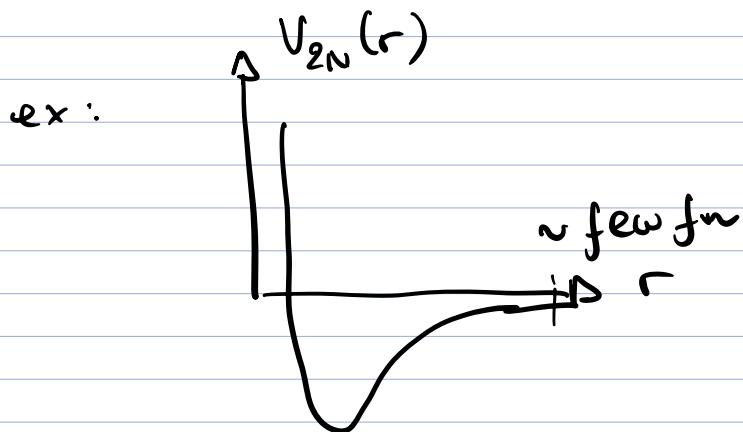
$\Rightarrow H$ is "3-local".

\Rightarrow In general the physical systems that we
want to describe are described by
local Hamiltonians.

→ How many terms L in the decomposition
of H ?

if H is c -local, i.e. at most
 c -body int $\Rightarrow L = O\left(\binom{n}{c}\right) = O(n^c)$
terms.

- * There is a stronger notion of locality:
"spatial / geometrical" locality



Typically in nature, particles interact only they are spatially close to each others.

A c-local Hamiltonian is also geometrically local if the c qubits on which the act can be organized in a small volume.

\Rightarrow in that case $L = \underline{O(n)}$

We are interested in Hamiltonians that are c-local and geometrically local.

→ we will show that quantum circuits can simulate quantum systems governed by such Hamiltonians efficiently:

dynamical evolution of an n-qubit system over time t can be simulated to cel accuracy with a circuit whose size is polynomial in both n and t .

② Time-Evolution of quantum systems.

Suppose we have a quantum syst in an initial state $| \Psi(0) \rangle$ and want to describe how it evolves in time.

The time evolution of a quantum syst is governed by a unitary operator $U(t)$:

$$| \Psi(t) \rangle = U(t) | \Psi(0) \rangle$$

where $U(t)$ satisfies:

$$\frac{d}{dt} U(t) = -iH(t) U(t)$$

$$\text{with } U(t=0) = I.$$

* if H is time-independent \Rightarrow

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

(* otherwise : $U(t) = T \left[e^{-i \int_0^t H(t') dt'} \right]$)

↳ time-ordering operator

Here : we will consider a time-independent H
but the discussion also applies to
time-dependent $H(t)$.

Ideally we would like to construct
a circuit which implements "the" time
evolution operator $U(t)$ -

But this becomes quickly untractable
for large n .

\rightarrow instead we will implement
some approximation $\tilde{U}(t)$

$$\Rightarrow \|\tilde{U}(t) - U(t)\| |\Psi(0)\rangle < \delta$$

\nwarrow accuracy required

$\underbrace{\quad}_{\text{Err}(\tilde{U}, U)}$

$\wedge |\Psi(0)\rangle$

when H is local it is possible to find an approx. \tilde{U} with efficient circuit (poly size).

As discussed in class the trick is to split the time t into small intervals

$$t = \Delta_t \times N_s$$

↓ ↓
 # steps time step size

and approx. the time evolution over t by a sequence of $N_s = \frac{t}{\Delta}$ steps.

$$\begin{aligned}
 \Rightarrow U(t) &= e^{-iHt} \\
 &= e^{-iHN_s \Delta} \\
 &= e^{-iH\Delta} e^{-iH\Delta} \dots e^{-iH\Delta} \\
 &\qquad\qquad\qquad \underbrace{\qquad\qquad\qquad}_{N_s \text{ times.}}
 \end{aligned}$$

$e^{-iH\Delta}$ is difficult to compute (H is very large \Rightarrow hard to exponentiate)

Now if H is local : $H = \sum_{k=1}^L H_k$

$\Rightarrow e^{-iH_k\Delta}$ is easier to compute.

(2, 3)

↓
acts on
c qubits
at the
same time.

but $[H_k, H_\ell] \neq 0$ in general.

$$\Rightarrow e^{-iH\Delta} = e^{-i(\sum_k H_k)\Delta}$$

$$\neq e^{-iH_1\Delta} e^{-iH_2\Delta} \dots e^{-iH_L\Delta}$$

However if Δ is small enough, this expression is approx true :

$$e^{-iH\Delta} \approx \prod_k e^{-iH_k\Delta}$$

Proof: denote $\underline{A_k} = -i H_k \Delta$.

$$\underline{e^{\sum_k A_k}} = -\prod_k e^{A_k}$$

$$= \left(\cancel{1} + \sum_k A_k + \frac{1}{2} \underbrace{\sum_{k \neq l} A_k A_l}_{\frac{1}{2} \sum_k A_k^2 + \frac{1}{2} \sum_{k < l} A_k A_l + \frac{1}{2} \sum_{k \neq l} A_k A_l} + \dots \right) \leftarrow$$

$$- \prod_k \left(\cancel{1} + A_k + \frac{1}{2} A_k^2 + \dots \right) \leftarrow$$

$$\left(\cancel{1} + \underline{A_1} + \frac{A_1^2}{2} + \dots \right) \left(\cancel{1} + \underline{A_2} + \frac{A_2^2}{2} + \dots \right)$$

$$\dots \left(\cancel{1} + \underline{A_L} + \frac{A_L^2}{2} + \dots \right)$$

$$= \cancel{1} + \underbrace{(A_1 + A_2 + \dots + A_L)}_{\sum_k A_k} + \frac{1}{2} \underbrace{\sum_k A_k^2}_{\frac{1}{2} \sum_k A_k^2 + \frac{1}{2} \sum_{k < l} A_k A_l + \dots}$$

$$\sum_k A_k$$

$$+ \sum_{k < l} A_k A_l + \dots$$

$$= -\frac{1}{2} \sum_{k < \ell} A_k A_\ell + \frac{1}{2} \underbrace{\sum_{k < \ell} A_k A_\ell}_{\sum_{k < \ell} A_\ell A_k} + \dots$$

$$= \frac{1}{2} \sum_{k < \ell} (A_\ell A_k - A_k A_\ell) + \dots$$

$$= -\frac{1}{2} \sum_{k < \ell} \underbrace{(A_k A_\ell - A_\ell A_k)}_{[A_k, A_\ell]} + \dots$$

$$= [A_k, A_\ell]$$

$$\Rightarrow e^{-i \sum_n H_n \Delta} - \prod_{k=1}^L e^{-i H_k \Delta}$$

$$= -\frac{1}{2} \sum_{k < \ell} [-i H_k \Delta, -i H_\ell \Delta] + \dots$$

$$= \frac{\Delta^2}{2} \sum_{k < \ell} [H_k, H_\ell]. + \dots$$

what is the error made when we approx

$$e^{-iH\Delta} \text{ by } \prod_{k=1}^L e^{-iH_k \Delta} ?$$

→ need to know how many non-vanishing $[H_k, H_\ell]$ there are.

if H is geometrically local : $L = O(n)$

we also consider the Hami to be bounded:

$$\|\underline{H_n}|4\rangle\| \leq \hbar \text{ cst.}$$

\Rightarrow Error :

$$\max_{|4\rangle} \left\| \left(e^{-iH\Delta} - \prod_L e^{-iH_k \Delta} \right) |4_0\rangle \right\| = O(L \hbar^2 \Delta^2)$$

$$\boxed{\begin{aligned} &= O(n \hbar^2 \Delta^2) \\ &= \text{error made in one time step.} \end{aligned}}$$

\Rightarrow The time evolution of one time step Δ requires a product of L local operations ($e^{-iH_L \Delta}$)

and leads to an error $O(L h^2 \Delta^2)$
 (adds linearly) $= O(n h^2 \Delta^2)$

\rightarrow each operation has error $O(h^2 \Delta^2)$

- To describe the evolution over time $t = N_s \Delta$ we need to repeat to repeat this procedure N_s times.

$$e^{-iHt} = (e^{-iH\Delta})^{N_s}$$

$$\text{U}(t) \approx \left(\prod_k e^{-iH_L \Delta} \right)^{N_s} \equiv \tilde{U}(t)$$

\Rightarrow The total error is:

$$\text{Err}(\tilde{U}, U) = N_s \stackrel{= t/\Delta}{=} O(n h^2 \Delta^2)$$

$$= O(t n \Delta h^2)$$

If we had considered time evolution without discretizing t into small steps, the error would have been

$$O(t^2 n h^2) \quad (\text{showed in class})$$

versus here $O(t \Delta n h^2)$

$$= O\left(\frac{t^2}{N_s} n h^2\right)$$

\Rightarrow we have divided the error by factor $\frac{1}{N_s}$!

. Now if we want to keep constant accuracy over the time evolution, say

$$\text{Err}(\tilde{u}, u) < \delta \Rightarrow \text{we need:}$$

$$\boxed{\Delta = O\left(\frac{\delta}{h^2 n t}\right)}$$

\rightarrow need smaller time steps for large t .

Efficiency of this approach?

- How many operations ($e^{-iH_0 \Delta}$) are required for the full circuit?

$$\underbrace{\left(\begin{array}{c} \# \text{ of operations /} \\ \text{step} \end{array} \right)}_{L = O(n)} \times N_s \approx \frac{t}{\Delta}$$

$$= O\left(nt \frac{h^2 nt}{s}\right)$$

$$= O\left((nt)^2 \times \left(\frac{h^2}{s}\right)\right)$$

\hookrightarrow cst.

$nt \sim$ volume of space-time that we are simulating.

as we increase the space-time volume (nt) that we simulate, the # of operations grows at $(nt)^2$.

- How many gates (from some approx. universal gate set) do we need for the full time evolution?

According to the Solovay - Kitaev thm (previous lecture) each operator $e^{-iH_k \Delta}$ can be implemented

up to accuracy ϵ (here $\epsilon = \Delta^2 h^2$) with a number of gates

that is $O(\text{poly}(\log(\frac{1}{\epsilon})))$

→ here: $O(\text{poly}(\log(\frac{1}{\Delta^2 h^2})))$

\Rightarrow for the total circuit we need

$$O(\text{poly}(\log(\frac{1}{\Delta^2 h^2})) \times O(n t)^2 \frac{h^2}{\delta})$$

||

$$\frac{h^2 n^2 t^2}{\delta^2}$$

$$\Rightarrow O\left(\left[\text{poly log}\left((nt)^2 \times \left(\frac{h^2}{\delta^2}\right)\right)\right] (nt)^2 \left(\frac{h^2}{\delta}\right)\right)$$

↓
 cst
 ↓
 cst

$$= O\left(\underline{(nt)^2} \text{poly}(\log((nt)^2))\right)$$

↳ size of the full circuit
 for the time evolution over t .

\Rightarrow Conclusion : although it is hard to
 do classically, we can simulate the
 time evolution of quantum systems
 with a circuit which scales polynomially
 in the # of qubits n and in t .

Note: what we derived is the leading-order (LO) term of the Suzuki-Trotter expansion.

$$e^{-i(H_1+H_2)t} = \lim_{N_S \rightarrow \infty} \left[e^{-iH_1 t/N_S} e^{-iH_2 t/N_S} \right]^{N_S}$$

In principle the exact time evolution can be recovered for infinite # of Trotter steps N_S -

But in practice, with current (noisy) quantum computers, one cannot apply too many Trotter steps because the circuit becomes too long and the computation would fail due to decoherence.

→ balance to find

(see Fig 17 PRA 99 052 335 2019)
Klo, Savage.

Next time: examples.