Day 4 - Quantum Simulation

There are a few common things we can do with quantum simulation:

① calculate lowest energy state of a system (ground state)

② study the time dynamics of a quantum system

I will mainly focus on ② today.

As I mentioned before, the observables of a quantum system are always probabalistic, due to superposition. So we will generally not be able to say: "after a time t, this electron will be at location X or this qubit will be measured as 1."

But . . . the wave function describing a quantum system does evolve deterministically with time. Wave functions evolve according to Schrödinger's equation (SE). The time-dependent SE is:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle$$

$\hat{H}(t)$: Hamiltonian of the system (total energy operator)

This type of differential equation has a simple solution. If we strip away the "quantumness" here, we have something like:

$$\frac{\partial}{\partial t} x = cx$$

A solution to this is:

$$x(t) = x(0)\, e^{ct}$$

Similarly, the solution to the time-dep. SE is:

$$(*) \quad |\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle$$

⚠ The above might not be true if $\hat{H}$ depends on time

So if we know the wavefunction at $t=0$ and the Hamiltonian $\hat{H}$, we know the wave function at all later points in time!

We point out that $(*)$ is the same as evolving under a unitary operator

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar}$$

$$\Rightarrow \quad |\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$$

In the case where $\hat{H} = \hat{H}(t)$, we can still find the wave function evolution, but the equations are more complicated.

What's the problem here?

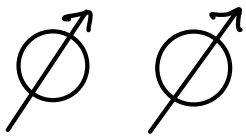
What is the "size" of a wavefunction?

Consider 1 spin-1/2 particle: ∅
(two level)

Since it has 2 levels, we can describe the system by a wavefunction:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$ (2 coefficients)

Now consider 2 spin-1/2 particles:



This whole system is described by a wave function:

$$|\psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$$

Now we have 4 coefficients, arising from the fact that a system of n two-level particles encodes 2^n classical bits of information, due to superposition.

Suppose you want to simulate a system of 80 spin-1/2 particles. Then you need to store $2^{80} \approx 10^{24}$ wavefunction coefficients in classical memory...

If you use single precision storage, this would require 3.2×10^{25} bits $\approx$ 3 YB (yottabyte)

The total amount of data stored in the world (predicted by 2025) will be:

$$175\ \text{ZB} \sim 1.4 \times 10^{24}\ \text{bits}$$

(zettabyte)

Clearly classical computing resources are not up to the challenge.

Why a quantum computer?

↳ a quantum computer inherently possesses the same exponential scaling as quantum systems

Two Main Types of Quantum Simulation:

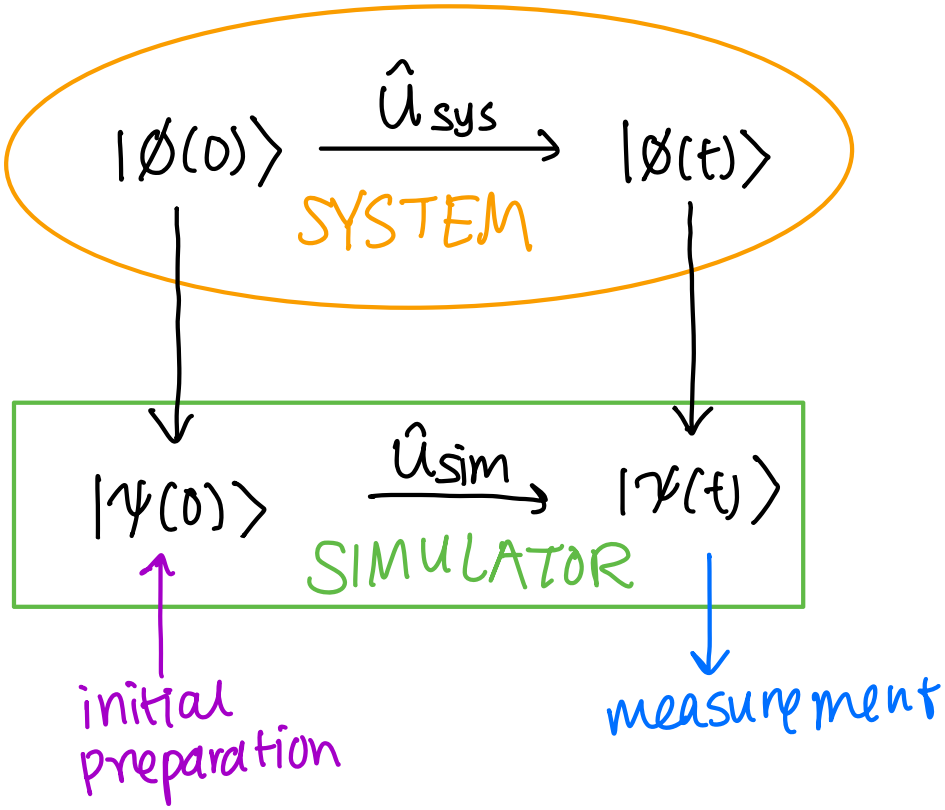
① Analog Quantum Simulation

↳ engineer the Hamiltonian of the simulator to emulate the desired Hamiltonian

↳ let the simulator evolve under the simulator Hamiltonian

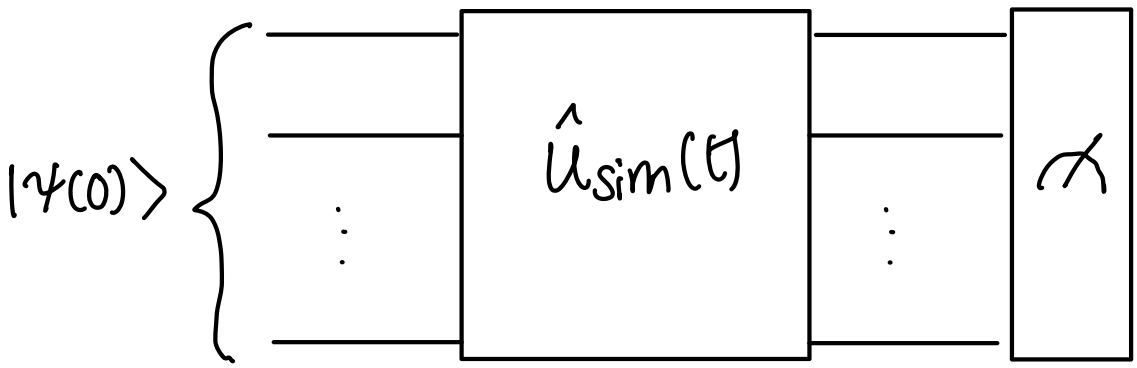
$$\hat{H}_{sys} \rightarrow \hat{H}_{sim}$$

$$\hat{U}_{sys}(t) \rightarrow \hat{U}_{sim}(t)$$



② Digital simulation

↳ use single and two-qubit gates to synthesize $\hat{U}_{sim}(t)$

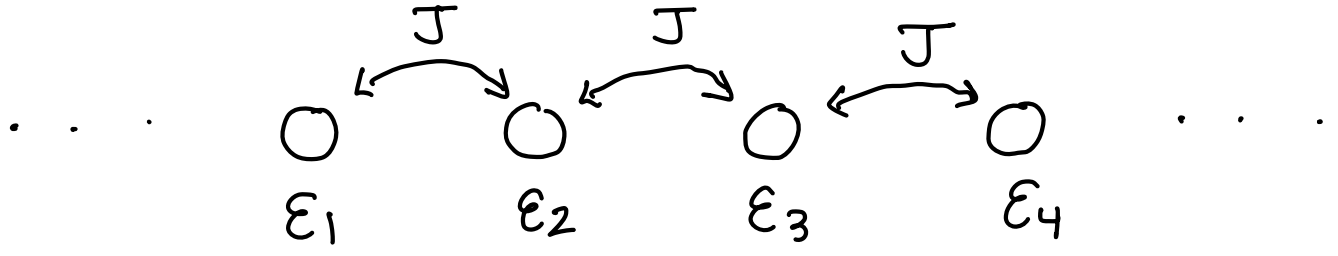


What is an example of an interesting Hamiltonian for analog simulation?

↳ Tight-binding Model: $\hat{H}_{TB}$

↳ describes electrons in solids

↳ explains some conductance properties of metals



Each site can be treated as a 2 level system:

$|0\rangle$ → no electron

$|1\rangle$ → electron

Energy of each site: $\hat{H}_{site} = -\frac{\varepsilon}{2}\sigma_z$

$$\hat{H}_{site}|0\rangle = -\frac{\varepsilon}{2} \equiv E_0$$

$$\hat{H}_{site}|1\rangle = \frac{\varepsilon}{2} \equiv E_1$$

$$\Delta E = E_1 - E_0 = \varepsilon$$

Exchange interaction between neighboring sites:

$$\hat{H}_{int} = -\frac{J}{2}\left(\sigma_x \sigma_x + \sigma_y \sigma_y\right)$$

$$\hat{H}_{int}\,|01\rangle = -\frac{J}{2}\left(\sigma_x \sigma_x |01\rangle + \sigma_y \sigma_y |01\rangle\right)$$

$$= -\frac{J}{2}\left(|10\rangle + |10\rangle\right)$$

$$= -J\,|10\rangle$$

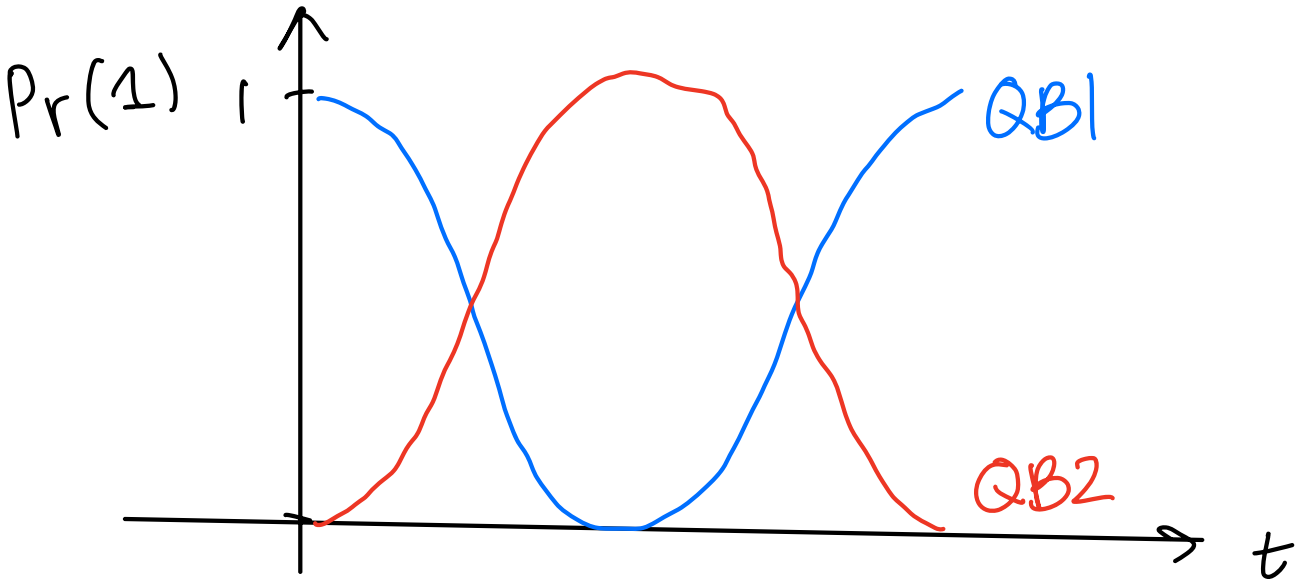
$$\hat{H}_{int}\,|10\rangle = -\frac{J}{2}\left(\sigma_x \sigma_x |10\rangle + \sigma_y \sigma_y |10\rangle\right)$$

$$= -\frac{J}{2}\left(|01\rangle + |01\rangle\right)$$

$$= -J\,|01\rangle$$

We also call this a "hopping" interaction, because the excitation hops back and forth between the 2 sites. When we evolve under $\hat{H}_{int}$ for

various times, we would see the excitation hopping back and forth:



So the total Hamiltonian generalized would be:

$$\hat{H}_{TB} = -\sum_{i=1}^{N} \frac{\varepsilon_i}{2} \sigma_z^i - \frac{1}{2} \sum_{\langle i,j \rangle} J_{ij} \left(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y \right)$$

Digital Quantum Simulation

Suppose we want to simulate:

$$\hat{H} = \sum_{\ell}^{m} \hat{H}_\ell$$

where $\hat{H}_\ell$ is a k-local Hamiltonian (only involves non-identity operations on k qubits)

Ex for 2-local: $\sigma_x^1 \otimes \sigma_z^2$

Ex for 3-local: $\sigma_x^1 \otimes \sigma_z^2 \otimes \sigma_y^3$

Most Hamiltonians of interest can be decomposed into such k-local Hamiltonians.

our unitary that we want to synthesize is:

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar}$$

$$= e^{-i\sum_{\ell}^{m} H_\ell t/\hbar}$$

If $[H_i, H_j] = 0$ for all $i,j \in \{1, 2, \cdots, m\}$

then:

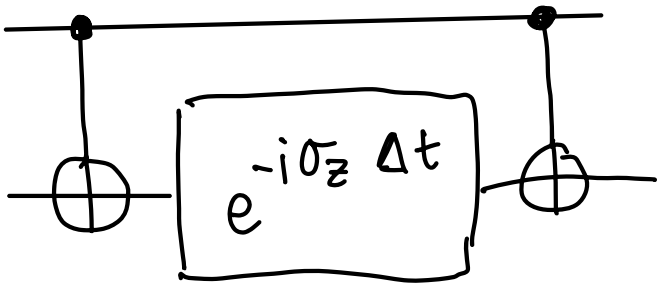
$$\hat{U}(t) = \prod_{l}^{m} e^{-iH_l t/\hbar}$$

we can construct this with gates

Examples of gate constructions:

$$H_l = \sigma_z^1 \otimes \sigma_z^2$$

$$\Rightarrow \hat{U}(\Delta t) = e^{-i\,\sigma_z^1 \otimes \sigma_z^2\,\Delta t}$$



$\mathbb{I}$ rotation around z for time Δt

Let's make sure we understand the idea behind this.

Suppose we are doing a θ rotation:

$$R_z(\theta) = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$$

OR $R_z(\theta) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}$ up to a global phase

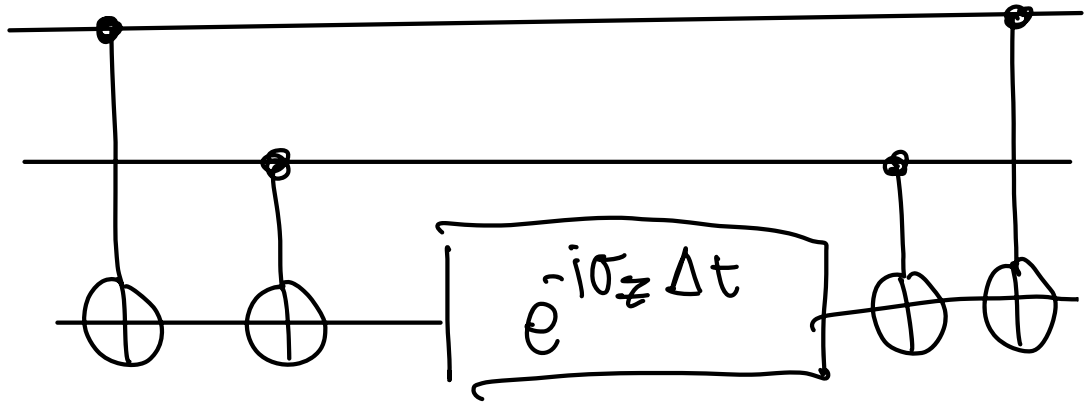
So: $|0\rangle \to |0\rangle$ and $|1\rangle \to e^{i\theta}|1\rangle$

Let's consider all four possible input basis states:

	after 1st CNOT	after $R_z(\theta)$	after 2nd CNOT
$\|00\rangle$	$\|00\rangle$	$\|0\rangle \otimes \|0\rangle$	$\|00\rangle$
$\|01\rangle$	$\|01\rangle$	$\|0\rangle \otimes e^{i\theta}\|1\rangle$	$e^{i\theta}\|01\rangle$
$\|10\rangle$	$\|11\rangle$	$\|1\rangle \otimes e^{i\theta}\|1\rangle$	$e^{i\theta}\|10\rangle$
$\|11\rangle$	$\|10\rangle$	$\|1\rangle \otimes \|0\rangle$	$\|11\rangle$

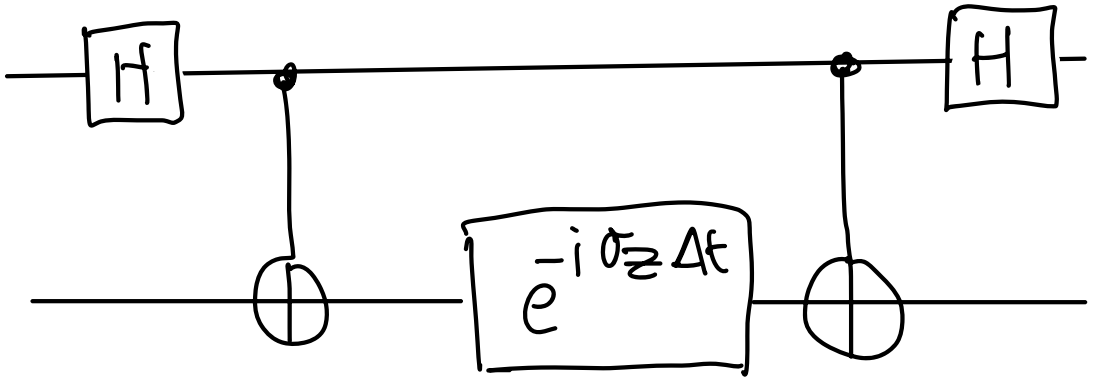
We wanted to apply $\sigma_z^1 \otimes \sigma_z^2$ which corresponds to a phase flip for $|01\rangle$ and $|10\rangle$ only, which we have.

The same works for $H_\ell = \sigma_z^1 \otimes \sigma_z^2 \otimes \sigma_z^3$



We can also generalize to other Paulis. Ex. $HZH = X$

So if $H_\ell = \sigma_x^1 \otimes \sigma_z^2$:



What if $[H_i, H_j] \neq 0$ for some of $i, j \in \{1, 2, \cdots, m\}$?

↳ $e^{\hat{A}+\hat{B}} \neq e^{\hat{A}} e^{\hat{B}}$

We have to use the Trotter-Suzuki formula:

$$\hat{U}(T) = e^{-i \sum_m^\ell \hat{H}_\ell T}$$

$$= \left(\prod_\ell^m e^{-i \hat{H}_\ell T/n} \right)^n + O\left(\frac{m^2 T^2}{n}\right)$$

This is called Trotterization.

The simulation becomes more accurate as we increase n.

Summary:

- Analog:
  - pros: does not require Trotter steps (i.e. potentially more accurate)
  - cons: limited by the possible $\hat{H}$ of your processor
- Digital:
  - pros: flexibility in terms of $\hat{H}_{sim}$
  - cons: requires Trotterization (which induces errors)