31/10/22

QUANTUM SIMULATION [Computational Quantum Physics]

Exact Diagonalization Approaches

- Interactions
- "N" particles that is large enough
- Interacting Spins
- Interacting Electrons

Solve Schrödinger Equation

$$i \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} \, |\Psi(t)\rangle$$

(Time Dependent S.E)

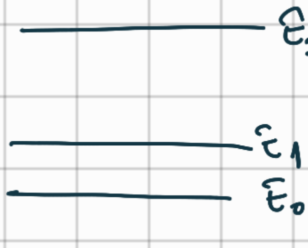
$|\Psi(0)\rangle$ = Initial Condition

Computational techniques allow to solve time dependent efficiently in some special cases

$$\hat{H} \, |E_k\rangle = E_k \, |E_k\rangle$$

→ Eigenkets

$$E_0 \leq E_1 \leq E_2$$



No efficient comp. techniq is known

Exact Diagonalization Approaches (Classical Methods)

$$\hat{H} = \sum_{i}^{N} J \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - \Gamma \sum_{i}^{N} \hat{\sigma}_i^x \rightarrow \text{transverse field}$$

$\searrow$ $2^N \times 2^N$ matrix

$$\hat{\sigma}_i^z = \underbrace{\hat{I} \otimes \hat{I} \otimes \hat{I} \cdots}_{i-1 \text{ identities}} \hat{\sigma}^z \underbrace{\cdots \otimes \hat{I} \cdots\cdots \otimes \hat{I}}_{N-i \text{ identities}}$$

$\downarrow$ $2^N \times 2^N$ matrix

$$\boxed{\sigma_{N+1}^z = \sigma_1^z}$$

$$\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \hat{\sigma}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Basis for the Eigenkets of $\hat{H}$

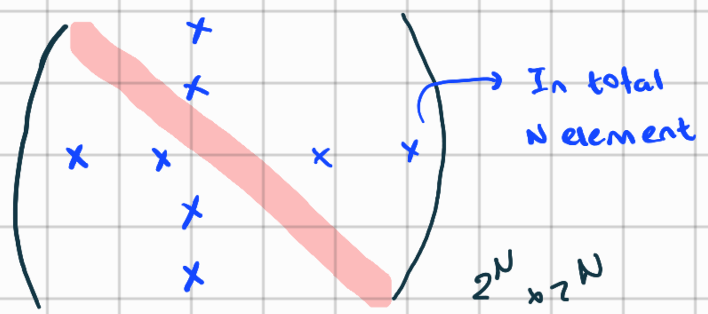
$$|\psi\rangle = \sum_{S_1 \ldots S_N} C_{S_1 \ldots S_N} |S_1 \ldots S_N\rangle$$

$$|S_1 S_2 \ldots S_N\rangle = |S_1\rangle \otimes |S_2\rangle \otimes \cdots \otimes |S_N\rangle$$

$$\hat{\sigma}_i^z |S_1 \ldots S_N\rangle = S_i |S_1 \ldots S_N\rangle$$

$\searrow$ ± 1 (eigen values)

Write Explicit Expression for the matrix elements

$\hat{H} =$ 

$\sum_i J\sigma_i^z\sigma_{i+1}^z$

$= \langle S_1 \ldots S_N | \hat{H} | S_1 \ldots S_N \rangle = \sum_{i=1}^{N} J\, S_i S_{i+1}$

$= \langle S_1 \ldots S_N | \hat{\sigma}_i^x | S_1' \ldots S_N' \rangle =$

$= \langle S_1| \otimes \langle S_2| \otimes \ldots \otimes \langle S_N| \; \hat{I}_1 \otimes \hat{I}_2 \ldots \otimes \hat{\sigma}^x \otimes \ldots I_{i+1} \otimes \hat{I}_N \; |S_1'\rangle |S_2'\rangle \ldots$

$= \langle S_1 | \hat{I}_1 | S_1' \rangle \langle S_2 | \hat{I}_2 | S_2' \rangle \ldots \langle S_i | \hat{\sigma}_x | S_i' \rangle \ldots \langle S_N | \hat{I}_N | S_N' \rangle$

$= \delta_{S_1,S_1'}\, \delta_{S_2,S_2'} \ldots \underset{\text{due to } \sigma_x^i}{\delta_{S_i,-S_i}} \ldots \delta_{S_N,S_N'}$

$\hat{\sigma}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\langle \uparrow | \sigma_x | \downarrow \rangle = 1$

$\langle \uparrow | \sigma_x | \uparrow \rangle = 0$

We have found that SPARSE MATRIX → Most of its matrix elements are 0.

$2^N \times 2^N$ MATRIX ELEMENTS $\rightarrow 2^N + N\,2^N \sim 2^N$

In software (eg Scipy. sparse)

Store the matrix elements (i, j, M_{ij}) → $M_{ij} \neq 0$ ↙ matrix elements are not zero

Memory Usage

N	Memory ($\|\psi\rangle$)
20	8 Megabytes
30	8 Gigabytes
40	8 Terrabytes

$$\text{Memory} = 2^N \times 8 \quad \text{BYTES}$$

Exploit Sparsity (only for Time-Dependent Sch. Eq.)

$$i \frac{\partial}{\partial t} C_{S_1, \dots S_N}(t) = \sum_{S_1' \dots S_N'} H(S_1 \dots S_N; S_1' \dots, S_N') \, C_{S_1' \dots S_N'}(t)$$

$$i \frac{\partial}{\partial t} \vec{c}(t) = \overleftrightarrow{H} \vec{c}(t) \qquad O(2^N)$$

$$\vec{c}(0) \longrightarrow \vec{c}(t) \qquad O(2^N)$$

What if I want the Ground State?

$$e^{-\tau \hat{H}} |\psi(0)\rangle = |\psi(\tau)\rangle \qquad \text{Imaginary Time}, \ \tau \in \mathbb{R}$$

$$e^{-it\hat{H}} |\psi(0)\rangle = |\psi(t)\rangle \qquad \text{Real Time}, \ t \in \mathbb{R}$$

$$|\psi(\tau)\rangle = \sum_k e^{-\tau\hat{H}} c_k |E_k\rangle \quad , \quad c_k = \langle E_k|\psi(0)\rangle$$

$$\hat{H} = E_k |E_k\rangle$$

$$\sum_k c_k e^{-\tau E_k} |E_k\rangle = c_0 e^{-\tau E_0} |E_0\rangle + \sum_{k\geq 1}^{2^N} c_k e^{-\tau E_k} |E_k\rangle$$

$$= e^{-\tau E_0}\left[c_0 |E_0\rangle + \sum_{k\geq 1} c_k e^{-\tau(E_k - E_0)} |E_k\rangle \right]$$

$$|\psi(\tau)\rangle \underset{\text{proportional}}{\propto} c_0 |E_0\rangle + \sum_{k\geq 1} c_k e^{-\tau\Delta_k} |E_k\rangle$$

$$\Delta_k = E_k - E_0 \geq 0$$

$\tau \to \infty$ $\quad c_0 |E_0\rangle$ will survive.

$$\tau \gg \frac{1}{\Delta_1} \quad , \quad |c_0| \neq 0$$

Algorithm

$$\frac{\partial}{\partial\tau} |\psi(\tau)\rangle = -\hat{H} |\psi(\tau)\rangle$$

$$\frac{\partial}{\partial\tau} c_{s_1 \dots s_N}(\tau) = -\sum_{s_1' \dots s_N'} H(s_1 \dots s_N ; s_1' \dots s_N') \, c_{s_1' \dots s_N'}(\tau)$$

$$\frac{\partial}{\partial\tau} \vec{c}(\tau) = -\overleftrightarrow{H} \cdot \vec{c}(\tau)$$ complexity $O\left(\frac{1}{\Delta_1} 2^N\right)$

Use a quantum computer —

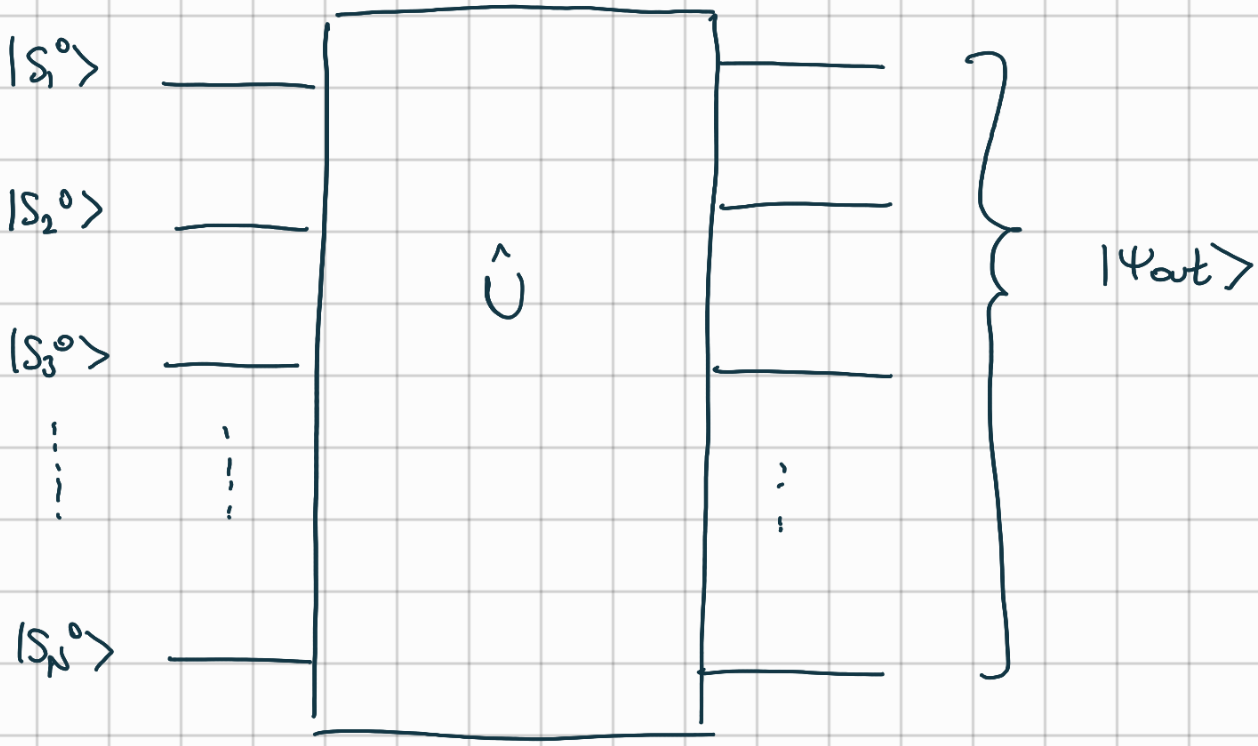
$|\Psi(t)\rangle = e^{-i\hat{H}t}|\Psi_0\rangle$, Only if $|\Psi(0)\rangle$ is a product state.

$$|\Psi(0)\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots\cdots |\phi_N\rangle$$

Single-Spin wave function (no entanglement)

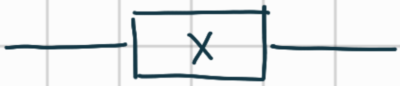
$c_{s_1^0 \cdots s_N^0} \neq 0$

Quantum Circuits

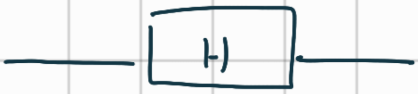


$\hat{U} = \hat{U}_L \cdots\cdots \hat{U}_2 \hat{U}_1$, $\hat{U}_i$ are k-local operations

1-Local Gates



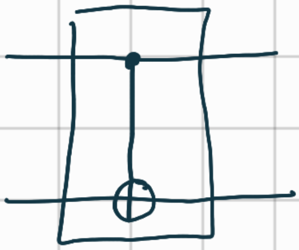
$$= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$



$$= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

2 qubit gates

CNOT



Trotter Decomposition of Unitary Dynamics

$$\hat{H} = \hat{H}_A + \hat{H}_B \quad , \quad [\hat{H}_A, \hat{H}_B] \neq 0 \ \text{(not commute)}$$

$$e^{-i\delta_t \hat{H}} = e^{-i\delta_t \hat{H}_a} e^{-i\delta_t \hat{H}_b} + \underset{\text{order}}{O}(\delta_t^2)$$

First Order Trotter-Suzuki Formula

$$e^{-i\delta_t \hat{H}} = e^{-i\frac{\delta_t}{2} \hat{H}_a} e^{-i\delta_t \hat{H}_B} e^{-i\frac{\delta_t}{2} \hat{H}_A} + O(\delta_t^3)$$

Second Order Formula

$$\hat{H} = \sum_k \hat{k}_k \quad , \quad \hat{k}_k \text{ are } K\text{-local}$$

"act only on few qubits"

$$e^{-i\delta_t \hat{H}} = \underbrace{e^{-i\delta_t \hat{k}_1}}_{U_1} \cdot \underbrace{e^{-i\delta_t \hat{k}_2}}_{U_2} \cdots \underbrace{e^{-i\delta_t \hat{k}_n}}_{U_n} + O(\delta_t^2)$$

$$e^{-it\hat{H}} |\psi(0)\rangle = e^{-i\delta_t \hat{H}} \cdot e^{-i\delta_t \hat{H}} \cdots e^{-i\delta_t \hat{H}} |\psi(0)\rangle$$

time-independent

divide to smaller time spaces

where $t = p \times \delta_t$

Total Error $O(\delta_t^2 \times p) = O(\delta_t \times t)$

time steps

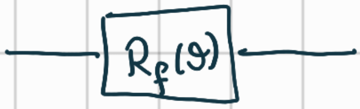
Example: The T.f. Ising Model

$$\hat{H} = -\Gamma \sum_i^N \hat{X}_i + J \sum_i^N \hat{Z}_i \hat{Z}_{i+1} \quad , \quad \hat{Z}_{N+1} = \hat{Z}_1$$

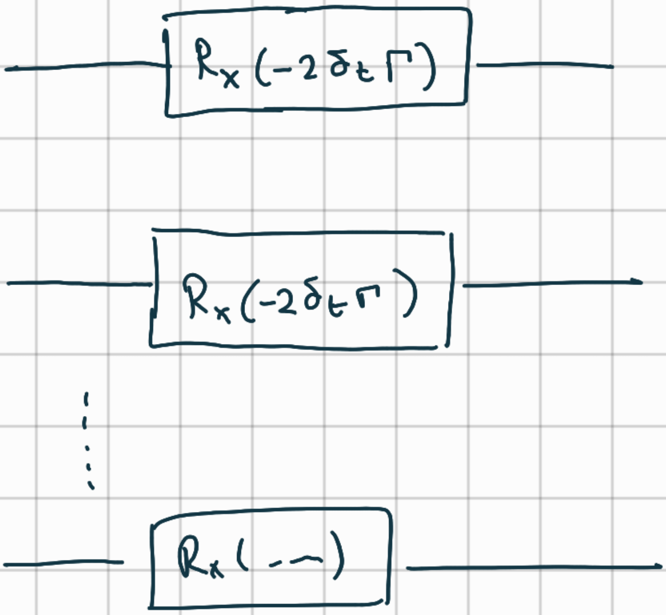
$\hat{k}_k \rightarrow$ I $\hat{X}_1, \hat{X}_2, \ldots, \hat{X}_N \rightarrow$ 1 qubit gates

II $\hat{Z}_1 \hat{Z}_2, \ldots \rightarrow$ 2 qubit gates

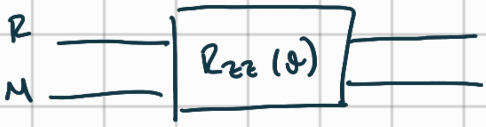
$$e^{+i\Gamma X_1 \delta_t} \dots e^{i\Gamma X_N \delta_t}$$

, $R_x(\theta) =$ 

$$\exp\left(-i X \frac{\theta}{2}\right)$$

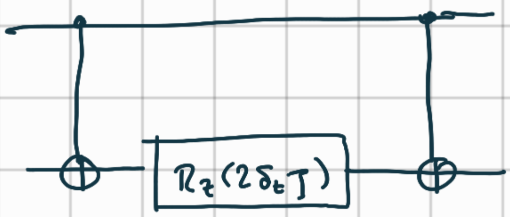


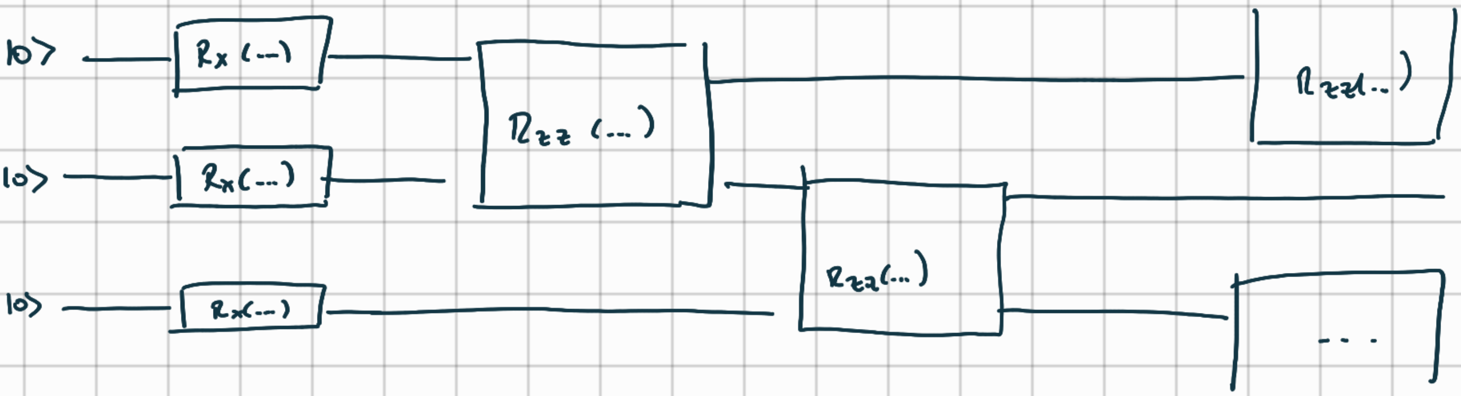
$$e^{-i\delta_t \hat{Z}_1 \hat{Z}_2} \quad e^{-i\delta_t \hat{Z}_2 \hat{Z}_3} \quad \dots\dots \quad e^{-i\delta_t \hat{Z}_N \hat{Z}_1}$$



$$\hat{R}_{zz}(\theta) = e^{-i\frac{\theta}{2}\hat{Z}_k \hat{Z}_M}$$

$$R_z(\theta) = e^{-i\frac{\theta}{2}\hat{Z}_k}$$



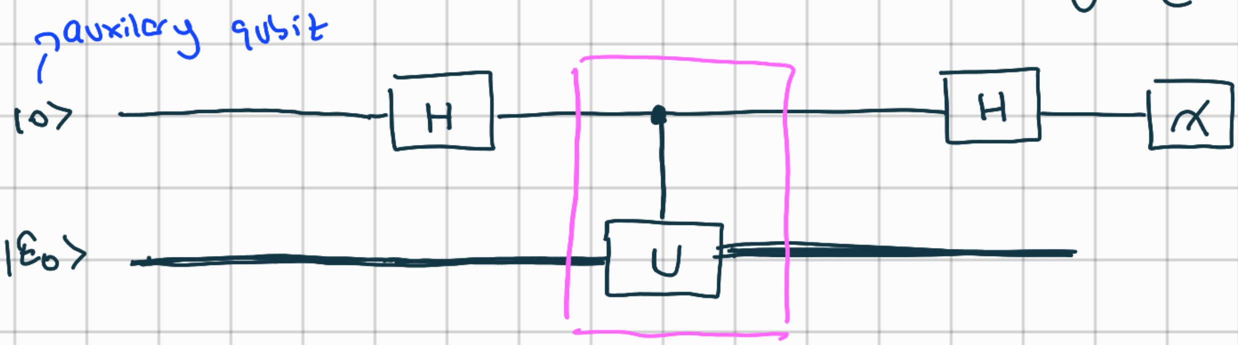


$$e^{-i\delta_t J Z_1 Z_3}\, e^{-i\delta_t Z_2 Z_3}\, e^{-i\delta_t J Z_1 Z_2}\, e^{i\delta_t \Gamma X_1}\, e^{i\delta_t \Gamma X_2}\, e^{i\delta_t \Gamma X_3}\, |000\rangle$$

QUANTUM PHASE ESTIMATION ☆

$|E_0\rangle$, Problem: Find E_0 , $|\psi_{IN}\rangle = |0\rangle|E_0\rangle$

$\hat{U} = e^{-it\hat{H}}$



$$\left(\begin{array}{cc|c} 1 & 0 & \\ 0 & 1 & 0 \\ \hline \multicolumn{2}{c|}{0} & U \end{array}\right)$$

$$|\psi_{IN}\rangle = |0\rangle|E_0\rangle$$

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle|E_0\rangle + |1\rangle|E_0\rangle\right)$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle|E_0\rangle + |1\rangle \, \underbrace{U}_{e^{-it\hat{H}}} |\hat{E}_0\rangle \right)$$

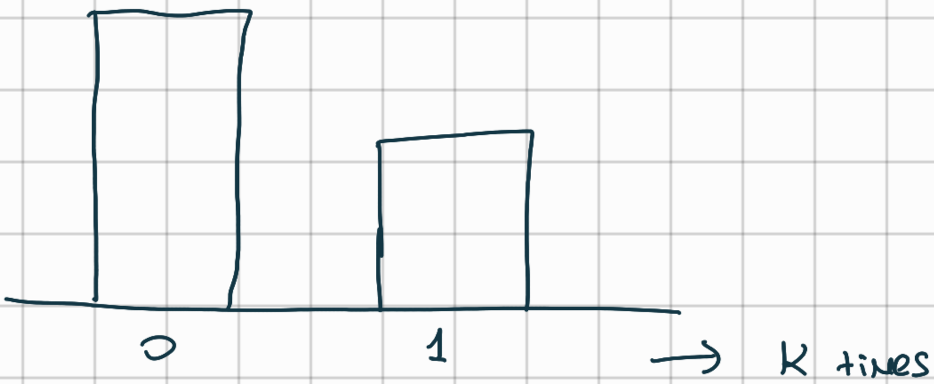
$$|\psi_2\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle|\hat{E}_0\rangle + e^{-it\hat{E}_0}|1\rangle|\hat{E}_0\rangle \right)$$

Applying H to the first qubit

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2}\, e^{-it\hat{E}_0} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 + e^{-it\hat{E}_0} \\ 1 - e^{-it\hat{E}_0} \end{pmatrix}$$

$$|\psi_3\rangle = \frac{1}{2}\left[(1+e^{-it\hat{E}_0})|0\rangle|E_0\rangle + (1-e^{-it\hat{E}_0})|1\rangle|E_0\rangle \right)$$

$$\mathrm{Prob}(0) = \frac{1}{4}\left| 1 + e^{-itE_0} \right|^2 = \cos\left(\frac{tE_0}{2}\right)^2$$

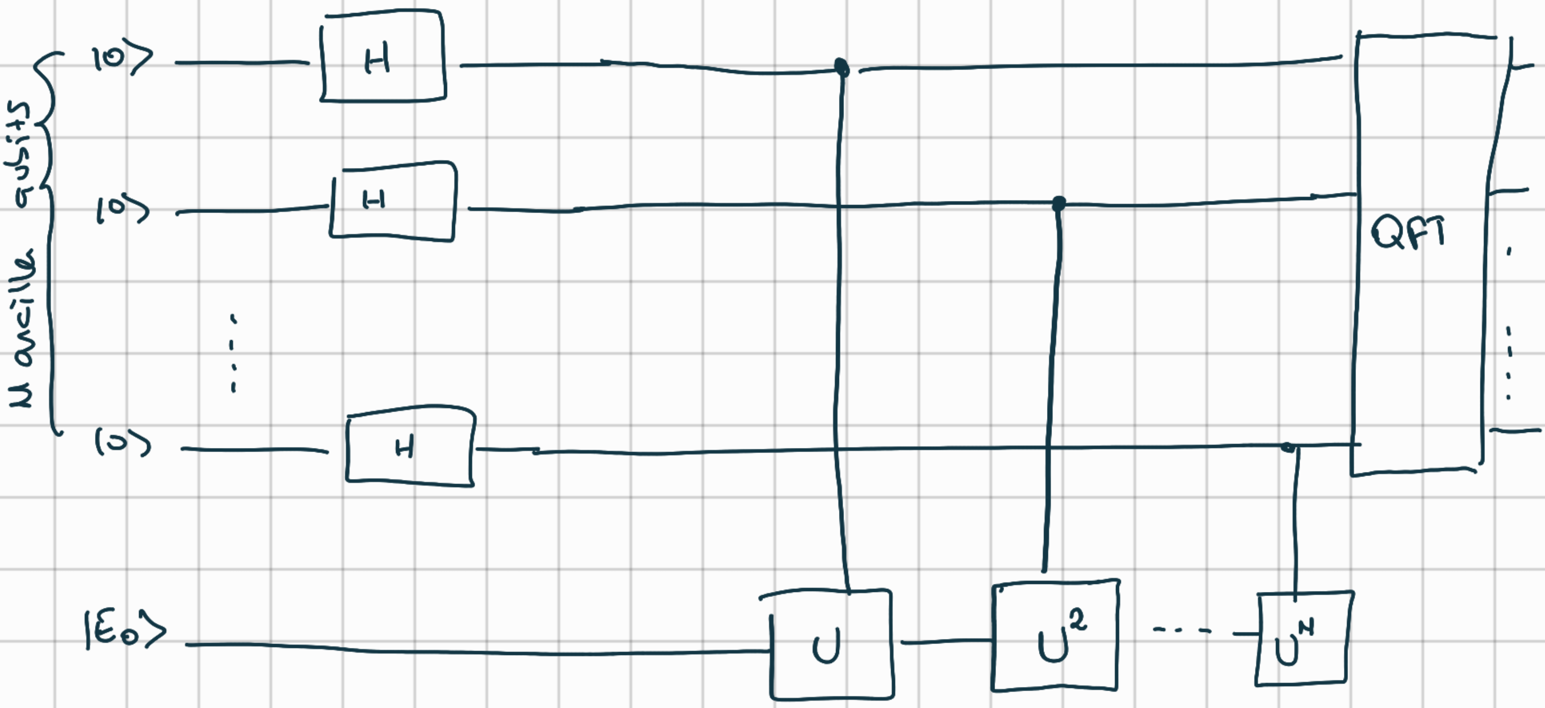


$\left(\frac{N_0}{K}\right)$ $\left(\frac{N_1}{K}\right)$

→ Proportional to the Prob (0)

FULL QUANTUM PHASE ESTIMATION

→ several peaks at eigenstates



↓ at time 2t

$$(e^{-it\hat{H}})^2 = e^{-i(2t)\hat{H}}$$

$$|\Psi_{out}\rangle = \frac{|E_0\rangle}{\sqrt{2^m}} \left[|0\rangle + e^{-itE_0} |1\rangle \right] \left[|0\rangle + e^{-i(2t)E_0} |1\rangle \right] \cdots \left[|0\rangle + e^{-i(Nt)E_0} |1\rangle \right]$$

$$|\Psi_{out}\rangle = \frac{1}{\sqrt{2^m}} \sum_{k=0}^{2^M-1} e^{-i(kt)E_0} |k\rangle |E_0\rangle$$

Fourier Transform

$$\text{PROB}(E_0) \sim |C_0|^2 \qquad C_0 \sim \frac{1}{\text{Poly}(N)}$$

$\to$ N qubits

$\to$ polynomial

$$\langle E_0 | \Psi(0) \rangle = C_0$$