Qiskit | Global Summer School 2022

Lecture 3

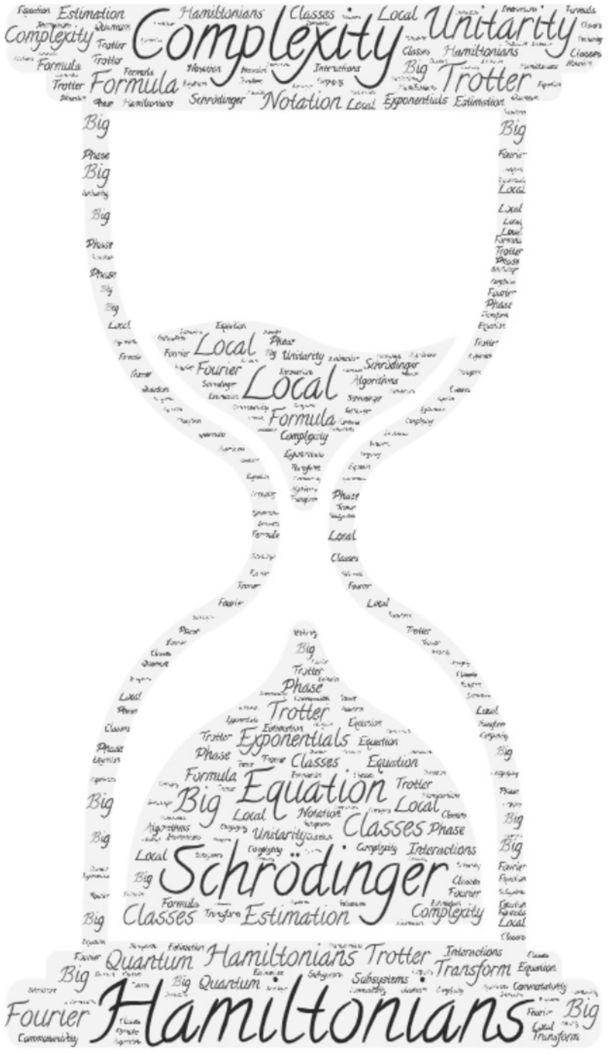
Time to evolve:

Hamiltonians and time-evolution of quantum systems

Quantum Simulation

Hamiltonians and time-evolution

- Hamiltonians
  - Schrödinger equation, unitarity, subsystems, local interactions, exponentials, commutativity, Trotter formula
- Algorithms
  - Quantum Fourier transform, quantum phase estimation
- Complexity
  - Complexity classes, big O notation



Schrödinger Equation

Hamiltonian.

$$i\hbar \frac{d|\psi\rangle}{dt} = \boxed{\hat{H}}\,|\psi\rangle$$

Planck's constant

$\hbar = 1$

Hermitian: $H^{\dagger} = H$

$$\begin{pmatrix} E_1 & \cdots & 0 \\ \vdots & E_2 & \vdots \\ 0 & \cdots & E_n \end{pmatrix}$$

$$H = \sum_k E_k \underbrace{|k\rangle}\langle k|$$

energy

energy eigenstates.

Lowest: Ground state energy

Ground state.

Example.

number

$$\hat{H} = \hbar \omega X$$

X-gate.

Eigenstates: $|+\rangle$, $\boxed{|-\rangle}$ ground state.

$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

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

$+\hbar\omega$ $\boxed{-\hbar\omega}$

Ground state energy

Exponential of a matrix

$$M = \sum_k e_k |k\rangle\langle k| \qquad f(M) = \sum_k f(e_k) |k\rangle\langle k|$$

$$\exp(M) = \sum_k \exp(e_k) |k\rangle\langle k|$$

$$M = \begin{pmatrix} e_1 & & 0 \\ & \ddots & \\ 0 & & e_N \end{pmatrix} \qquad \exp(M) = \begin{pmatrix} \exp(e_1) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \exp(e_N) \end{pmatrix}$$

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \exp(\theta Z) = \begin{pmatrix} \exp(\theta \times 1) & 0 \\ 0 & \exp(\theta \times -1) \end{pmatrix} = \begin{pmatrix} \exp(\theta) & 0 \\ 0 & \exp(-\theta) \end{pmatrix}$$

$$|\psi(t)\rangle = \exp\left[-\frac{iH\boxed{t}}{\hbar}\right]|\psi(0)\rangle$$

$$\boxed{i\hbar\frac{d|\psi\rangle}{dt} = H|\psi\rangle}$$

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = i\hbar\frac{d}{dt}\left(\exp\left[-\frac{iHt}{\hbar}\right]|\psi(0)\rangle\right)$$

$$= -i\hbar\frac{i}{\hbar}H\exp\left[\frac{iHt}{\hbar}\right]|\psi(0)\rangle$$

$$= H|\psi(t)\rangle$$

$$\boxed{|\psi(t_2)\rangle = \exp\left[-\frac{iH(t_2-t_1)}{\hbar}\right]|\psi(t_1)\rangle}$$

$$U(t_1,t_2) = \exp\left[-\frac{iH(t_2-t_1)}{\hbar}\right]$$

$$|\psi(t_2)\rangle = U|\psi(t_1)\rangle$$

Checking unitarity

$$[H, H] = 0$$

$$U = \exp\left[-\frac{iH(t_2 - t_1)}{\hbar}\right]$$

$$U^\dagger U = \exp\left[-\frac{iH(t_2 - t_1)}{\hbar}\right]^\dagger \exp\left[-\frac{iH(t_2 - t_1)}{\hbar}\right]$$

$$= \exp\left[\frac{+iH^\dagger(t_2 - t_1)}{\hbar}\right] \exp\left[\frac{-iH(t_2 - t_1)}{\hbar}\right]$$

$H^\dagger = H$

works only if operators commute.

DANGER

$$= \exp\left[+i\frac{H(t_2 - t_1)}{\hbar} - \frac{iH(t_2 - t_1)}{\hbar}\right] = \exp[0] = \mathbb{1}.$$

Commutability

$\hat{A}, \hat{B}$ Commute. $AB = BA$

$$\underbrace{AB - BA}_{[A,B]} = 0$$

commutator.

Anti-commute. $AB = -BA$

$$AB + BA = 0$$

$$\{A, B\} = 0$$

anti-commute.

Exponentials with commutativity

$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$|+\rangle, |-\rangle$ $|0\rangle, |1\rangle$

$\exp(A)\exp(B)$

$[A, B] = 0$ $A = \sum_k a_k |k\rangle\langle k|$ $B = \sum_k b_k |k\rangle\langle k|$

$$\exp(A)\exp(B) = \exp\left(\sum_k a_k |k\rangle\langle k|\right) \exp\left(\sum_k b_k |k\rangle\langle k|\right)$$

$$= \sum_k \exp(a_k) |k\rangle\langle k| \sum_k \exp(b_k) |k\rangle\langle k|$$

$$= \sum_k \exp(\underbrace{a_k + b_k}) |k\rangle\langle k| = \exp(A+B)$$

$$\underbrace{|k\rangle\langle k|k\rangle\langle k|}_{|k\rangle\langle k|} \quad |k\rangle\underbrace{\langle k|k\rangle}_{1}\langle k|$$

Unitary gates $\longleftrightarrow$ Hamiltonians

Hermitian

$$U = \exp(iK)$$

any unitary

$$U^\dagger U = \mathbb{1}$$

eigenvalues of unitary

$e^{i\varphi}$

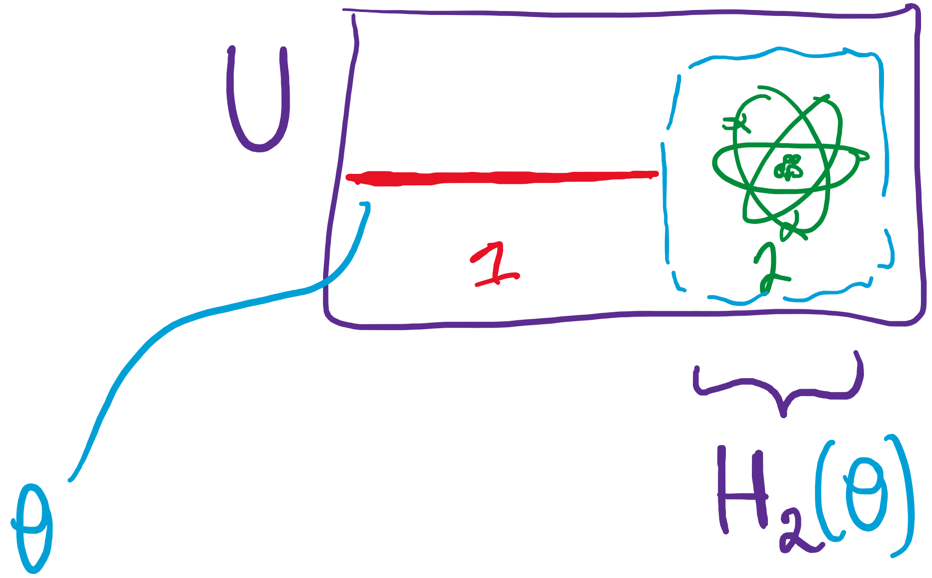
$$K = -i \log U$$

$$= -i \log \sum_k u_k |k\rangle\langle k|$$

$$= -i \sum_k \log u_k |k\rangle\langle k|$$

$$= -i \sum_k \log e^{i\varphi_k} |k\rangle\langle k| = -i \sum_k i\varphi_k |k\rangle\langle k| = \underbrace{\sum_k \varphi_k |k\rangle\langle k|}_{} = K^\dagger$$

Evolution of subsystems



H_{12}.

vary over time.

Simulating Hamiltonians

Classically: very inefficient!

$$i\hbar \frac{d|\psi\rangle}{dt} = H|\psi\rangle$$

$$\langle x|\psi\rangle = \psi(x)$$

$$i\hbar \frac{\partial}{\partial t}\psi(x) = \underbrace{\left[-\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]}_{\text{Hamiltonian}}\psi(x)$$

Use quantum computers!

approximations...

1 qubit: $|0\rangle, |1\rangle$ 2 equation.

2 qubits: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$ 4 eq^ns.

n qubits: $|0\ldots0\rangle, \ldots, |1\ldots1\rangle$ 2^n eq^ns

exponential!

Local interactions

H time-independent. $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$ ← Hamiltonian.

$$H = \sum_{k=1}^{L} H_k \qquad H_1 = X_3 X_4 \qquad H_2 = Z_5$$

$\boxed{\text{Good news!}}$

$e^{-iH_k t}$

↑ smaller subsystem.

→ easier approximate q circuits

$\boxed{\text{Bad news!}}$

$$\underbrace{e^{-iHt} = e^{-i\sum_k H_k t} \neq e^{-iH_1 t} e^{-iH_2 t} \cdots e^{-iH_L t} = \sum e^{-iH_k t}}_{\text{if } H_k \text{ don't commute,}}$$

Trotter formula

Hermitian: A, B

$$\lim_{n\to\infty}\left(e^{i\frac{At}{n}}e^{i\frac{Bt}{n}}\right)^n = e^{i(A+B)t} \leftarrow \text{for real } t$$

$$e^{i(A+B)\Delta t} = e^{iA\Delta t}e^{iB\Delta t} + O(\Delta t^2)$$

$$e^{i(A+B)\Delta t} = e^{\frac{iA\Delta t}{2}}\, e^{iB\Delta t}\, e^{\frac{iA\Delta t}{2}} + O(\Delta t^3)$$

Schrödinger equation

$-d \qquad d$

$|-d\rangle \longrightarrow |+d\rangle$

$$H = \frac{p^2}{2m} + V(x)$$

$$|\psi\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\psi\rangle \, dx = \sum_{k=-\frac{d}{\Delta x}}^{\frac{d}{\Delta x}} a_k \underbrace{|k\Delta x\rangle}_{n}$$

$$\frac{2d}{\Delta x} + 1 = 2^n$$

$$n = \log\left(\frac{2d}{\Delta x} + 1\right)$$

$$\left[V(x), \frac{p}{2m}\right] \neq 0$$

$$|k\rangle \to e^{-iV(k\Delta x)\Delta t} |k\rangle$$

$$U_{FFT}\, x\, U_{FFT}^{\dagger} = p$$

$$\longrightarrow \quad |k\rangle \longrightarrow U_{FFT}\, e^{-\frac{ix^2}{2m}}\, U_{FFT}^{\dagger} |k\rangle$$

Fourier transform

$$\text{difficult} \xrightarrow{FT} \text{Solvable}$$

$$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} \qquad \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix}$$

do on a QC!

Discrete FT:

$$a_1, a_2, \ldots, a_N \longrightarrow b_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} a_j e^{\frac{2\pi i jk}{N}}$$

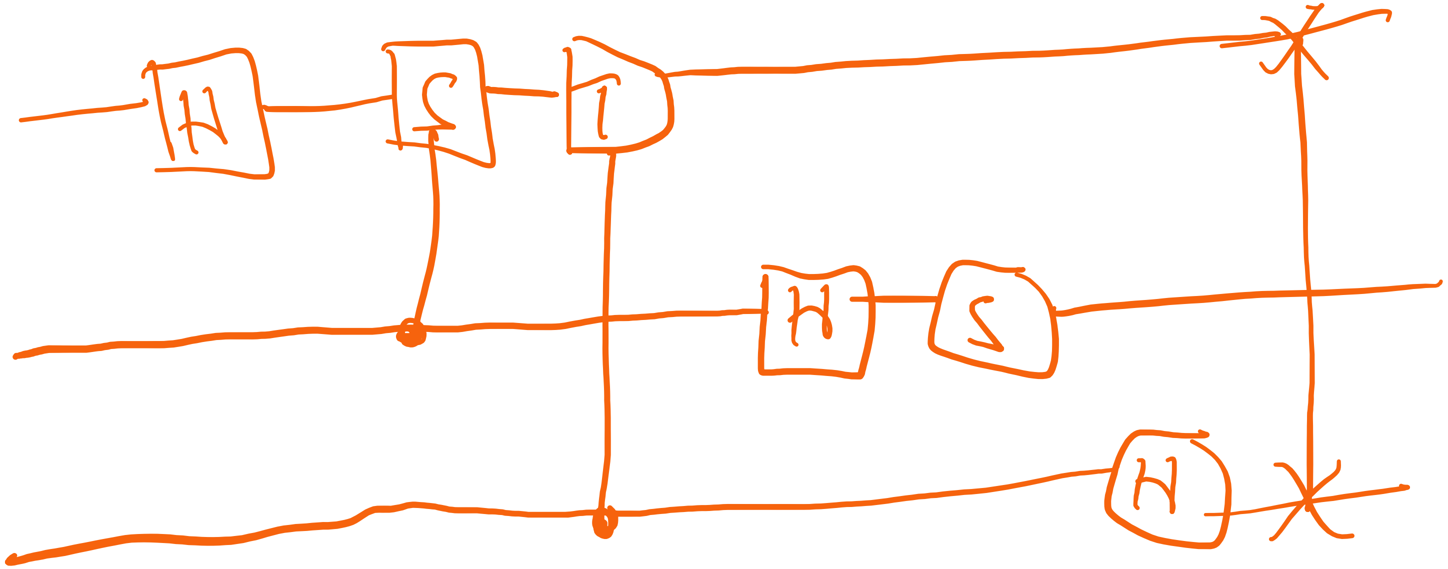
Quantum FT:

$$|0\rangle, \ldots, |N-1\rangle \longrightarrow$$

$$|j\rangle \longrightarrow \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{\frac{2\pi i jk}{N}} |k\rangle$$

$$\sum_{j=0}^{N-1} a_j |j\rangle \longrightarrow \sum_{k=0}^{N-1} b_j |k\rangle$$

unitary!



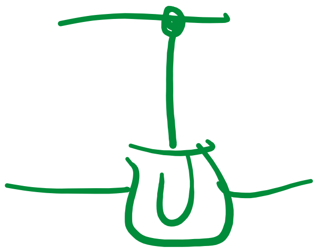
3 FT

Phase estimation.

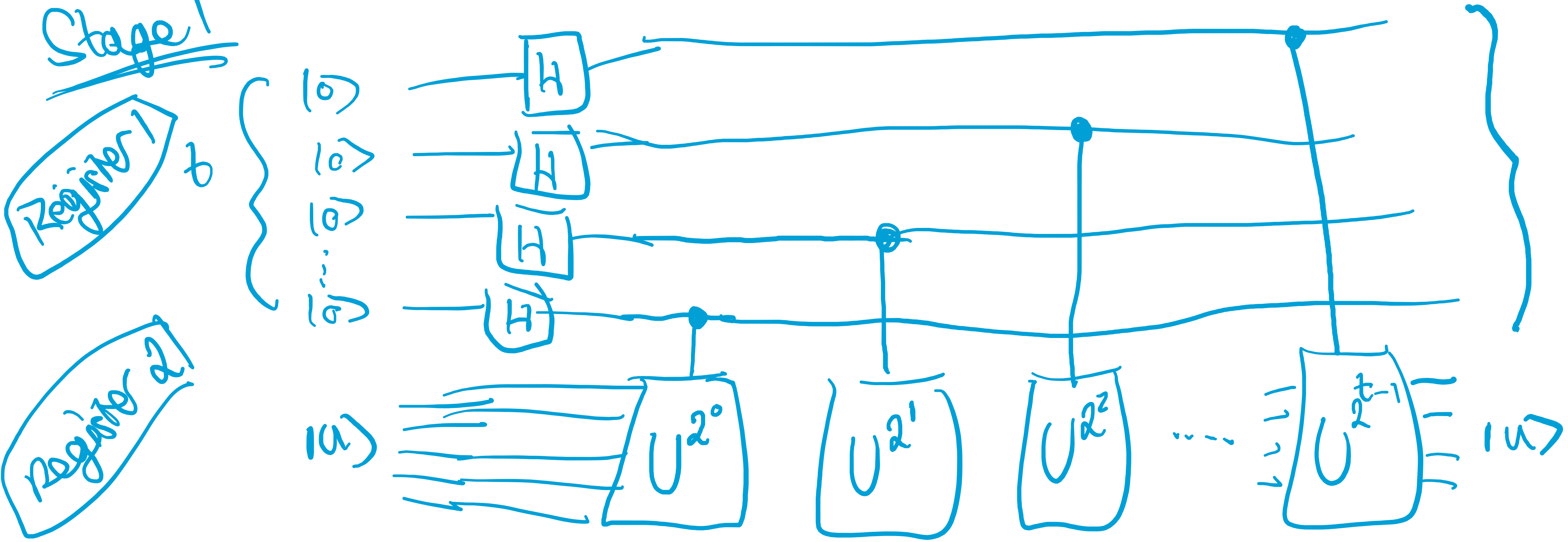
$$\underbrace{U|u\rangle}_{\text{prepare.}} = e^{2\pi i\varphi}|u\rangle$$

???

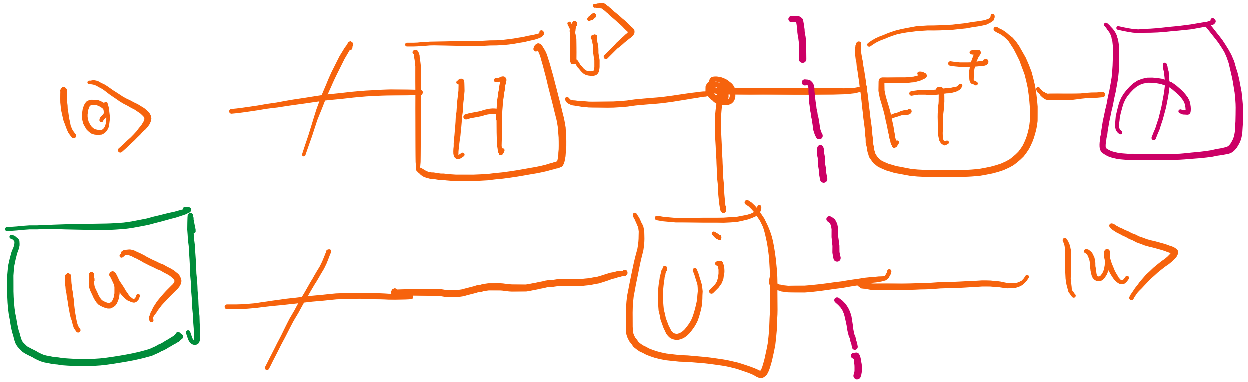
Controlled-U^{2^j}



Stage 1



Overall phase estimation



$$|\psi\rangle = \sum_u c_u |u\rangle$$

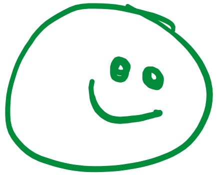
$|c_u|^2 \leftarrow$ prob. of correct outcome.

correction from lecture

$\varphi = 0.\varphi_1\varphi_2\cdots\varphi_t$ t bits

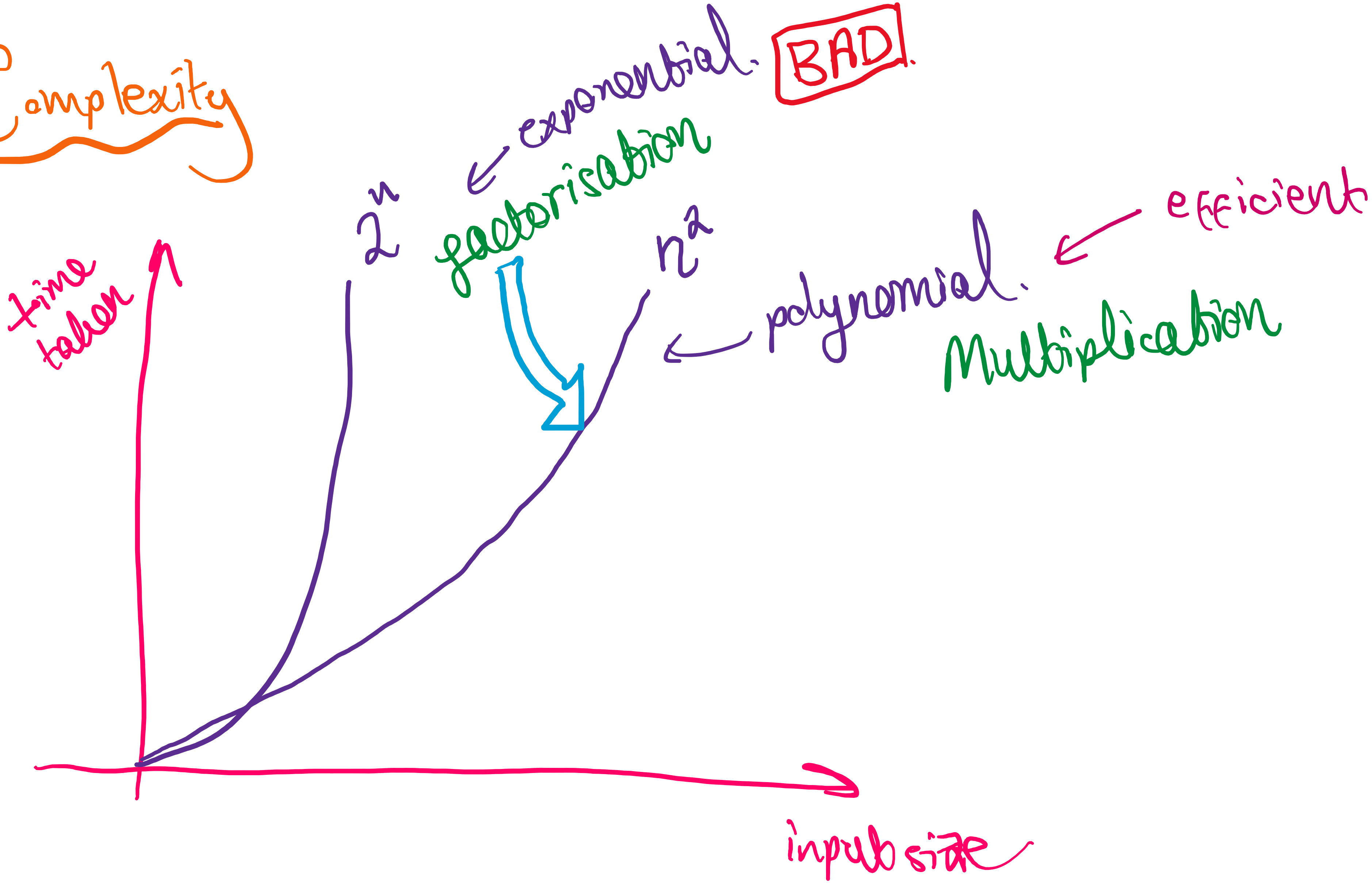
1st stage: $$\frac{1}{2^{t/2}}\left(|0\rangle + e^{2\pi i\, 0.\varphi_t}|1\rangle\right)\left(|0\rangle + e^{2\pi i\, 0.\varphi_{t-1}\varphi_t}|1\rangle\right)\cdots\left(|0\rangle + e^{2\pi i\, 0.\varphi_1\varphi_2\cdots\varphi_t}|1\rangle\right)$$

inverse FT $\longrightarrow$ $|\varphi_1\varphi_2\cdots\varphi_t\rangle$

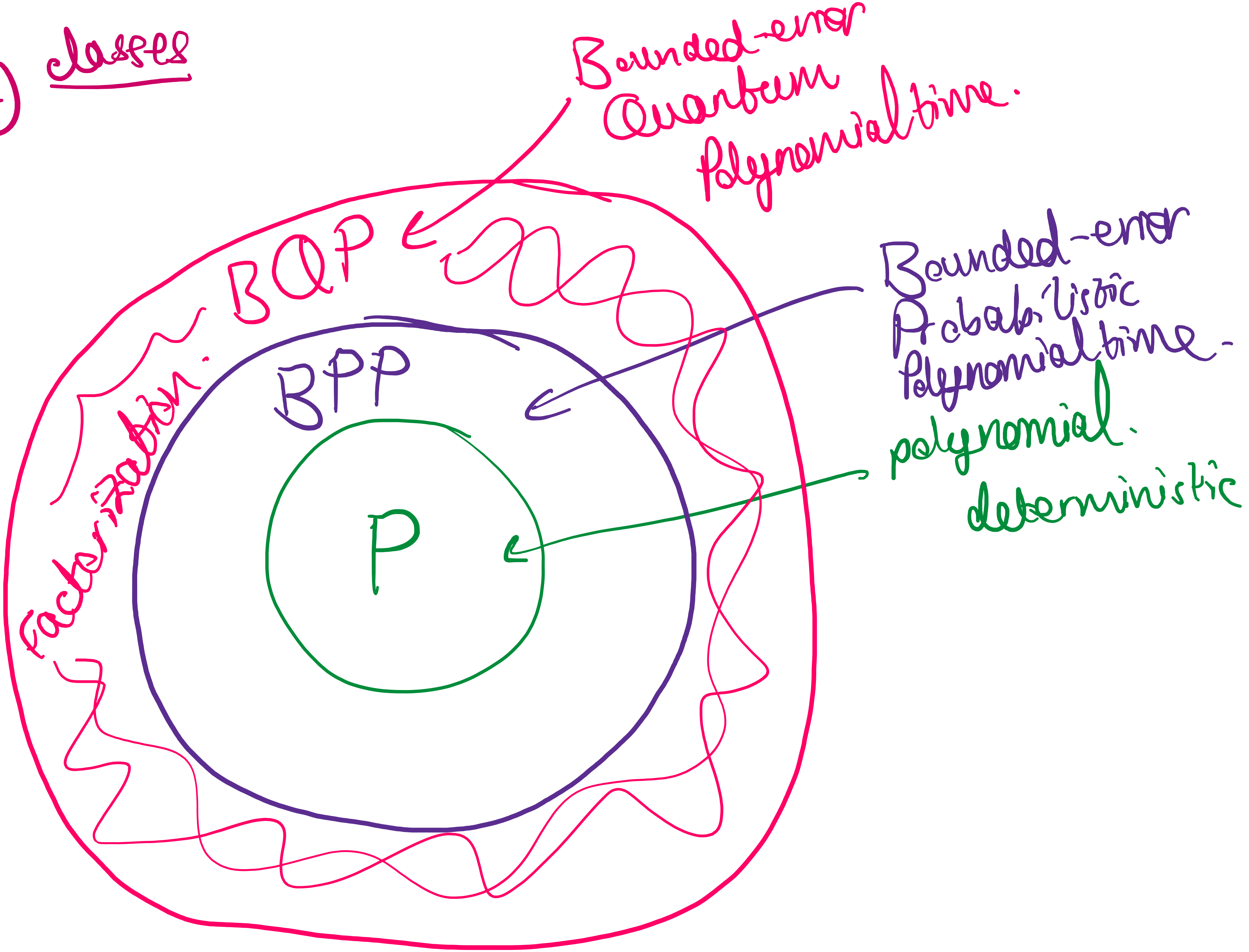


↳ Measure in comp. basis

Complexity


time taken
input size
2^n
n^2
exponential.
BAD
factorisation
polynomial.
efficient
Multiplication

Complexity classes



Big O notation

n: $n + 3n + n^4$

$3n^2$

Classical

$O(n^4)$

$O(n^2) \leftarrow$ Multiplication

$O(n) \leftarrow$ Addition

$O(e^{n^{1/3}}) \leftarrow$ Factorization

$O(n^2)$