

Lecture 3

Time to evolve:

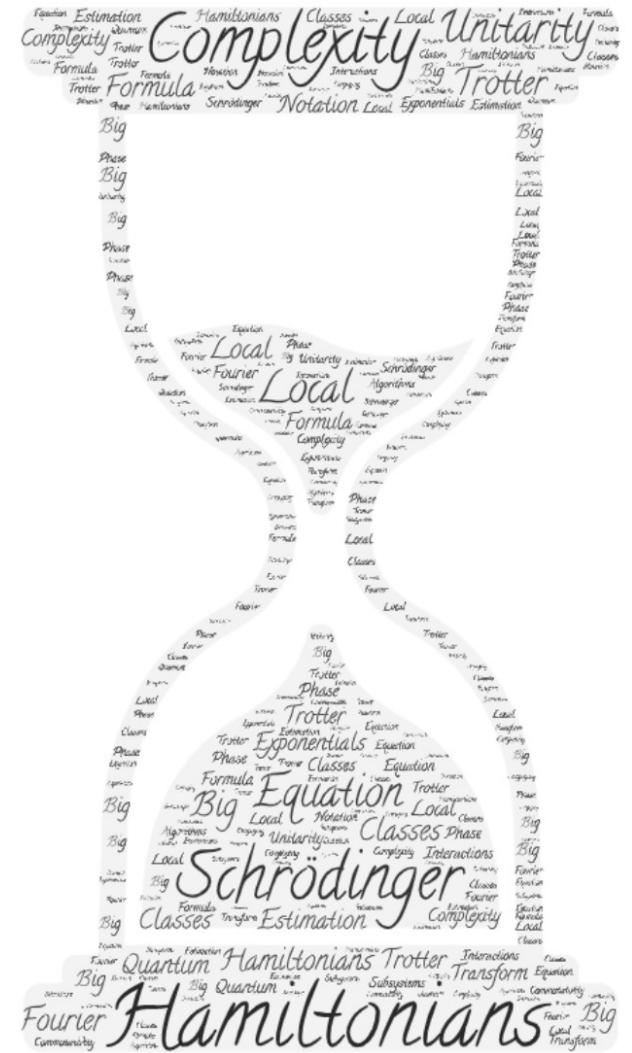
Hamiltonians and time-evolution of quantum systems



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.

$$i\hbar \frac{d|\Psi\rangle}{dt} = [\hat{H}]|\Psi\rangle$$

Planck's constant

$$\hbar = 1$$

Hermition: $H^+ = H$

$$\begin{pmatrix} E_1 & - & - & 0 \\ ; & E_2 & - & ; \\ ; & . & . & . \\ 0 & - & - & - E_n \end{pmatrix}$$

$$H = \sum_k E_k |k\rangle \langle k|$$

energy eigenstates.

lowest: Ground state energy

Ground state

Example - number

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

x-gate.

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

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

$+\hbar\omega$ $- \hbar\omega$ Ground state energy

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

Exponential of a matrix

$$M = \sum_k e_k \quad |k \times k| \quad f(M) = \sum_k f(e_k) \quad |k \times k|$$

$$\exp(M) = \sum_k \exp(e_k) \quad |k \times k|$$

$$M = \begin{pmatrix} e_1 & & 0 \\ & \ddots & \\ 0 & & e_N \end{pmatrix}$$

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

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

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

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

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

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

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

$$\stackrel{?}{=} H |\psi(t)\rangle$$

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

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

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

Checking unitarity

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

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

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

$\stackrel{H}{\approx}$

DANGER

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

$$[H, H] = 0$$

works only if
operators commute.

Commutativity

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

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

Anti-commute. $AB = -BA$

$$\begin{gathered} AB + BA = 0 \\ \{A, B\} = 0 \end{gathered} \quad \xleftarrow{\text{anti-commute,}}$$

Exponentials with commutativity

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

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

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

$$\begin{aligned} \exp(A) \exp(B) &= \exp\left(\sum_k a_k |k\rangle\langle k|\right) \exp\left(\sum_{k'} b_{k'} |k'\rangle\langle k'|\right) |k\rangle\langle k| \\ &= \sum_k \exp(a_k) |k\rangle\langle k| \sum_{k'} \exp(b_{k'}) |k'\rangle\langle k'| \\ &= \sum_k \underbrace{\exp(a_k + b_k)}_{\sim} |k\rangle\langle k| = \exp(A+B) \end{aligned}$$

Unitary gates \longleftrightarrow Hamiltonians

$$U = \exp(iK)$$

any unitary

$$K = -i \log(U)$$

$$= -i \log \sum_k u_{kk} |k\rangle\langle k|$$

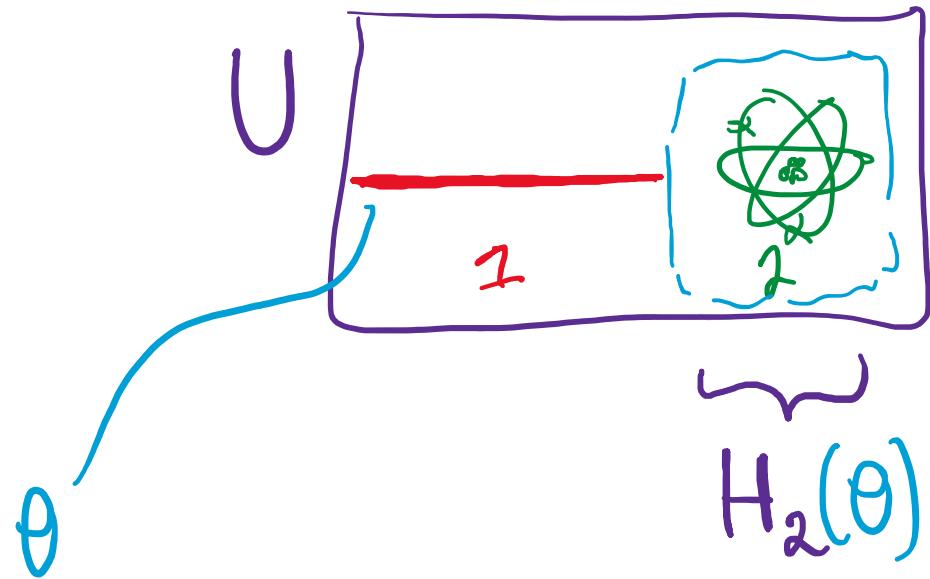
$$= -i \sum_k \log u_{kk} |k\rangle\langle k|$$

$$= -i \sum_k \log e^{i\phi_k} |k\rangle\langle k| = -i \sum_k i\phi_k |k\rangle\langle k| \stackrel{\text{def}}{=} \sum_k q_k |k\rangle\langle k| = K^*$$

eigenvalues of unitary
 $e^{i\phi}$

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

Evolution of subsystems



H_{12} .

\uparrow vary over time.

Simulating Hamiltonians

Classically: very inefficient!

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

$$= \langle \psi | \hat{H} \rangle$$

Hamiltonian

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

Use quantum computers!

$$i\hbar \frac{\partial}{\partial t} \Psi(x) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \Psi(x)$$

1 qubit: $|0\rangle, |1\rangle$

2 equations.

2 qubits: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$ 4 eqns.

n qubits: $|0\dots 0\rangle, \dots, |1\dots 1\rangle$

2^n eqns

approximations..

\prod

exponentially!

Local interactions

H time independent.

$$H = \sum_{k=1}^L H_k \quad \rightarrow \quad \begin{aligned} H_1 &= X_3 X_4 \\ H_2 &= Z_5 \end{aligned}$$

Good news!

$e^{-iH_k t}$

↑

smaller subsystem.

$$|\Psi(t)\rangle = e^{-i\frac{Ht}{\hbar}} |\Psi(0)\rangle$$

Hamiltonian.

Bad news!

$$e^{-iHt} = e^{-i\sum_k H_k t}$$

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

$$= \sum e^{-iH_k t}$$

if H_k don't commute,

* Trotter formula *

Hermitian: A, B

$$\lim_{n \rightarrow \infty} \left(e^{\frac{iA\Delta t}{n}} e^{\frac{iB\Delta t}{n}} \right)^n = e^{i(A+B)t} \leftarrow \text{for real } t$$

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

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

Schrödinger equation

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

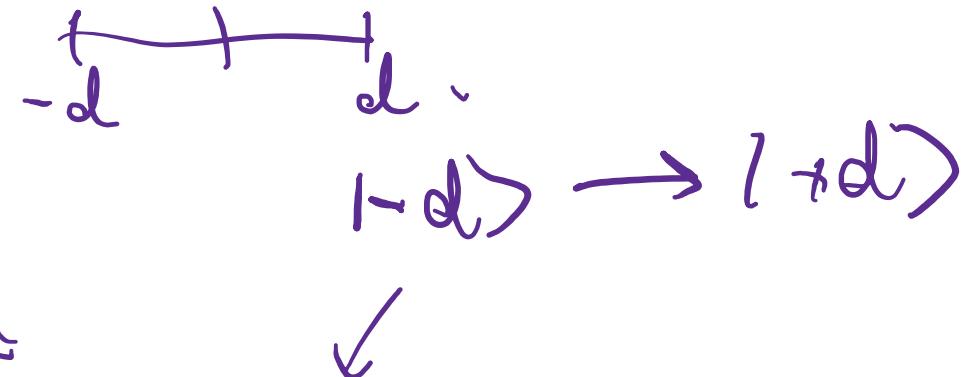
$$|\psi\rangle = \int_{-\infty}^{\infty} |x\rangle \times x |\psi\rangle dx.$$

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

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

$$U_{FFT} \propto U_{FFT}^\dagger = P$$

$$\rightarrow |k\rangle \rightarrow U_{FFT} e^{-\frac{i\omega^2}{2m}} U_{FFT}^\dagger |k\rangle$$

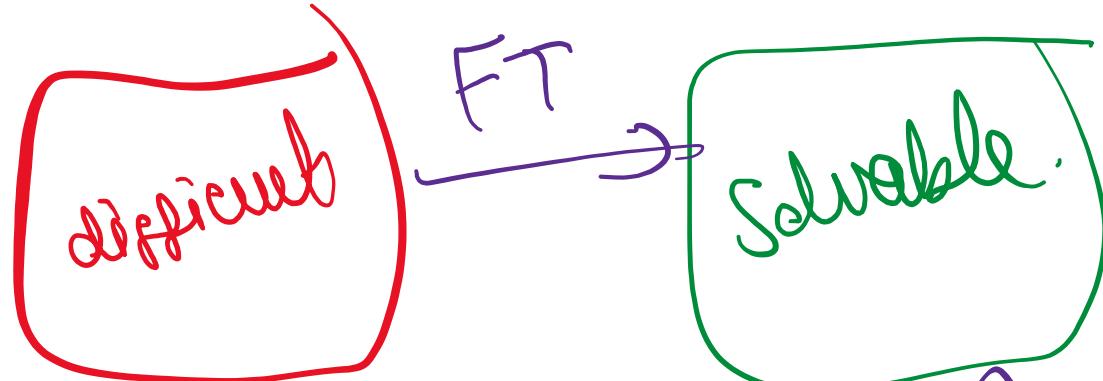


$$\sum_{k=-\frac{d}{\Delta x}}^{\frac{d}{\Delta x}} a_k |k\Delta x\rangle$$

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

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

Fourier transform



$$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

$$\begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix}$$

do on a
QC!

Discrete FT:

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

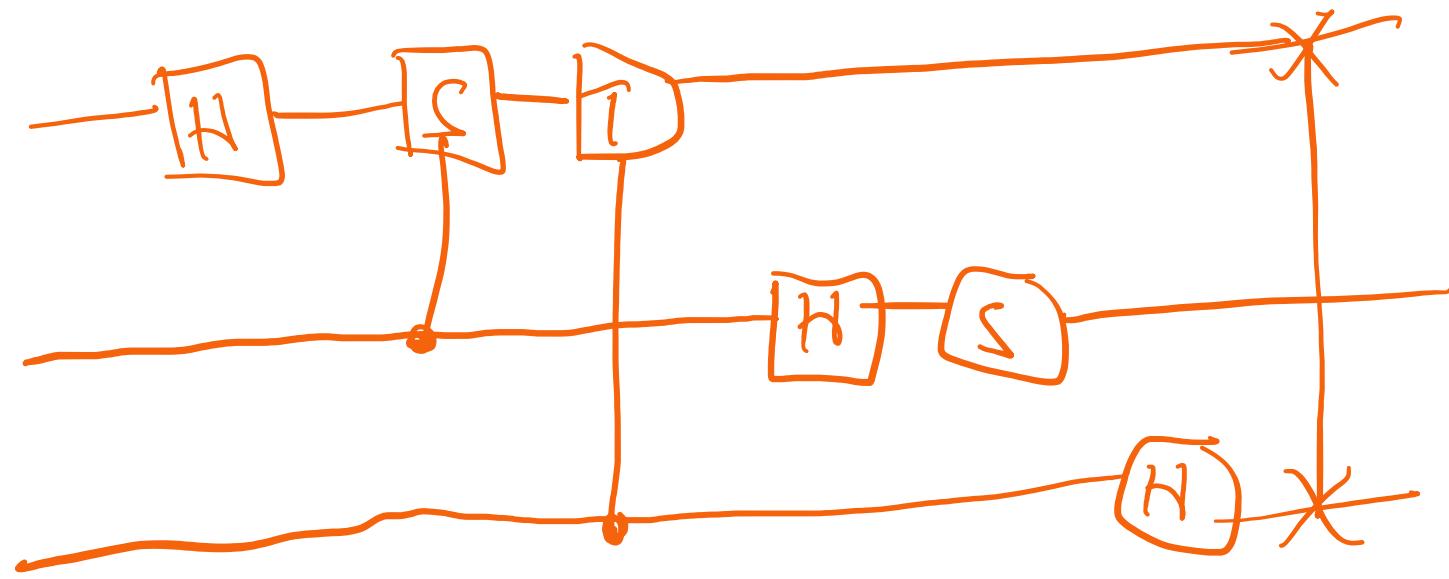
Quantum FT:

$$|0\rangle, \dots, |N-1\rangle \rightarrow$$

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

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

unitary!



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ET

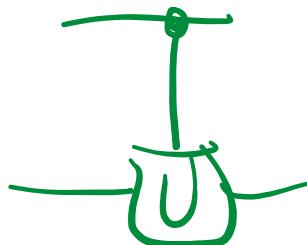
Phase estimation-

$$|U(u)\rangle = e^{2\pi i q} |u\rangle$$

$|u\rangle$
prepare.

• ? ? ?

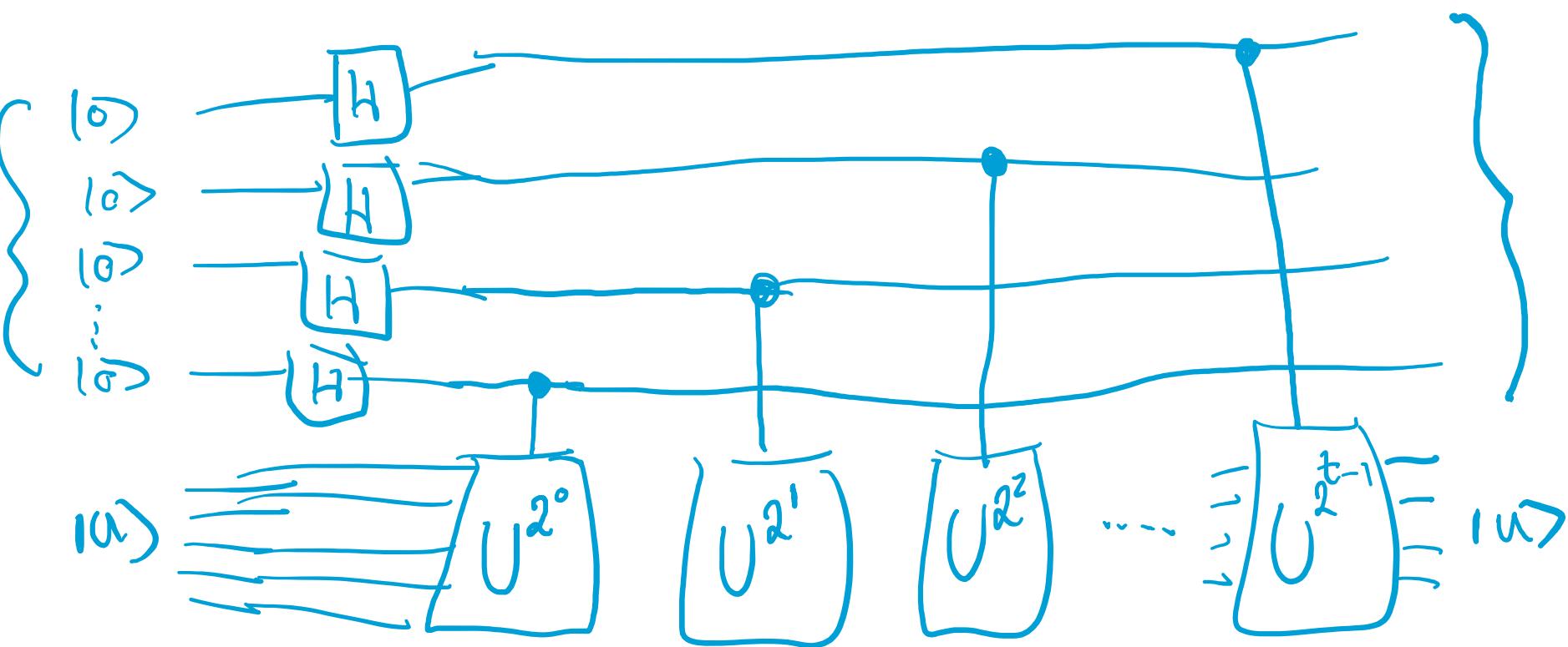
Controlled- V^{zj}



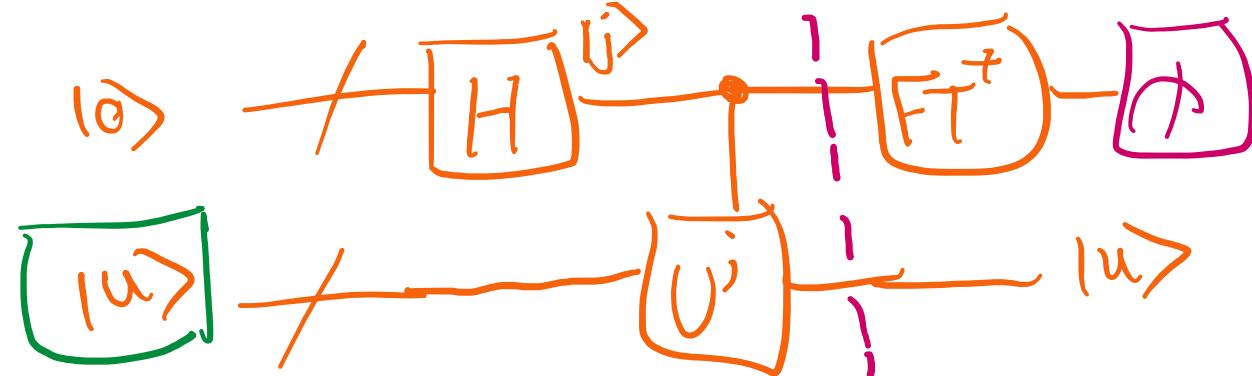
Stage 1

Reinier

Beginner 2



Overall phase estimation



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

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

correction from lecture
 $\varphi = 0.\varphi_1\varphi_2\dots\varphi_t$ t bits

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

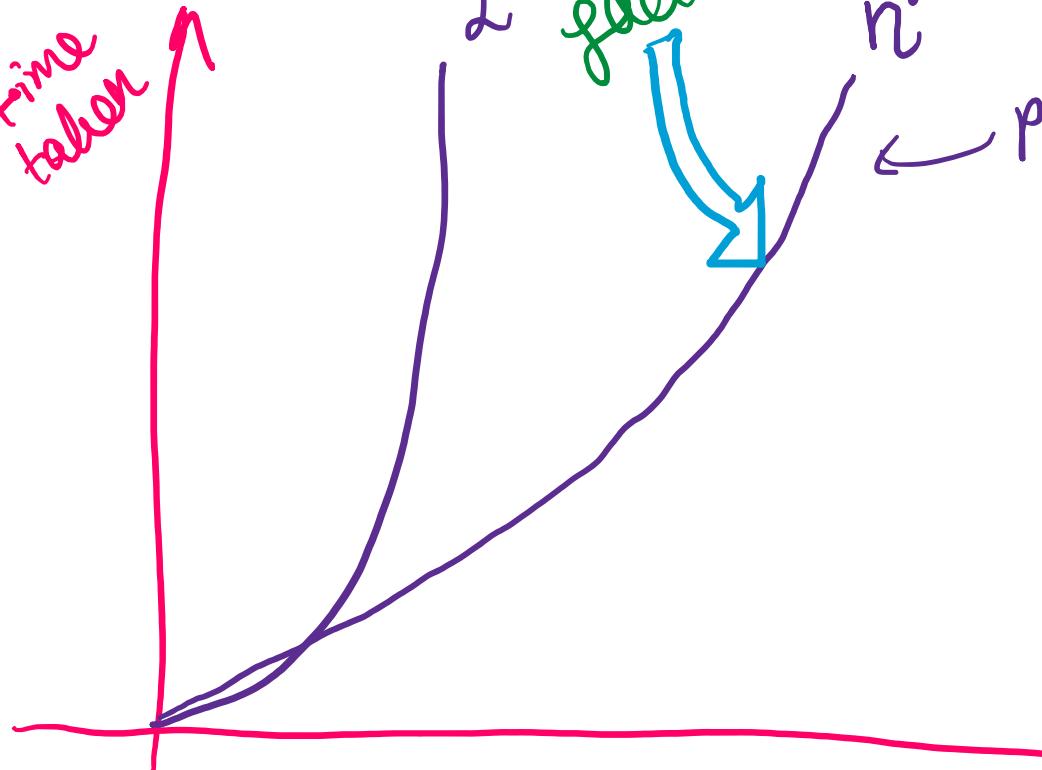
inverse FT
 $\rightarrow | \varphi_1 \varphi_2 \dots \varphi_t \rangle$



Measure in comp. basis

Complexity

Time taken



2^n exponential. **BAD!**

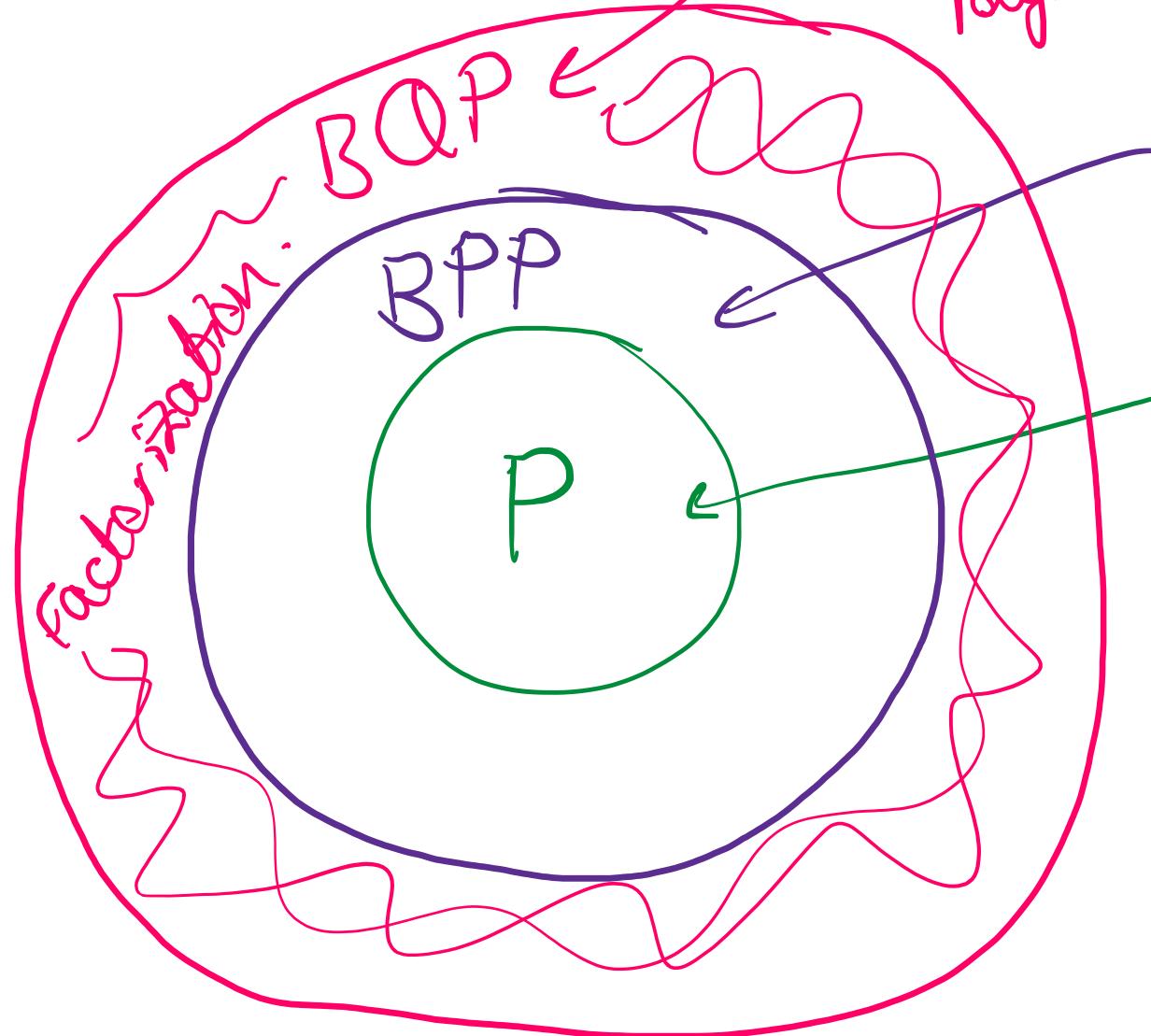
$n!$ factorisation

n^2

polynomial. **efficient**

Multiplication

Complexity classes



Bounded-error
probabilistic
polynomial-time -
polynomial.
deterministic

Bounded-error
Quantum
polynomial time.

Big O notation

$n:$ $n + 3n + n^4$
 $3n^2$

$O(n^4)$ Classical
 $O(n^2)$ Multiplication
 $O(n)$ Addition
 $O(e^{n^3})$ Factorization
 $O(n^2)$