### Quantum computing

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#### **Motivation**

The basic unit of information in classical computing is a bit

that can take two symbolic values: 0 and 1

Quantum computing works with quantum bits (or qubits)

that can be simultaneously 0 and 1 — in various proportions!

By the end of today we'll be storing information on qubits and running programs on quantum computers

# **Spoiler warning**

This is what our first quantum computer program will look like:

$$q[0] - |0\rangle - H - \chi^{2}$$

$$c1 = 0$$

To make sense of what it does, we first need to review some concepts and formalism

from Quantum Mechanics



Quantum systems

Dirac formalism

Quantum bits

#### **Recall: Wave function**

A quantum system can be described by a (complex-valued) wave function  $\Psi(\mathbf{x},t)$  satisfying Schrödinger's equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi + V \Psi$$

where

- $\Delta = \sum_{i} \frac{\partial^2}{\partial x_i^2}$  is the Laplacian operator,
- $V(\mathbf{x}, t)$  the potential function representing the environment.

### **Stationary states**

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\Delta\Psi+V\Psi$$

Let's assume that the potential  $V = V(\mathbf{x})$  is independent of t and look for *separable* solutions of the form

$$\Psi(\mathbf{x},t) = \chi(t)\,\phi(\mathbf{x}).$$

The equation becomes:

$$i\hbar \frac{\partial \chi}{\partial t} \phi = \chi \left( -\frac{\hbar^2}{2m} \Delta \phi + V \phi \right)$$

or

$$\frac{i\hbar}{\chi}\frac{\partial\chi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\Delta\phi}{\phi}+V.$$

# Separable solutions

$$\frac{i\hbar}{\chi}\frac{\partial\chi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\Delta\phi}{\phi} + V = \text{constant} =: E$$

reduces to

$$\begin{cases} \frac{\partial \chi}{\partial t} = \frac{\chi E}{i\hbar} = -\frac{iE}{\hbar} \chi \\ -\frac{\hbar^2}{2m} \Delta \phi + V \phi = E \phi \end{cases}$$

$$\begin{cases} \chi(t) = A e^{-\frac{iE}{\hbar}t} \text{ and} \end{cases}$$

 $\implies \begin{cases} \chi(t) = A \, \mathrm{e}^{-\frac{iE}{\hbar}t} & \text{and} \\ \\ \widehat{H} \, \phi = E \, \phi & \text{where} & \widehat{H} = -\frac{\hbar^2}{2m} \Delta + V \end{cases}$ 

### Quantization

Given boundary conditions on  $\phi(\mathbf{x})$ , the reduced Hamiltonian operator  $\widehat{H}$  only has countably many (real) eigenvalues:

$$E_1 \leq E_2 \leq \cdots \leq E_n \leq \cdots,$$

corresponding to countably many eigenfunctions:

$$\phi_1, \quad \phi_2, \quad \dots \quad \phi_n, \quad \dots$$

hence we get countably many separable solutions

$$\Psi_n(\mathbf{x},t) = A_n e^{-\frac{iE_n}{\hbar}t} \phi_n(\mathbf{x}).$$

### **Quantum states**

In general, the state of a quantum system can be written as a linear combination

$$\Psi(\mathbf{x},t) = \sum_{n} A_n e^{-i\frac{E_n}{\hbar}t} \phi_n(\mathbf{x})$$

where the  $\phi_n$  are eigenfunctions for the reduced Hamiltonian operator:

$$\widehat{H}\,\phi_n=E_n\,\phi_n.$$

These eigenstates are orthogonal with respect to the Hermitian product

$$\langle \phi | \psi \rangle = \int \phi(\mathbf{x})^* \, \psi(\mathbf{x}) \, \mathrm{d}\mathbf{x}$$

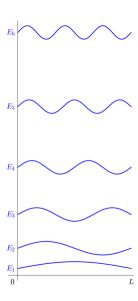
## Remember the 1-D infinite potential well

$$V(x) = \begin{cases} 0 & 0 \le x \le L \\ +\infty & \text{elsewhere} \end{cases}$$

$$\implies \phi_n(x) = \sin \frac{n\pi x}{L}$$

with energy

$$E_n = \frac{\pi^2 \hbar^2 n^2}{2mL^2}$$



Quantum systems

Dirac formalism

Quantum bit

#### **Braket notation**

The instantaneous states  $\phi(\mathbf{x}) = \Psi(\mathbf{x}, t_0)$  form a vector space  $\mathcal{V}$  spanned by the  $\phi_n$ :

$$\phi(\mathbf{x}) = \sum_{n} \alpha_n \phi_n(\mathbf{x})$$
 with  $\alpha_n \in \mathbb{C}$ .

Hermitian product: if the  $\phi_n$  are **normalized** ( $\|\phi_n\| = \sqrt{\langle \phi_n | \phi_n \rangle} = 1$ ) then for

$$\phi = \sum_{n} \alpha_{n} \phi_{n}, \qquad \psi = \sum_{n} \beta_{n} \phi_{n},$$

we have

$$\langle \phi | \psi \rangle = \sum_{n} \alpha_{n}^{*} \beta_{n} = \begin{bmatrix} \alpha_{1} & \alpha_{2} & \dots \end{bmatrix}^{*} \begin{bmatrix} \beta_{1} \\ \beta_{2} \\ \vdots \end{bmatrix} = |\phi\rangle^{\dagger} |\psi\rangle$$

#### Measurement

When we measure a mixed state

$$|\phi\rangle = \sum_{n} \alpha_{n} |\phi_{n}\rangle \in \mathcal{V} \setminus \{\mathbf{0}\}:$$

it gets projected on the **pure state**  $|\phi_n\rangle$  with energy  $E_n$  with probability

$$\mathbb{P}[\mathcal{M}|\phi\rangle = |\phi_{n}\rangle] = \frac{|\langle\phi|\phi_{n}\rangle|^{2}}{\|\phi\|^{2}} = \frac{|\alpha_{n}|^{2}}{\|\phi\|^{2}}.$$

If  $|\phi\rangle$  is normalized, this is just

$$\mathbb{P}[\mathcal{M}|\phi\rangle = |\phi_n\rangle] = |\langle\phi|\phi_n\rangle|^2 = |\alpha_n|^2.$$

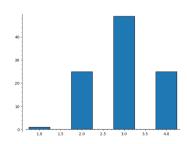
#### **Exercise**

We measure the mixed quantum state

$$|\phi\rangle = |\phi_1\rangle + (3+4i)|\phi_2\rangle + 7|\phi_3\rangle + 5i|\phi_4\rangle.$$

What do we expect to see ?

#### **Answer:**



Quantum systems

Dirac formalism

Quantum bits

## Computational quantum systems

*N*-level quantum system: when dim<sub>C</sub>  $\mathcal{V} = N$ .

Basis of pure (eigen) states  $|\phi_1\rangle$ ,  $|\phi_2\rangle$ , ...,  $|\phi_N\rangle$ .

Computational basis: to simplify notation let us write

$$|n\rangle := |\phi_{n+1}\rangle \qquad (0 \le n < N)$$

and  $V_N$  for the standard N-level state space with pure states

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

## N=2: Quantum bits (or qubits)

The state of a qubit can be thought of as a nonzero linear combination

$$|\phi\rangle = \alpha |0\rangle + \beta |1\rangle \qquad \alpha, \beta \in \mathbb{C}.$$

When we measure it:

$$\mathbb{P}\big[\,\mathcal{M}|\phi\rangle = |0\rangle\,\big] = \frac{|\alpha|^2}{|\alpha|^2 + |\beta|^2}, \qquad \mathbb{P}\big[\,\mathcal{M}|\phi\rangle = |1\rangle\,\big] = \frac{|\beta|^2}{|\alpha|^2 + |\beta|^2}.$$

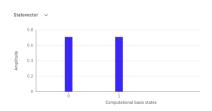
For a normalized state,  $|\alpha|^2 + |\beta|^2 = 1$  so this is just

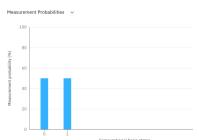
$$\mathbb{P}\big[\,\mathcal{M}|\phi\rangle = |0\rangle\,\big] = |\alpha|^2, \qquad \mathbb{P}\big[\,\mathcal{M}|\phi\rangle = |1\rangle\,\big] = |\beta|^2.$$

# **Example**

$$|\phi 
angle = |0 
angle + |1 
angle, \qquad | ilde{\phi} 
angle = rac{|0 
angle + |1 
angle}{\sqrt{2}} \ ext{normalized}$$

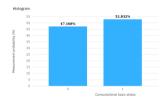
$$\mathbb{P}ig[\,\mathcal{M}|\phi
angle = |0
angle\,ig] = \mathbb{P}ig[\,\mathcal{M}|\phi
angle = |1
angle\,ig] = rac{1}{2}$$



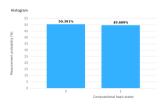


# IBM Q Experience results

Result of 1024 simulations:



Result of 1024 executions on ibmq\_armonk (a real physical qubit):



#### For next time

Start messing around with qubits yourself by creating an account on

https://quantum-computing.ibm.com/

Suggestion:

yields 
$$|\phi
angle = rac{|0
angle + |1
angle}{\sqrt{2}}$$