


QUANTUM COMPUTING


what why how



About Me

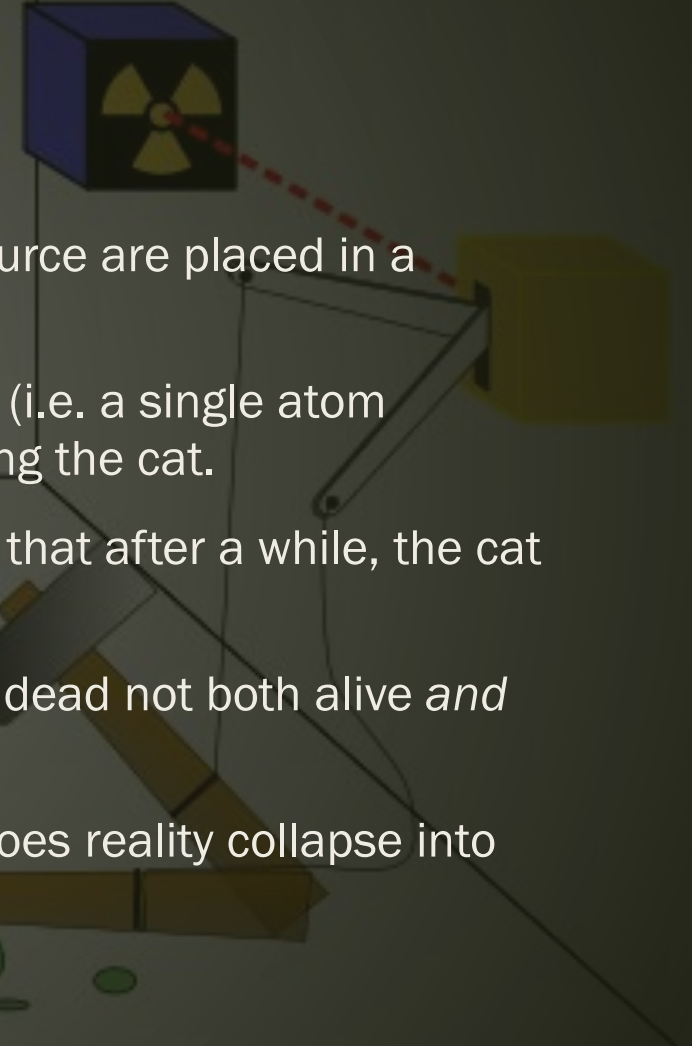
- Software Engineer
- Commercial Software Engineering @ Microsoft
- Quantum Enthusiast

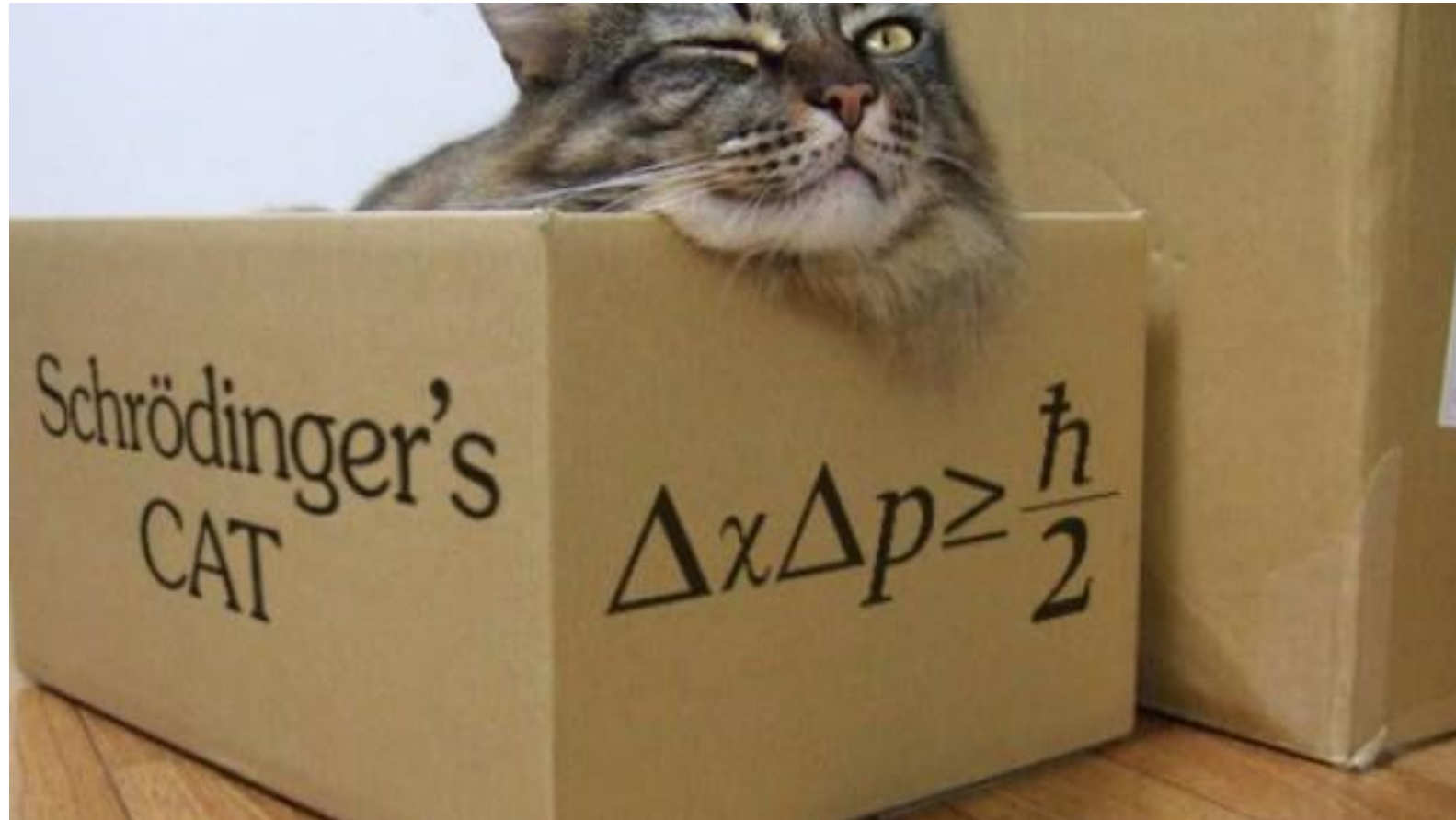
@xtellurian 

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Schrödinger's Cat: Dead or Alive?

1. Schrödinger's cat: a cat, a flask of poison, and a radioactive source are placed in a sealed box.
2. If an internal monitor (e.g. Geiger counter) detects radioactivity (i.e. a single atom decaying), the flask is shattered, releasing the poison, and killing the cat.
3. The Copenhagen interpretation of quantum mechanics implies that after a while, the cat is *simultaneously alive and dead*. [**Superposition**]
4. Yet, when one looks in the box, one sees the cat *either alive or dead* not both alive *and* dead. [**Measurement**]
5. So when exactly does quantum superposition end, and when does reality collapse into one possibility or the other?





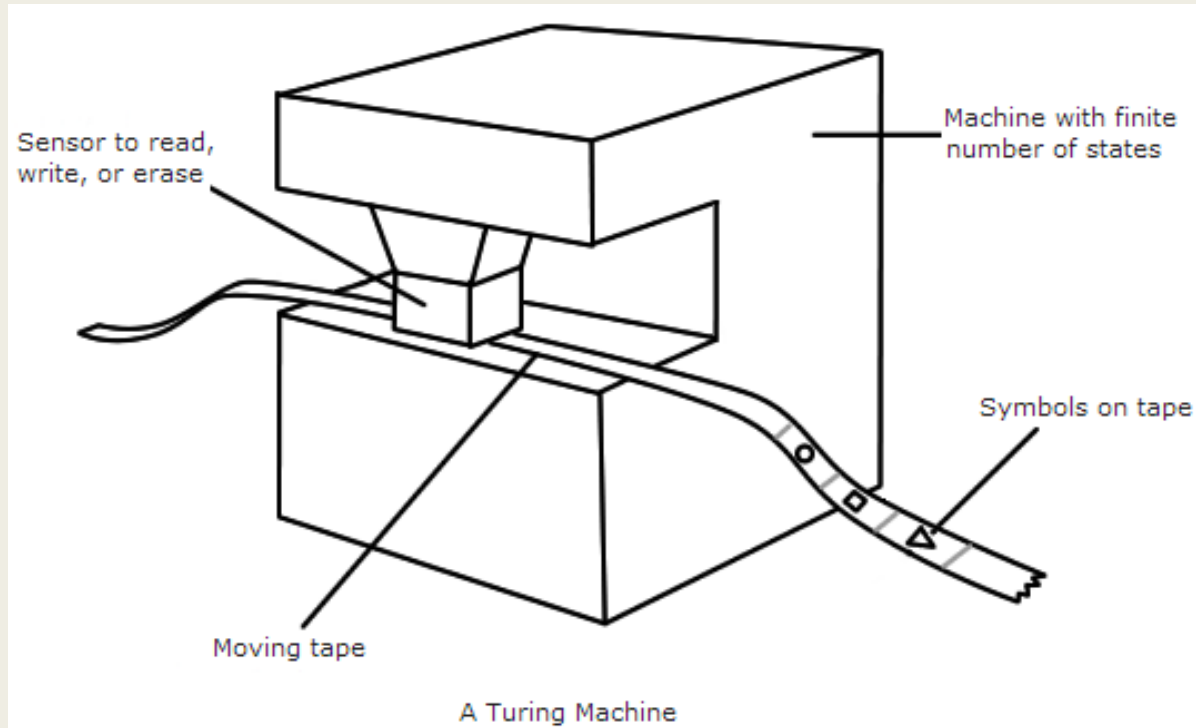


WHAT?



What is classical computing?

- Information is stored in **bits**, which take the discrete values 0 and 1.
 - *Bits are composed into larger numbers. 1001 => 9*
 - *Allowed values are discrete, rational numbers.*
- Calculations are done essentially the same way as “by hand”
 - *Everything is addition*
- Physically implemented by **transistors** and **logic gates**
 - *There are billions of transistors in your phone.*
 - *von Neumann architecture implements the Turing machine*



TURING MACHINE

Computational Complexity (Classical)

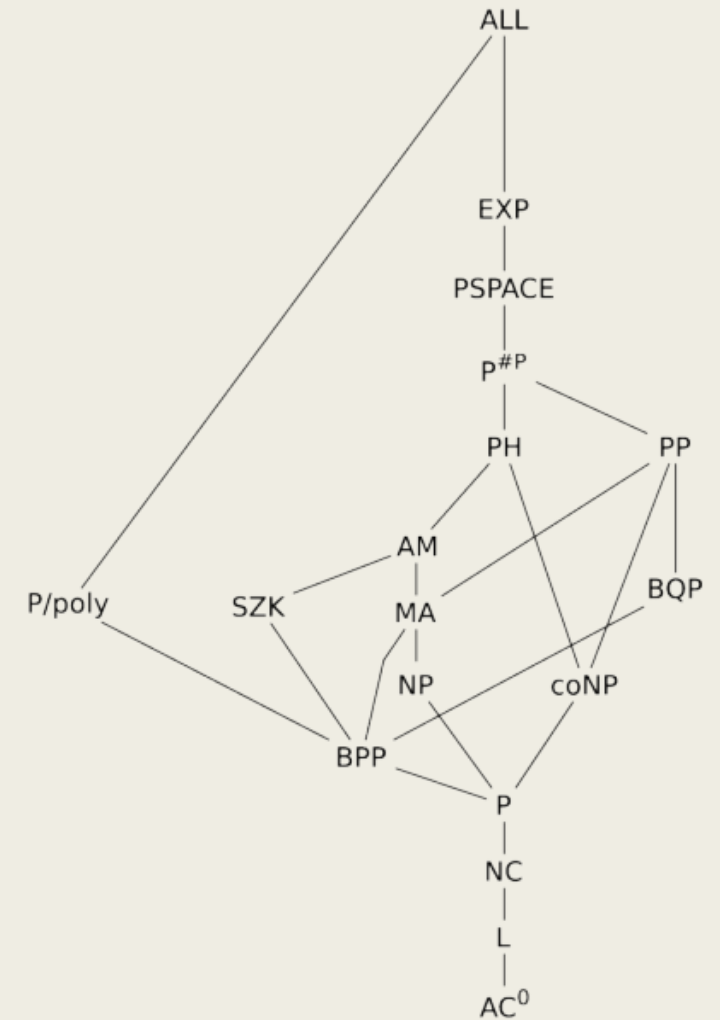
what can my computer do, and when will it be finished?

- Given some well defined problem, how hard is it to solve?
 - *Expressed as a function $n \rightarrow f(n)$, where n is the size of the input.*
 - *How much space (i.e. memory) is required?*
 - *How much time is required?*
- Classical computers (i.e. Turing machines) can solve problems in the complexity class **BPP** (**b**ounded-error **p**robabilistic **p**olynomial time)

Complexity Classes

Complexity classes are related to each other, and some classes are entirely contained within others.

- **P**: The class of problems which we can solve efficiently using a conventional algorithm -> class of all problems solvable by a deterministic Turing machine bounded in time by a polynomial function of the input length.
- **NP**: the set of problems such that someone can convince you of a yes answer in a reasonable amount of time.
- **BPP**: The class of problems that are solvable efficiently by randomized algorithms.
- **BQP**: The class of all problems that admit an efficient solution by quantum computers.



What is Quantum Computing?

The really short version

- A quantum computer **exploits fundamental laws** of the cosmos to do computational tasks
 - *Simulating quantum mechanics is hard*, so let's use quantum mechanics to perform hard* computation.*
- Physical implementations
 - *Superconducting electron qubits or topological qubits*
 - *Quantum gates and circuits*
- Information is stored as quantum bits, a.k.a. **qubits**

Quantum States

- Vector of norm 1 in n-dimensional Hilbert space
 - *Hilbert space: generalizes the notion of Euclidean space.*
 - *Complex numbers*
 - Vector *amplitudes encode probability* of measurement outcomes
- Quantum operators interact with quantum states
 - *E.g. a measurement, transformation, or time evolution*
 - *Represented as matrices in Hilbert space*
- Dirac notation
 - *a,b are complex amplitudes*
 - *and u,d are complex vectors*

$$|\psi\rangle = a|u\rangle + b|d\rangle.$$

Qubits

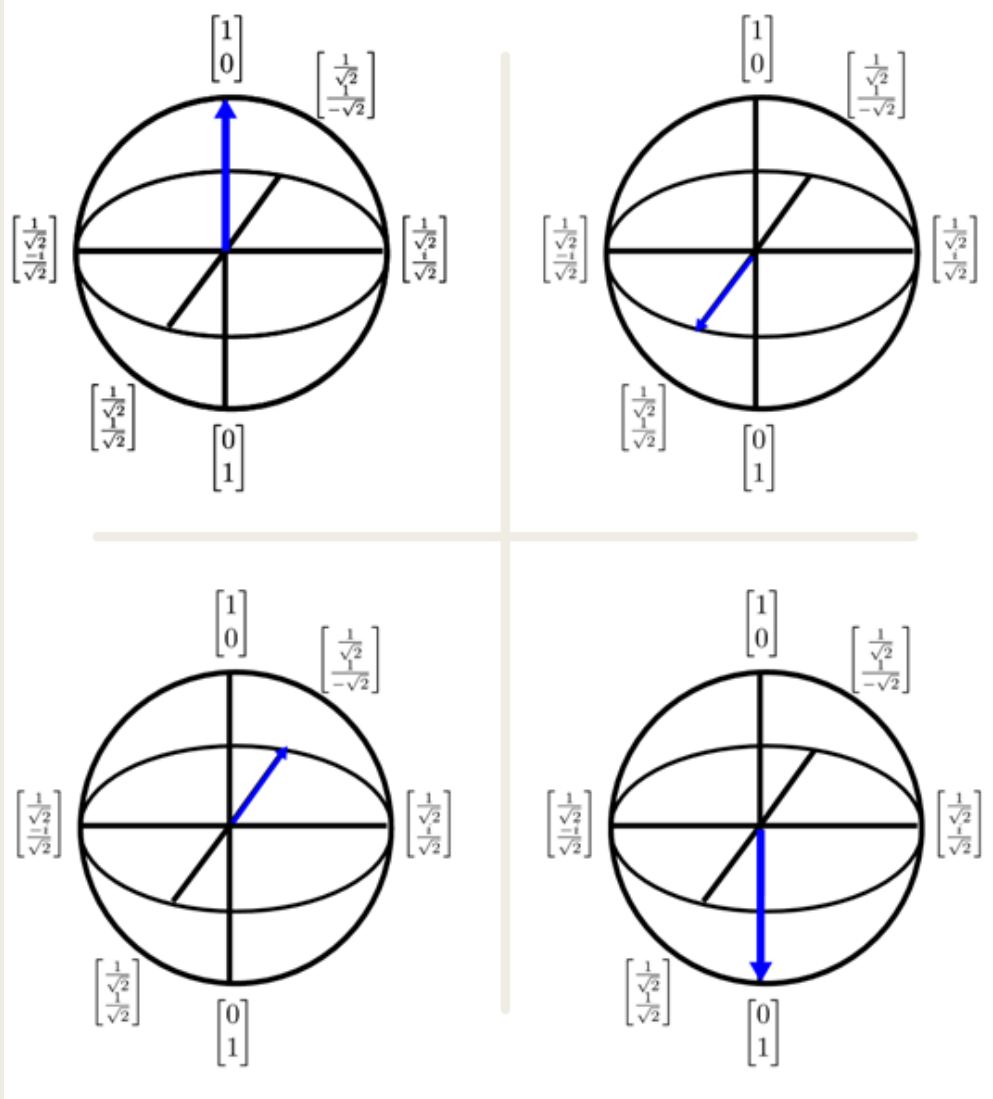
- Qubits are the simplest quantum state
- The standard basis is called the **computational basis**

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

- Note that the numbers inside the *kets* $|\cdot\rangle$ are just labels. Any state of this system is thus represented as a superposition of these two basis states:

$$|\Psi\rangle = a |0\rangle + b |1\rangle$$

Qubit Intuition



Bloch Sphere

- Definitely a **One**

$$|x\rangle = 0|0\rangle - 1|1\rangle$$

- Definitely a **Zero**

$$|y\rangle = 1|0\rangle + 0|1\rangle$$

- A half-dead cat

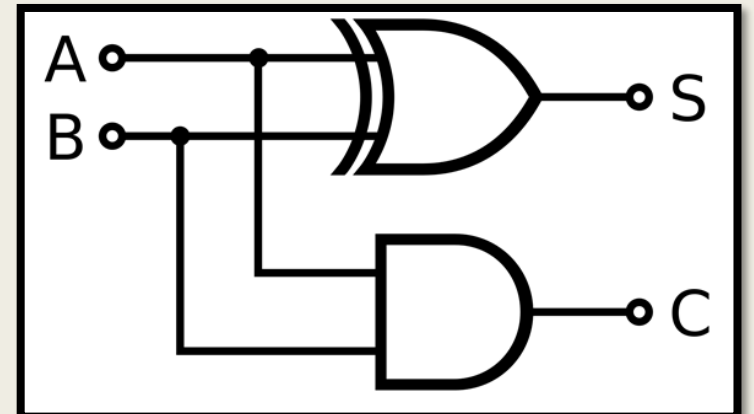
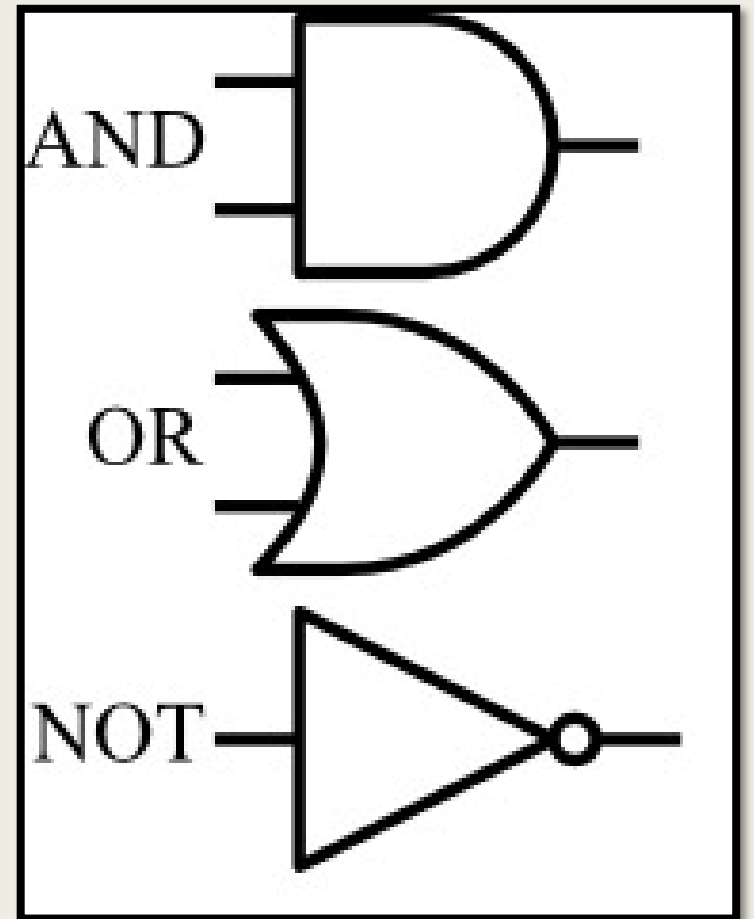
$$|snuggles\rangle = \frac{1}{\sqrt{2}}|dead\rangle - \frac{1}{\sqrt{2}}|alive\rangle$$




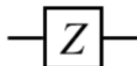
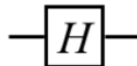
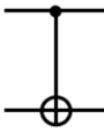
Logic Circuits

the classical version

- Logic gates take bits as input, and produce a bit as output
- Implemented in silicon via transistors
 - All gates can be implanted by a *universal logic gate* i.e. the NAND and NOR gates.
- Gates are *composed* to form logical circuits (e.g. the half-adder)



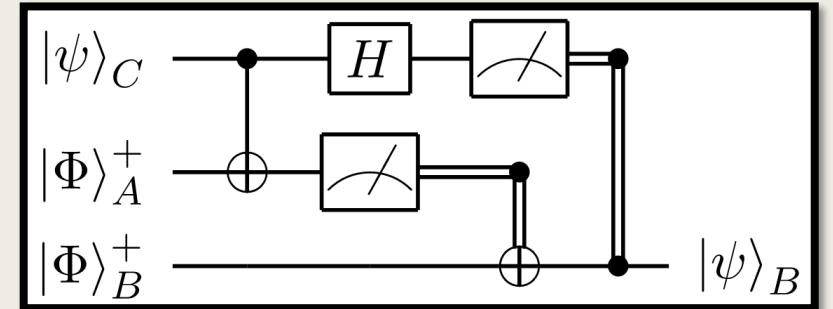
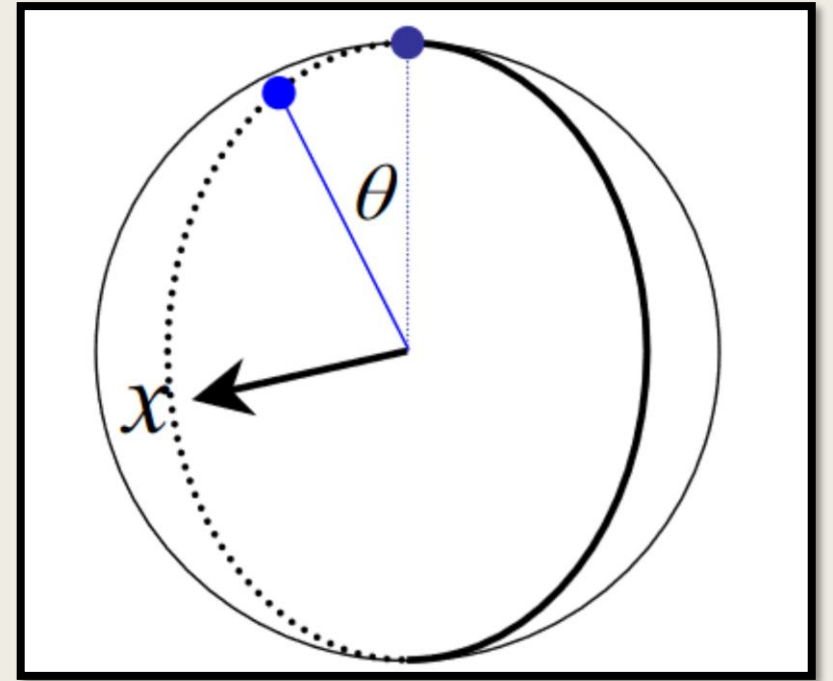
QUANTUM GATES

Gate	Notation	Matrix
NOT (Pauli- X)		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Z		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard		$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
CNOT (Controlled NOT)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

Logic Circuits

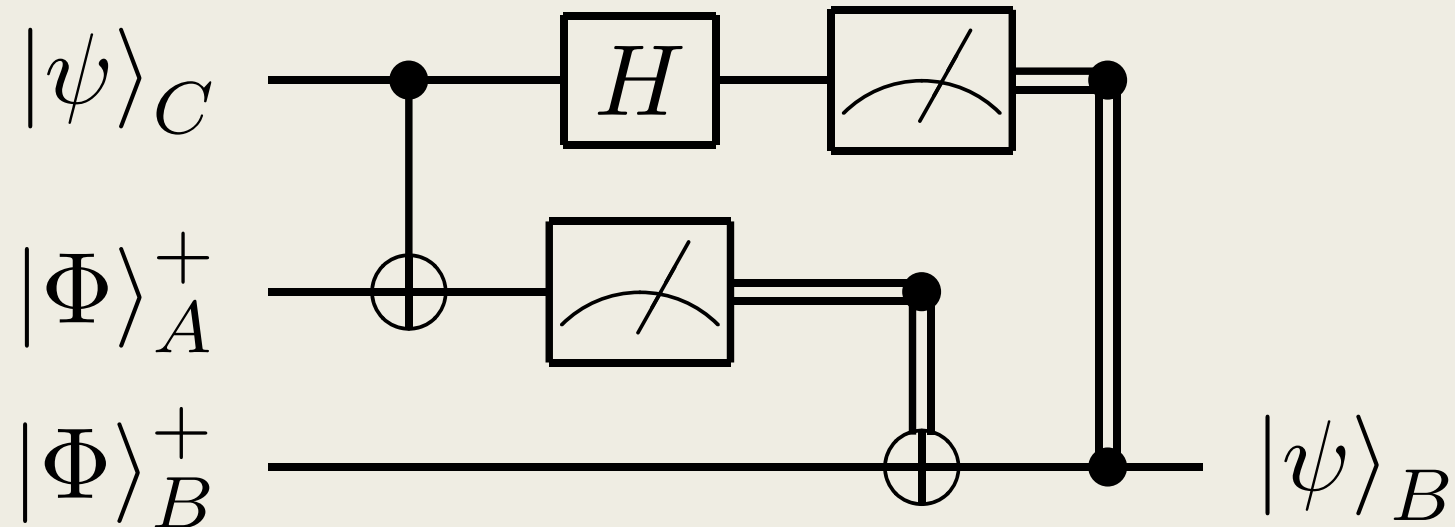
the quantum version

- Example: The X-Gate
 - $X = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$
 - Names: Pauli X, X, NOT, bit flip, σ_x
 - Perform equivalent of NOT gate in traditional computing
- All quantum gates are *rotations* around an axis on the Bloch sphere.
- Quantum gates are composed into quantum circuits



Entanglement

- Two qubits with correlated measurement outcomes
- We can create entangled qubits!
- Used for **control** and **execution** of quantum **operations**



What is Quantum Computing?

Again

- Implements quantum circuits
 - From *universal quantum gates* we can approximate any quantum gate.
- Model any quantum system
 - *with less effort than the equivalent simulation on a classical computer.*
- Quantum circuits implement quantum algorithms
 - *Some class of problems (BQP) are much easier to solve.*
- Solves *hard* problems*

What Quantum Computing is NOT

- NOT a really fast computer
- NOT a massively parallel computer
- NOT, for most problems, better than classical computers
- NOT cheap
- NOT magic



WHY?



Challenges and Opportunities



NITROGEN
FIXATION



CARBON
SEQUESTRATION



ANTIBIOTIC
RESISTANCE



CRYPTOGRAPHY

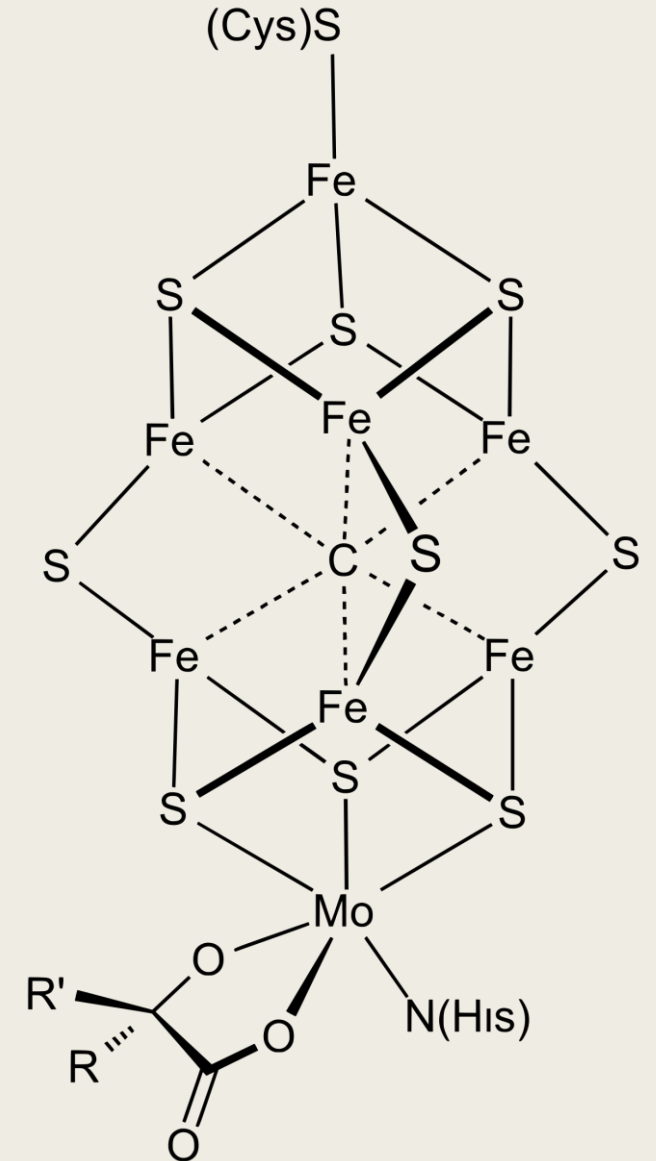


ARTIFICIAL
INTELLIGENCE

Nitrogen Fixation

or how to feed the world

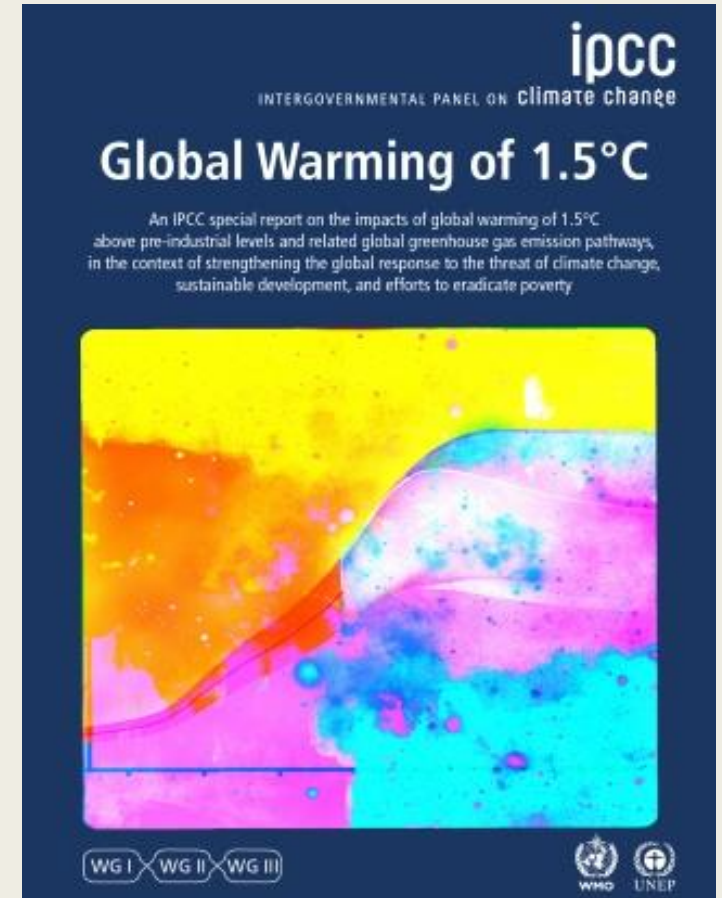
- Crops consume nitrogen as fertiliser
- The Haber-Bosch process
 - *Converts atmospheric nitrogen (N_2) to ammonia (NH_3)*
 - *Uses 1-2% of global annual energy supply*
- FeMoco
 - *Catalyses the conversion of atmospheric N_2 into ammonia (NH_3) a.k.a. nitrogen fixation.*
 - *200 qubits can simulate FeMoco*



Carbon sequestration

combat climate change

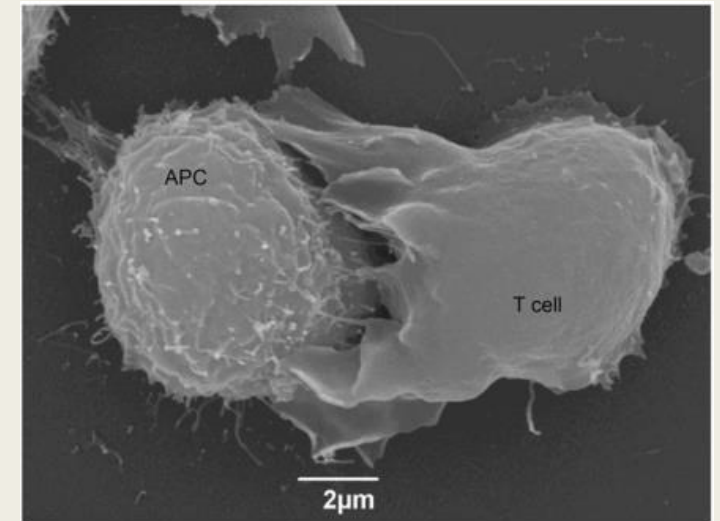
- Current State of the Art in carbon sequestration is ineffective and inefficient
- Can we find a low energy catalyst for carbon sequestration?
 - *Capture atmospheric or oceanic carbon*



Antibiotic Resistance

molecular modelling

- Antigens are important molecules for fighting disease
 - *Usually proteins, peptides (amino acid chains) and polysaccharides*
 - *Vaccines are examples of antigens*
 - *Antigens bind to foreign/ infected cells*
 - *T cells selectively recognize the antigens, based on HLA proteins*
- Can we model antigen/ pathogen interaction?
 - *Potentially thousands of atoms*
 - *We can do it (with enough qubits)*



Quantum Cryptography

Perfectly Private Communication

- Quantum Key Exchange
 - *enables two parties to produce a shared random secret key known only to them.*
- Alice and Bob can detect the presence of any third party attempting to intercept comms
- Exploits quantum *entanglement*
 - “spooky action at a distance” – Einstein
 - Two quantum states that, when measured, will have correlated outcomes **regardless of distance.**



Artificial Intelligence

optimising machine learning

Quantum software to enable machine learning that is faster than that of classical computers.

- Grover's Search
- Linear algebra simulation with quantum amplitudes
- Enhanced reinforcement learning
- Fast sampling from generic probabilistic models



Quantum Supremacy

- Quantum supremacy means:
 - Solving a *really hard* problem* on a **quantum** computer
 - Not solving that same problem on a **classical** computer
 - Some confidence that the problem is **classically not solvable**.



HOW?



Quantum Hardware

- Superconducting Qubits (Rigetti, Google, IBM)
- Topological Qubits (Microsoft)
- Advantages of a topological qubit
 - *Longer decoherence time*
 - *Robust to noise = scale with fewer resources*
 - *Information is stored non-locally, meaning fewer errors*
 - *Less overhead on long (i.e. useful) computations*
- Quantum Compute Stack
 - *Quantum Processor*
 - *Cryogenic Control Machine*
 - *Application Computer*



Quantum Software



Cirq - Python library for writing, manipulating, and optimizing quantum circuits



Qiskit - for developing quantum computing applications and working with NISQ (Noisy-Intermediate Scale Quantum) computers such as IBM Q.



pyQuil - library for easily generating Quil programs to be executed using the Rigetti Forest platform.

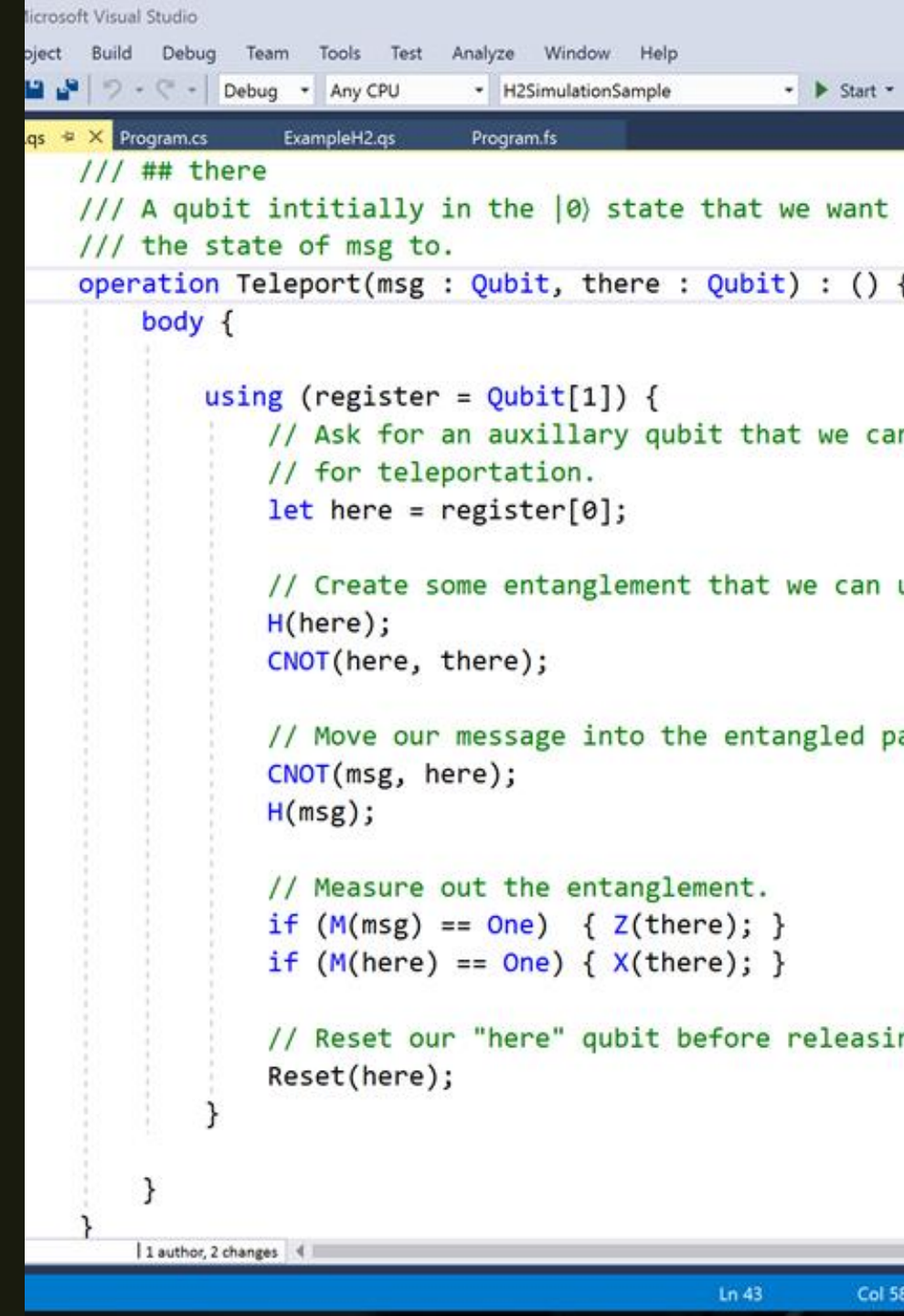


QDK – Quantum Development Kit including Q# language, simulators and libraries

Q#

Quantum-focused Programming Language

- Built ground-up for Quantum
- Native type system
- Windows, MacOS and Linux
- Fully integrated into Visual Studio and VS Code
- Python interoperability



The screenshot shows the Microsoft Visual Studio IDE with a Q# script open. The script defines a teleportation operation. The code is as follows:

```
/// ## there
/// A qubit initially in the  $|0\rangle$  state that we want
/// the state of msg to.
operation Teleport(msg : Qubit, there : Qubit) : () {
    body {
        using (register = Qubit[1]) {
            // Ask for an auxillary qubit that we can
            // for teleportation.
            let here = register[0];

            // Create some entanglement that we can u
            H(here);
            CNOT(here, there);

            // Move our message into the entangled pa
            CNOT(msg, here);
            H(msg);

            // Measure out the entanglement.
            if (M(msg) == One) { Z(there); }
            if (M(here) == One) { X(there); }

            // Reset our "here" qubit before releasin
            Reset(here);
        }
    }
}
```

The status bar at the bottom indicates "1 author, 2 changes" and the current position is "Ln 43 Col 58".

Quantum Simulator

Run locally or in the cloud



Local simulator

Simulate a 30 qubit computer

Visual Studio and VS Code integration

Full debugging support



Azure simulator

Available for up to 40 qubits – with 16TB of memory!

QDK

Libraries and Samples



New Features

New chemical simulation library

Q# language improvements

Improved developer experience



Samples

Database search and integer factorisation

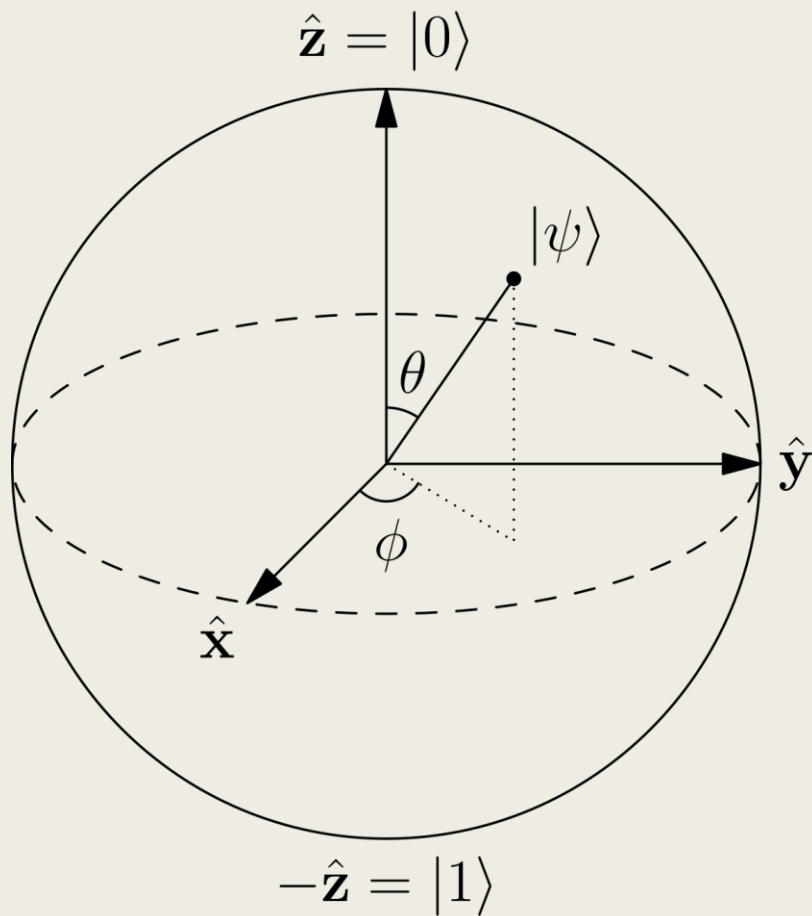
H2 molecular simulation

Ferromagnetic simulation

Interop with Qiskit and OpenQasm

Quantum as a Service

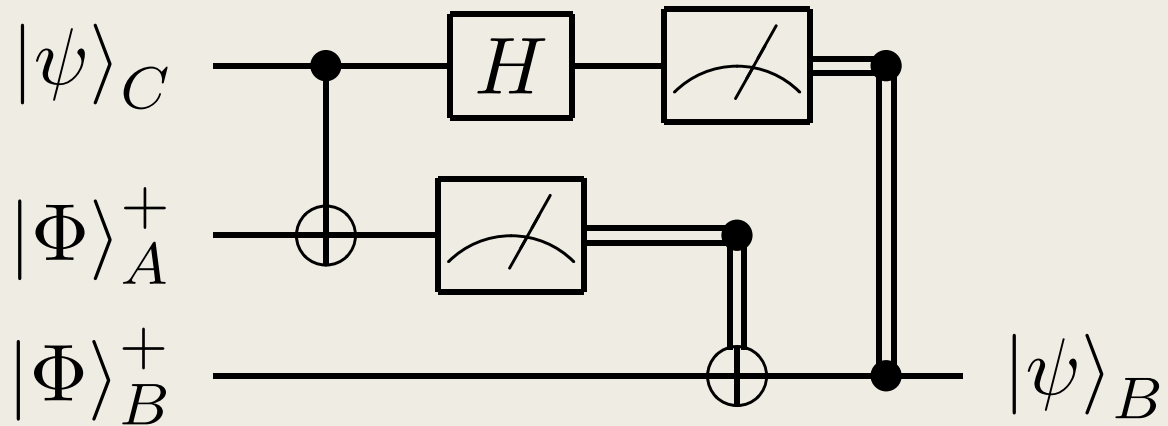
- Quantum computing will be provided as an auxiliary service, similar to:
 - *FPGA's (Project Brainwave)*
 - *Graphics Cards*
 - *Cognitive Services*
- It's a 'back-end' service
 - *You won't have a quantum computer in your pocket!*



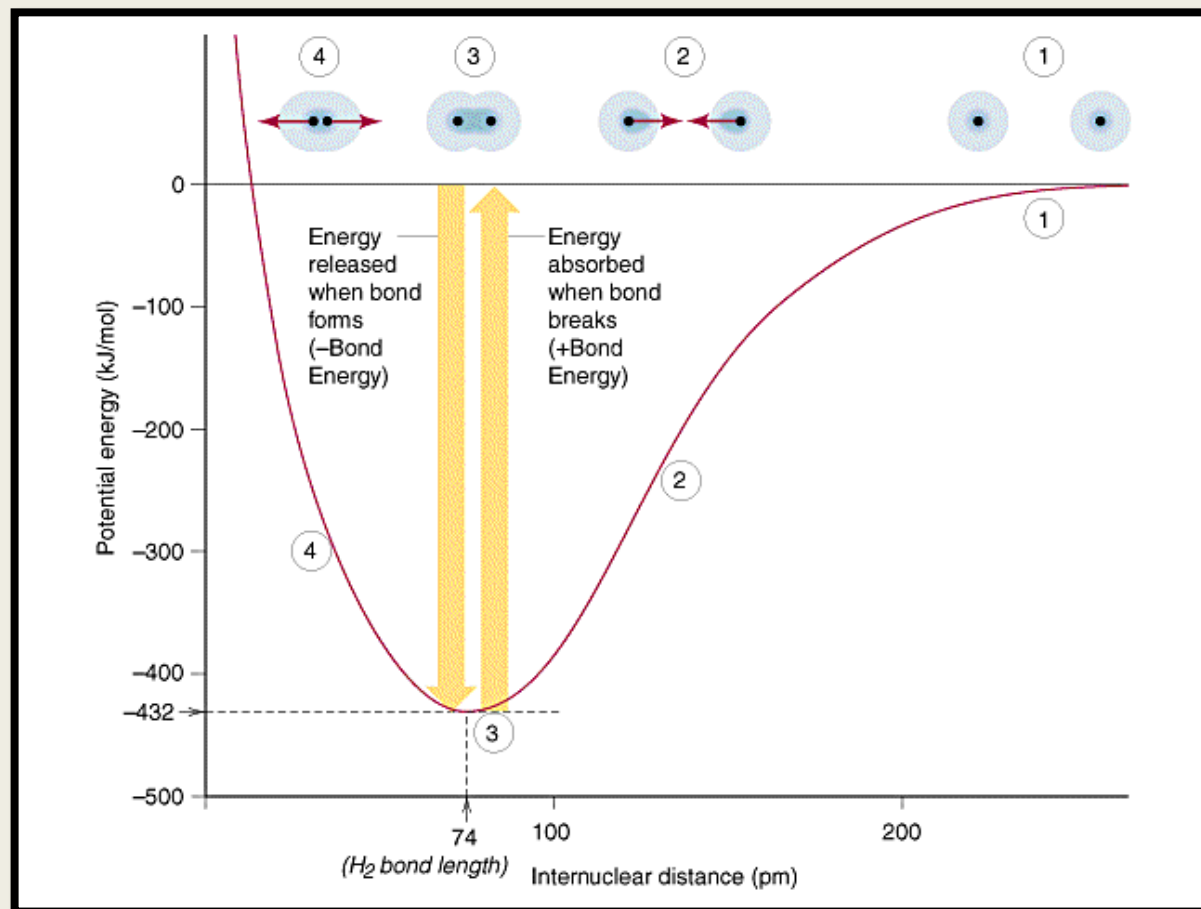
DEMO

MEASUREMENT

Hadamard transformation: 180 degree rotation around the diagonal $X+Z$ axis of the Bloch sphere.



DEMO
TELEPORTATION



DEMO

H₂ BOND ENERGY



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