Quantum computing and QML

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Meaning of classical

Classical can mean:

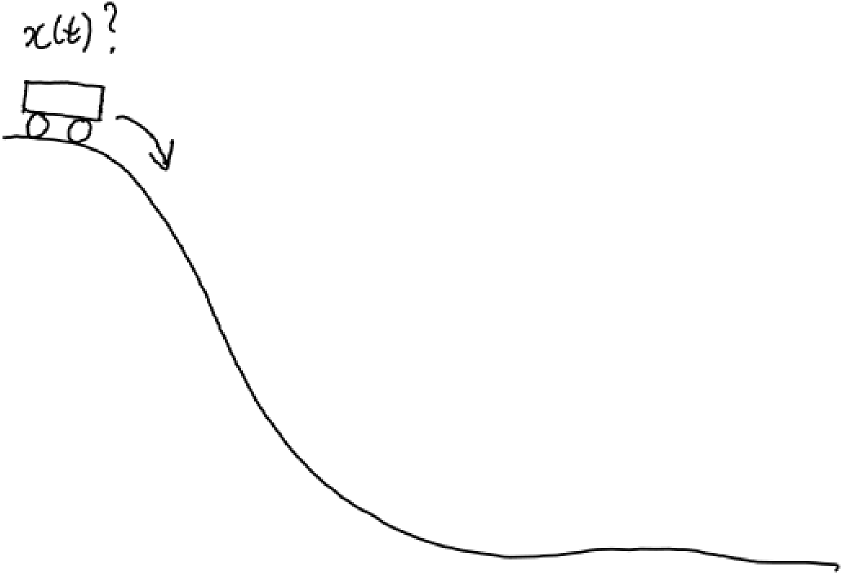
- Non-relativistic
- Non-quantum mechanical
- Newtonian mechanics

Usually a contrasting term

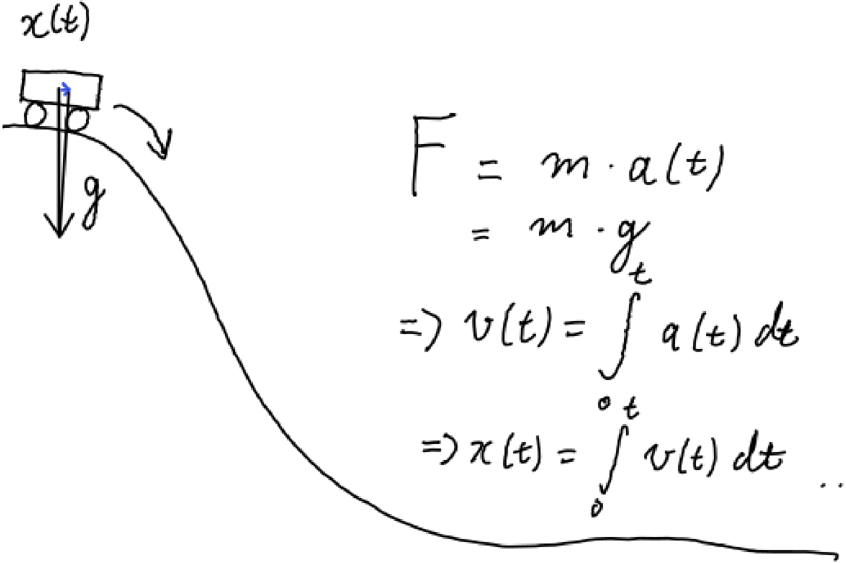
Quantum weirdness

- Quantized properties
- Superposition
- Entanglement

Classical systems



Classical systems



$$F = m \cdot a(t)$$
$$= m \cdot g_t$$
$$\Rightarrow v(t) = \int_0^t a(t)\, dt$$
$$\Rightarrow x(t) = \int_0^t v(t)\, dt \quad \ldots$$

Continuous properties

Cart has continuous properties:

- Velocity
- Position
- Acceleration

Continuous properties

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- Velocity
- Position
- Acceleration
- Mass?

Quantum systems

For small particles, different equation that determines behaviour:

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$$

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- ψ: Wave function

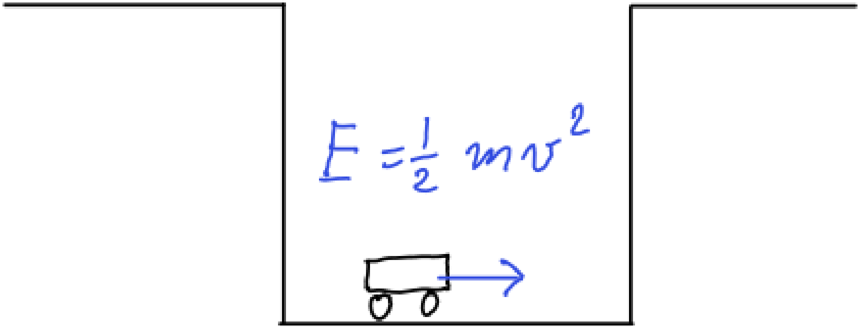
Quantum systems

For small particles, different equation that determines behaviour:

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$$

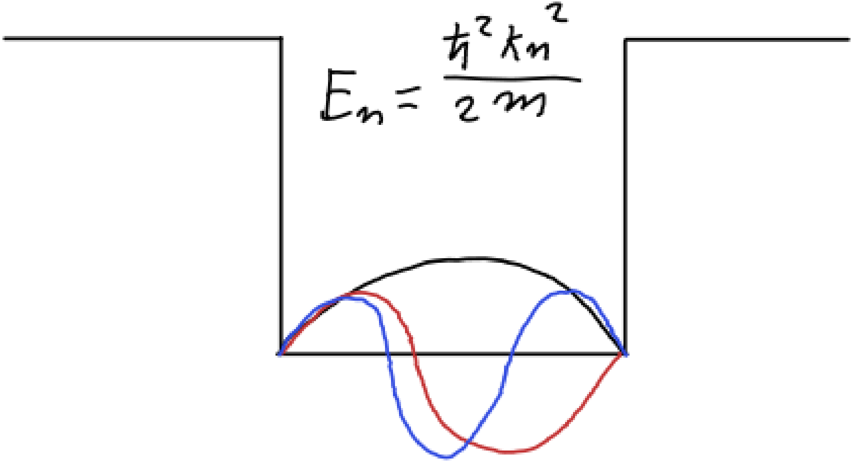
- $i = \sqrt{-1}$
- $\hbar$: constant
- ψ: Wave function
- $\hat{H}$: Hamiltonian, or **energy** operator

Classical: continuous energy

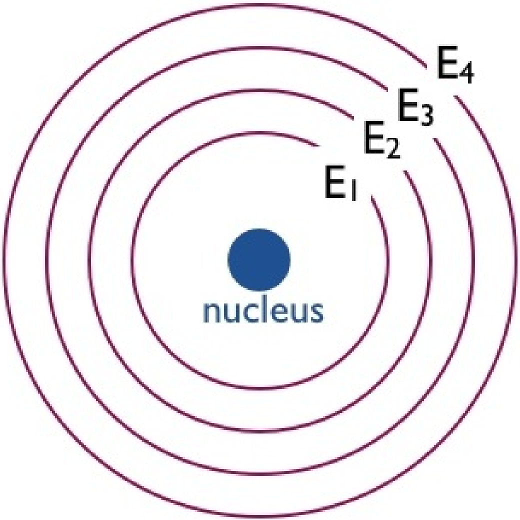


$$E = \frac{1}{2} m v^2$$

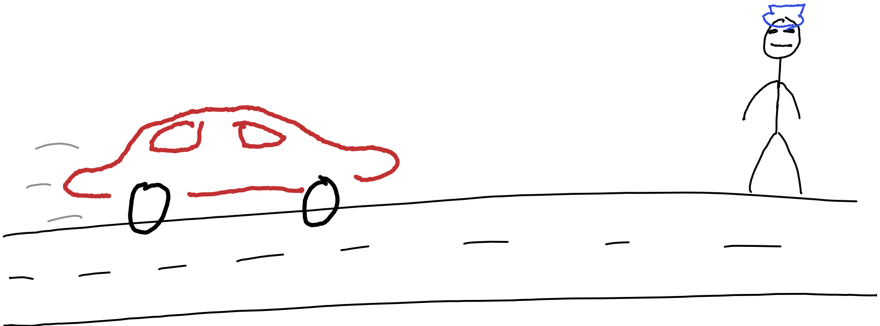
Quantum: Discrete energies



Quantum: Orbitals



Observation in physics



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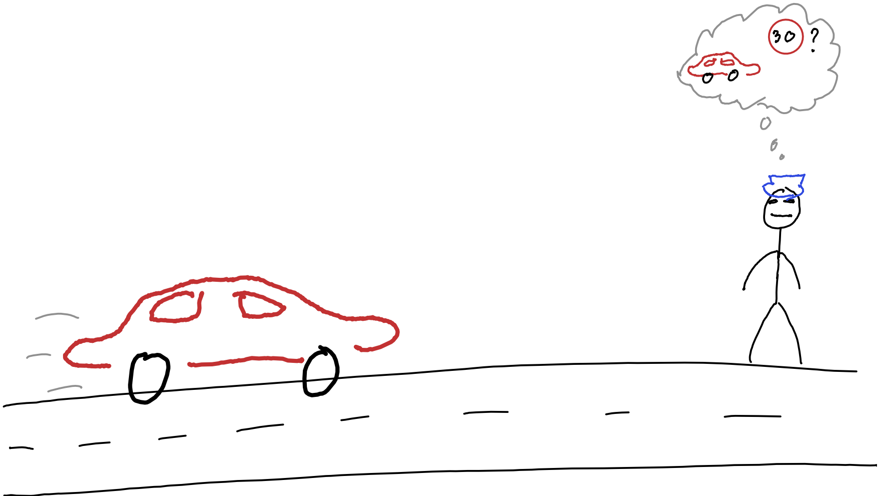

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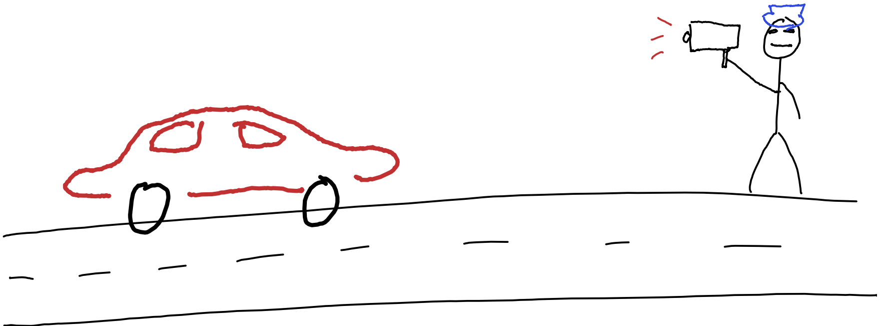

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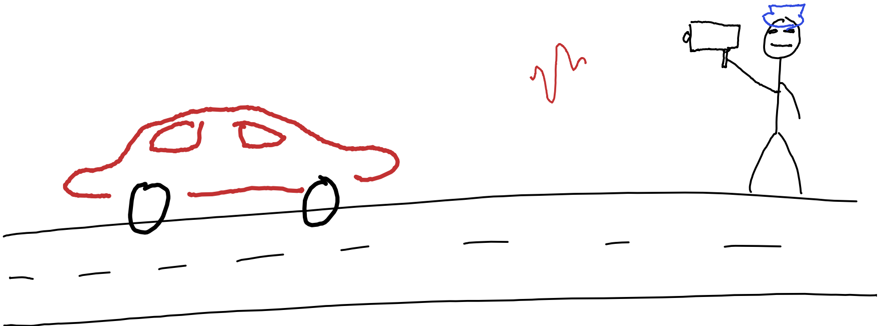

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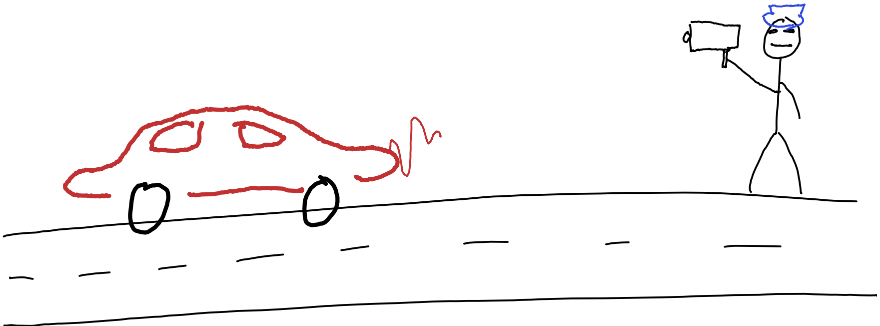

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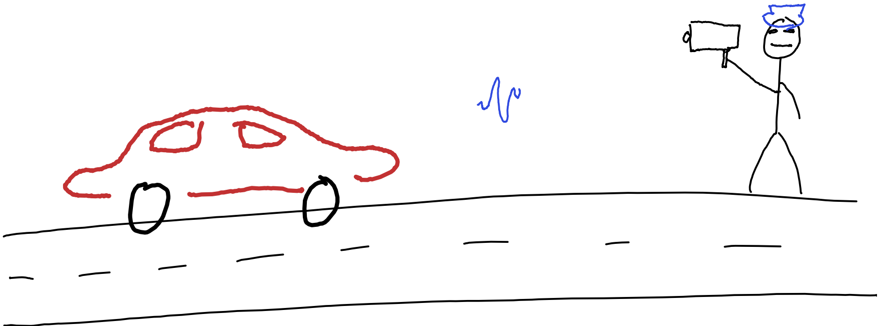

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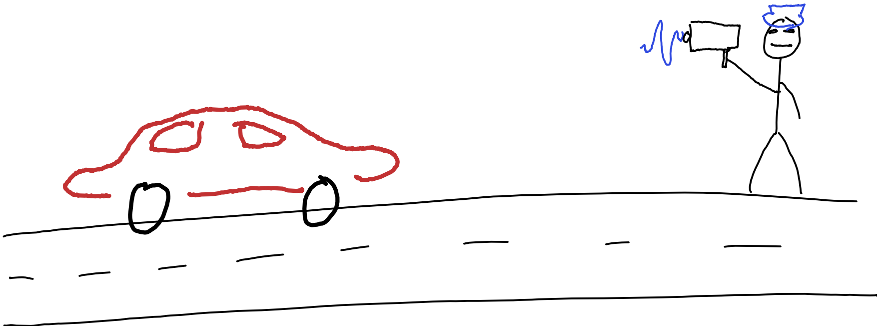

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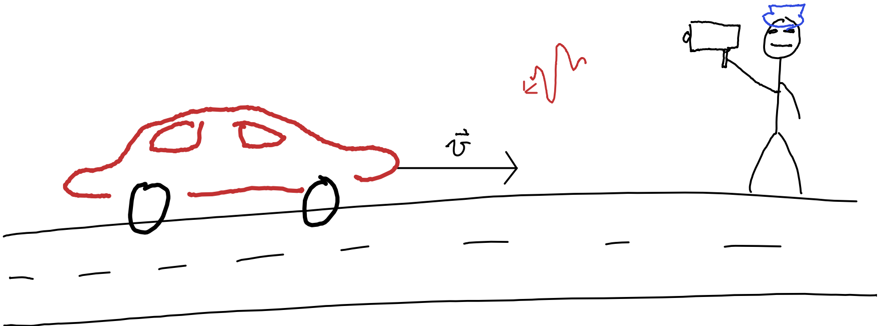

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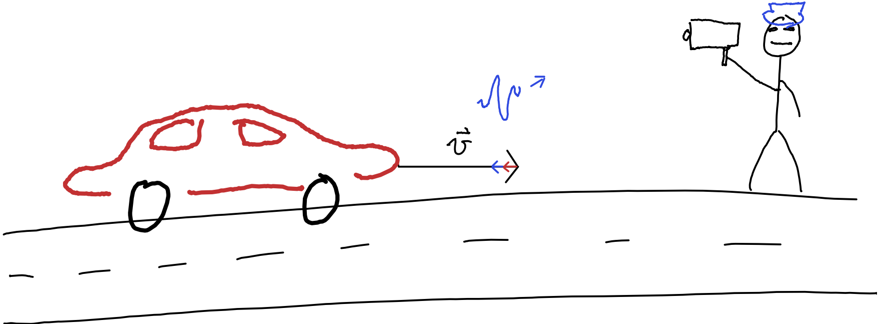

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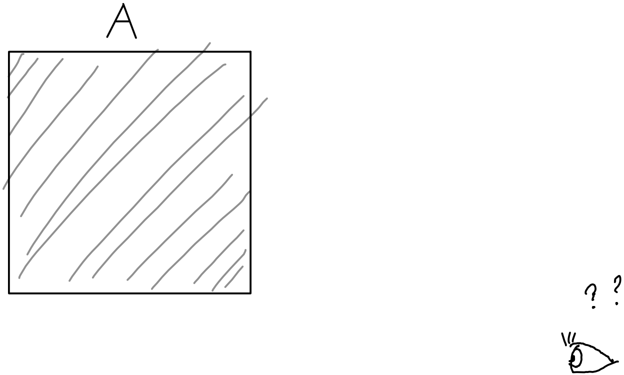

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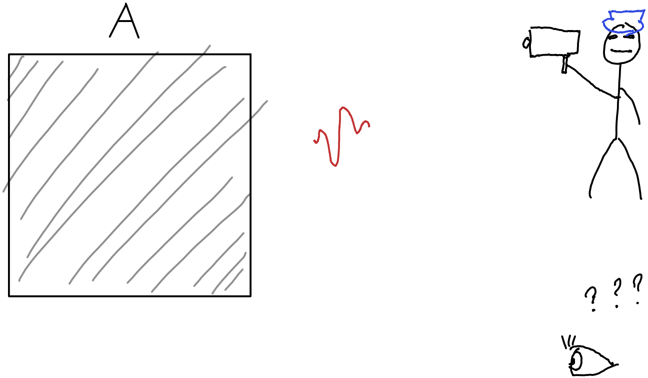

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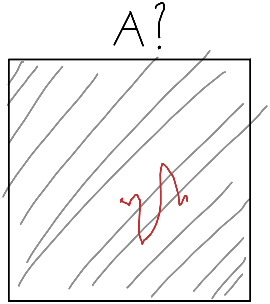

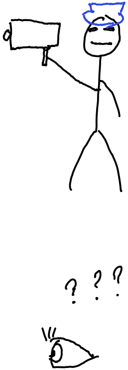

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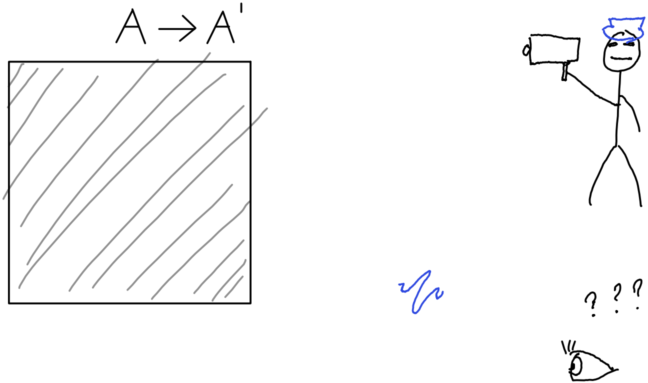

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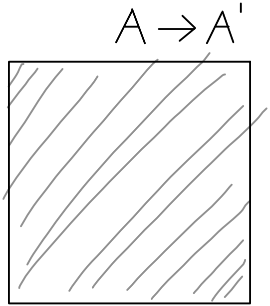

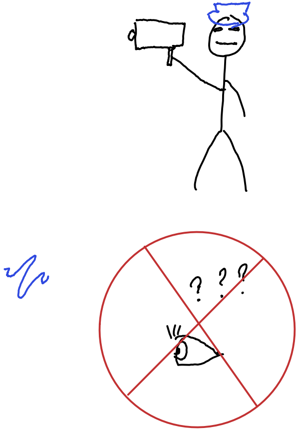

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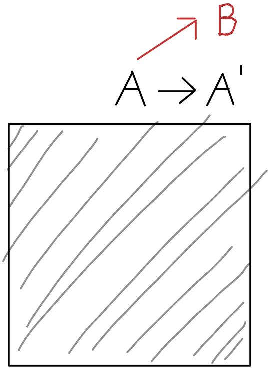
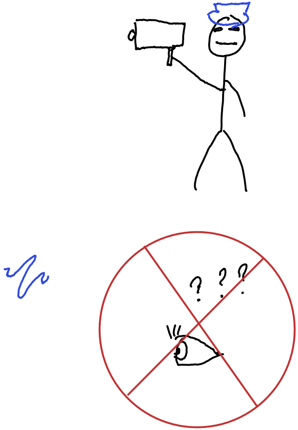


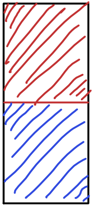


Classical measurements

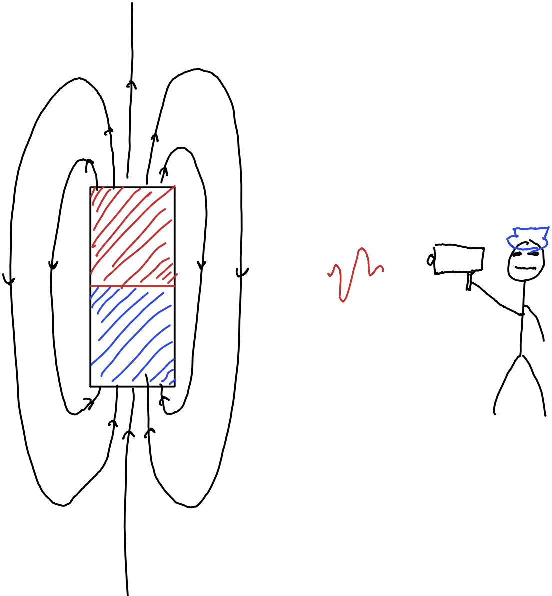
Car has well-defined:

- Velocity
- Position
- Energy
- Magnetization
- etc...

Classical magnet



Classical magnet



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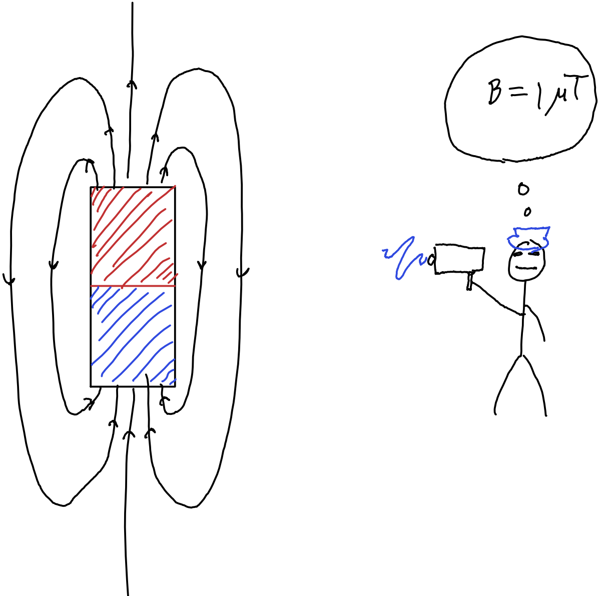
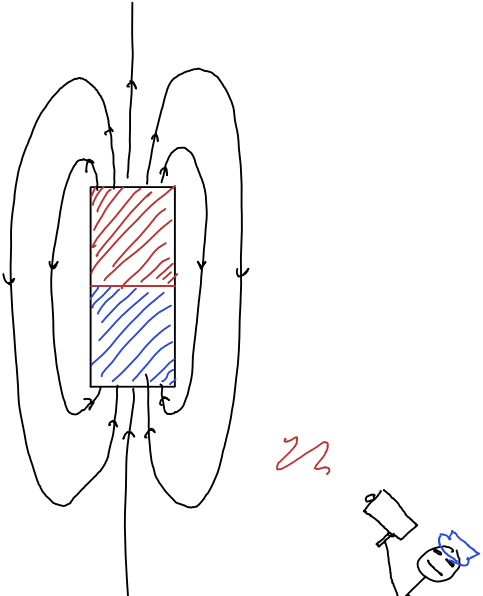
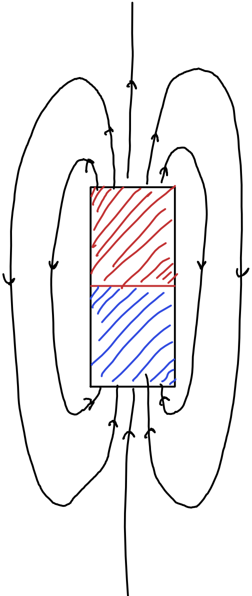


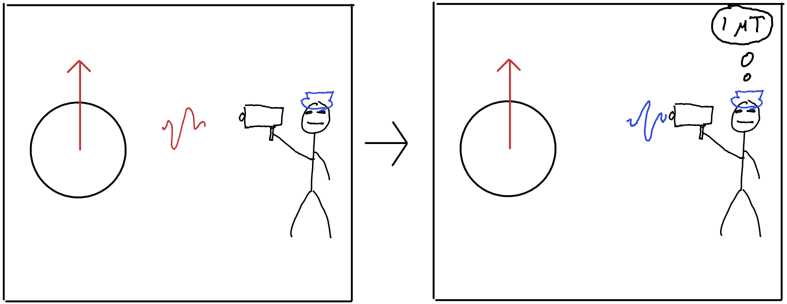
Classical magnet



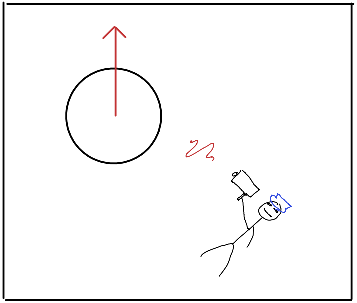
Classical magnet



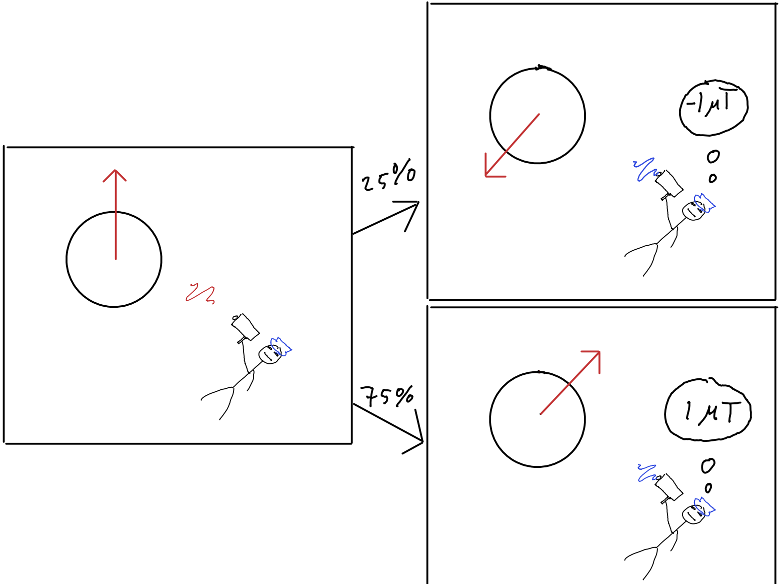
Quantum magnet



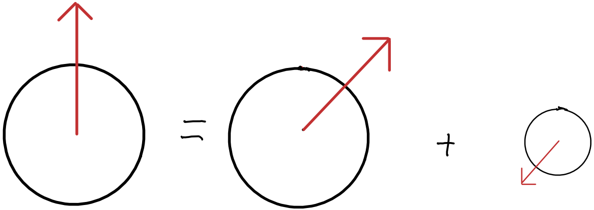
Quantum magnet



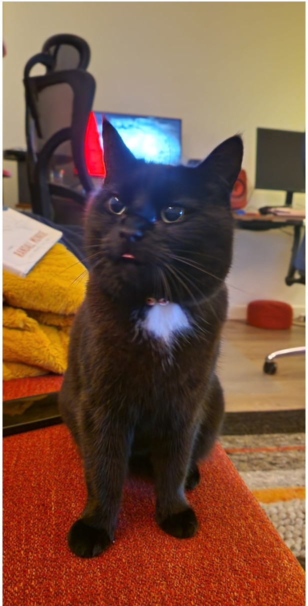
Quantum magnet



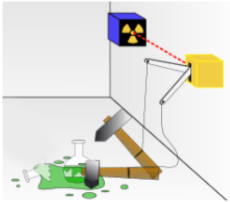
Quantum magnet



Schödinger's cat

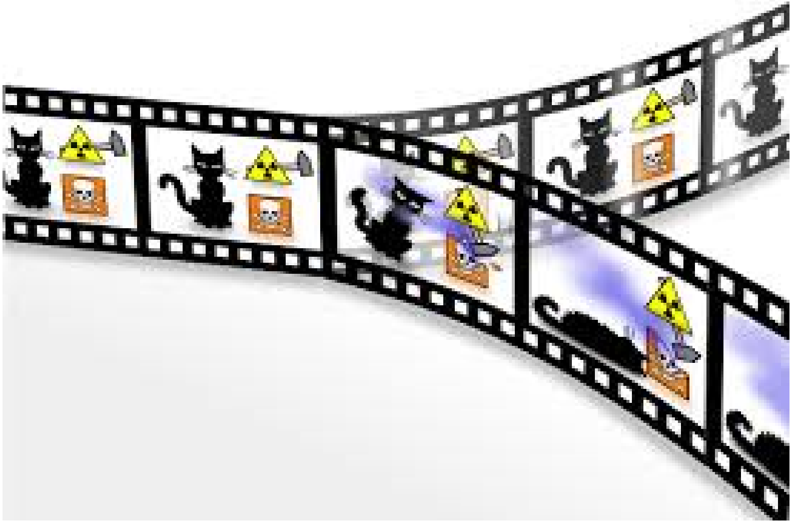


$\Leftarrow$



$\Rightarrow$

Interpretation

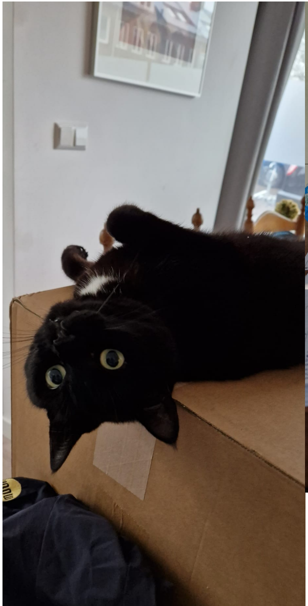


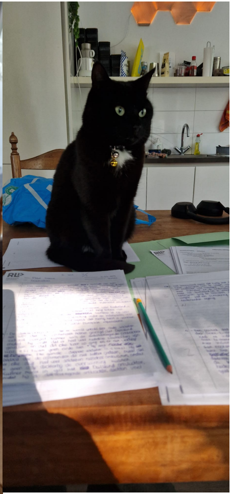
Quantum measurements - Heisenberg's uncertainty principle

- Superposition: properties are not always well-defined
- Sometimes QM particles can be 'in between'
- ome properties are not well-defined at the same time

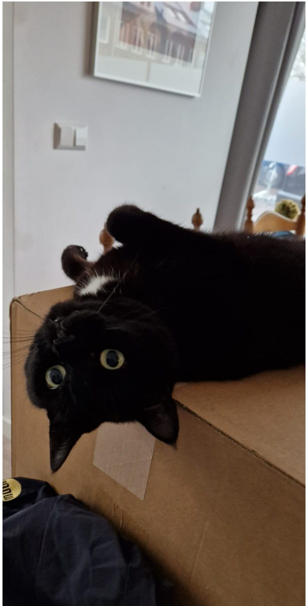
$$\Delta\hat{x}\Delta\hat{p} \geq \frac{\hbar}{2}$$

Measuring is influencing





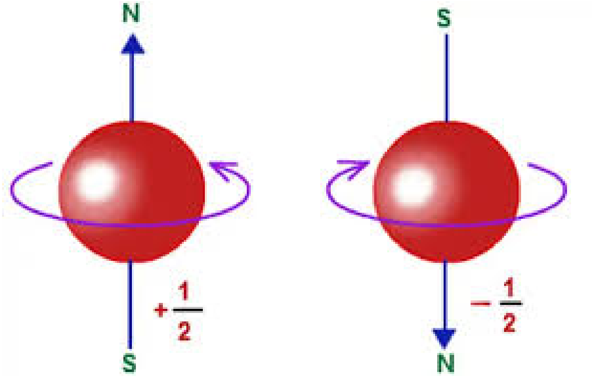
$\Rightarrow$



Classical bits

```
11110100 11011001 01000101 01001110 11010100 10111100 00010110 01011110
10000110 00110100 11110001 10111111 11000001 00100101 01101110 00010111
00000101 01111110 11011100 00100001 00101000 10111000 00011101 10000011
11000101 10111111 11110001 00010000 01101010 10000101 11011110 10001000
11011001 11010011 01110011 10011111 10110101 00111100 01101111 00001000
01010010 10100011 00000000 01100111 01110100 00100110 11110011 11011000
10101010 01111111 10100100 01110100 01101110 01110001 01010010 11011111
01111010 01101111 01100101 01111110 01011110 01010101 10010010 10101111
00010011 10000101 10101001 00100111 10000101 11110010 10101111 11001101
10011101 11011111 10011011 00010001 11001100 11100011 10100100 10111001
00010111 01111100 01010010 11011010 11011011 11001001 10010001 11111000
10100001 00101011 00001111 11111110 01001010 11011001 01100011 11101000
01100111 10100011 00110001 00000101 00101111 11100011 00011000 11110010
01101111 00100010 01010110 10111011 00110010 11101010 10110001 10001010
10011110 00000010 11111010 00011000 00111101 00100101 01001111 10100001
```

Spin



Spin

- Spin is quantized: discrete values
- Whole or half integer
- Spin-n particle: $\{-n, -n+1, -n+2, ... n-1, n\}$
- For $n = \frac{1}{2}$: $\left\{-\frac{1}{2}, \frac{1}{2}\right\}$

example: electron

Dirac notation

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

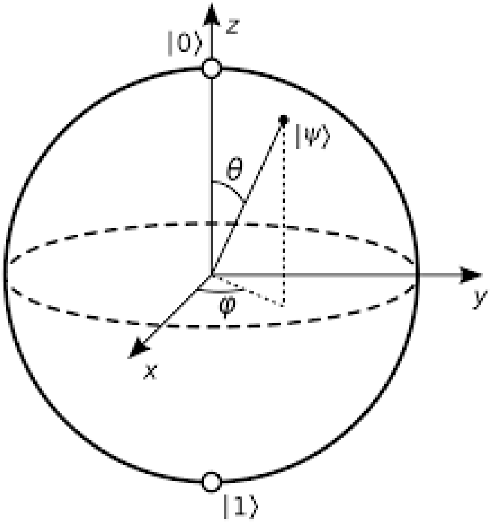
$$\langle\uparrow| = \begin{pmatrix} 1 & 0 \end{pmatrix}$$

Measurements

Observables in QM: operators/matrices

$$H\,|{\uparrow}\rangle = E_1\,|{\uparrow}\rangle$$

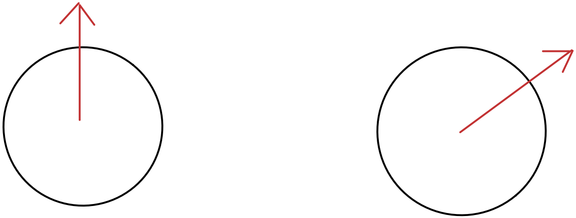
Bloch sphere



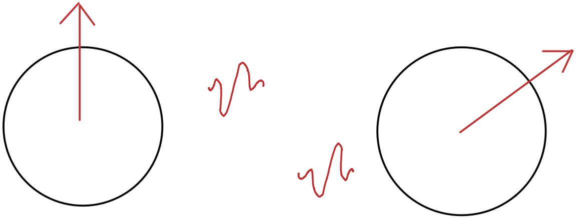
Qubit states

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
$$|\downarrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Entanglement



Entanglement



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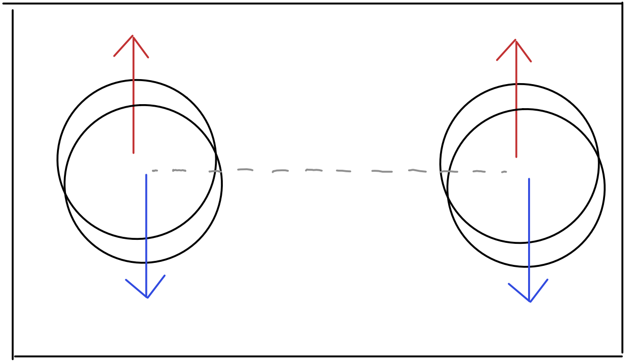

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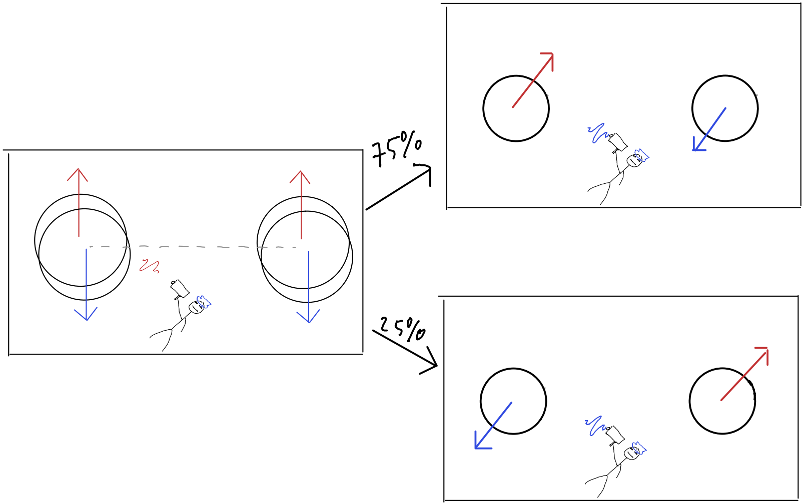
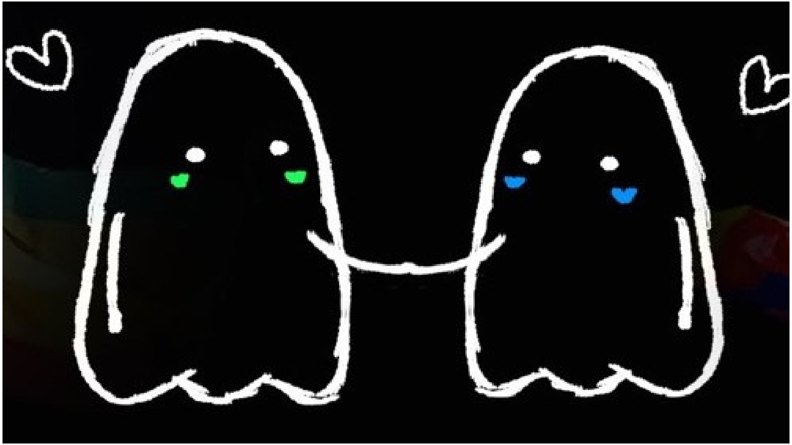


Spooky action at a distance

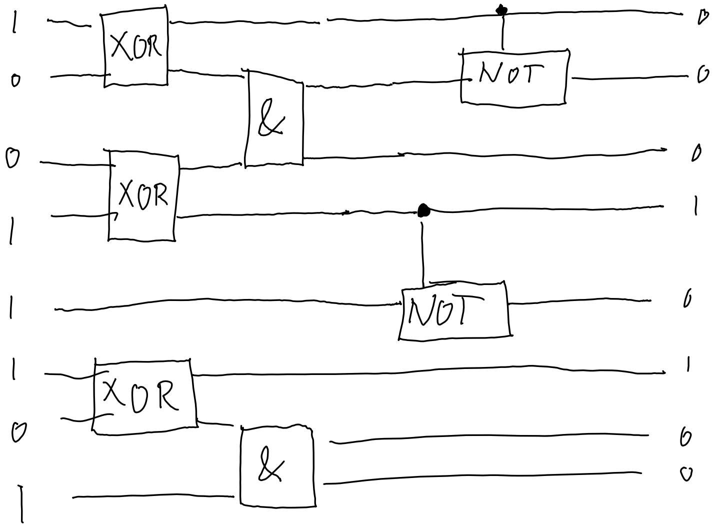


Logical operations on bits

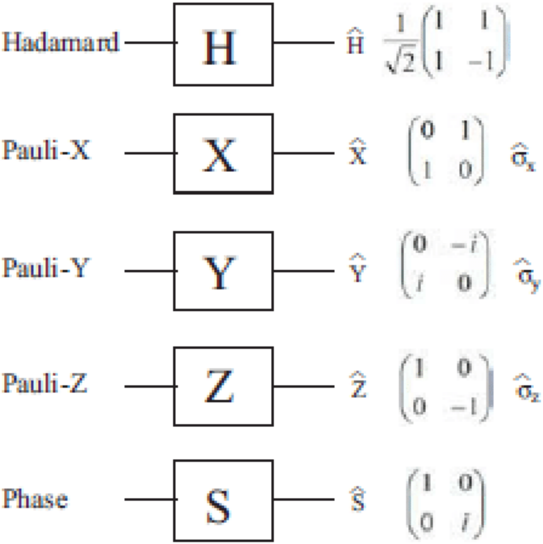
Bit 1	Bit 2	&	|	^
1	0	1	1	0
1	0	0	1	1
0	1	0	1	1
0	0	0	0	0

bit	~
1	0
0	1

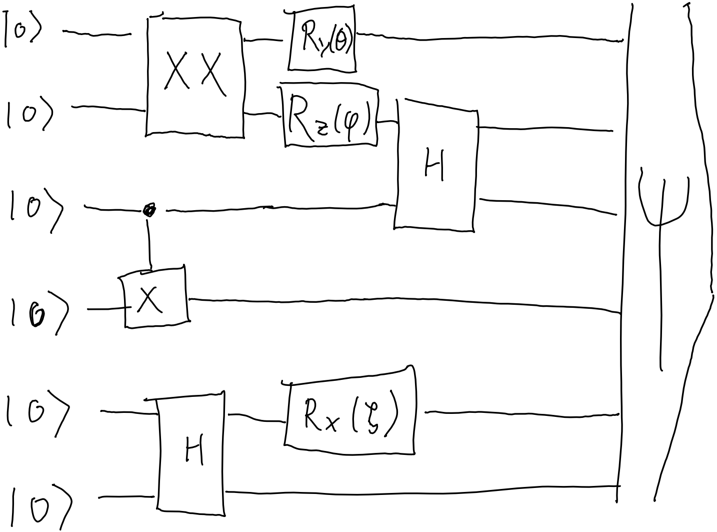
Classical computer programs



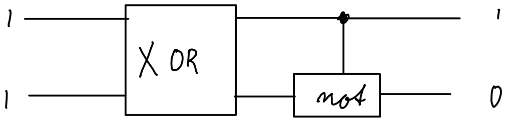
Operations on qubits



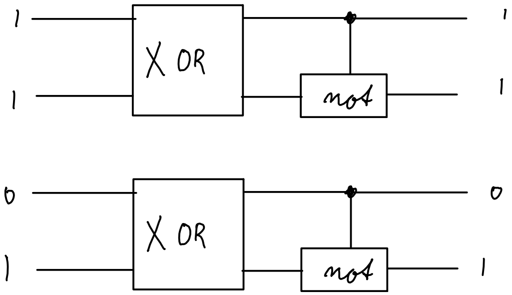
Gated quantum computers



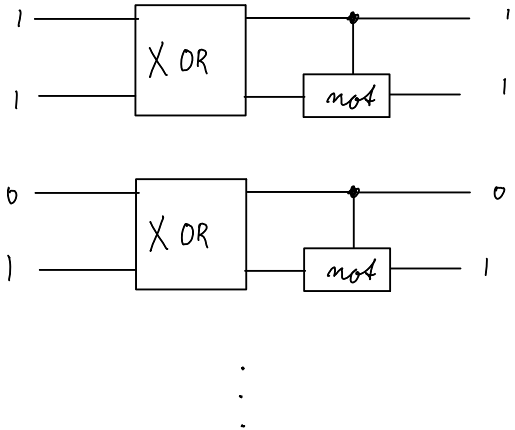
Classical operations



Classical operations



Classical operations



Classical operations

$$|\psi\rangle = |\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle$$

Classical operations

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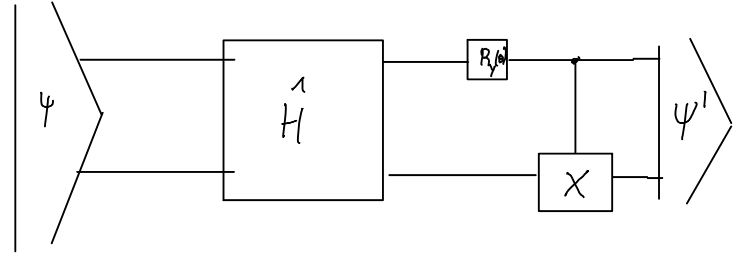
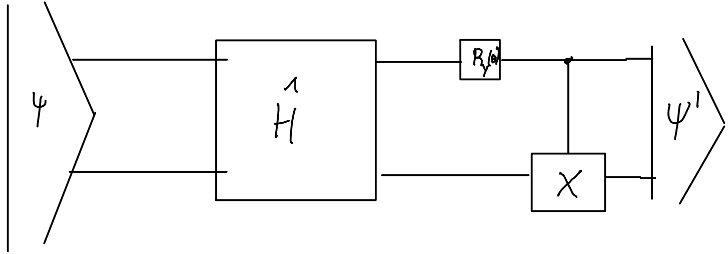


Classical operations

$$|\psi\rangle = |\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle$$

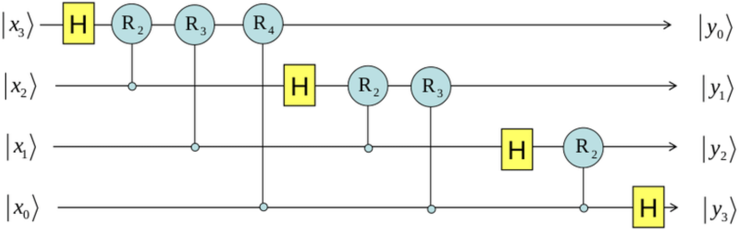


how much of $|\uparrow\uparrow\rangle$ in Alice?

$$\langle \uparrow\uparrow | \psi' \rangle$$

Quantum fourier transform

Quantum Fourier Transform

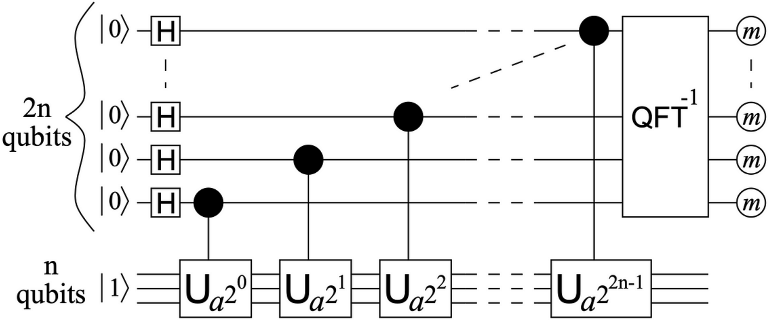


$$|x\rangle \rightarrow \frac{1}{\sqrt{2^n}} \sum_y e^{\frac{2\pi i}{2^n}xy} |y\rangle$$

Uniform family of networks

n Hadamard gates and n(n-1)/2 phase shifts, the size of the network = n(n+1)/2

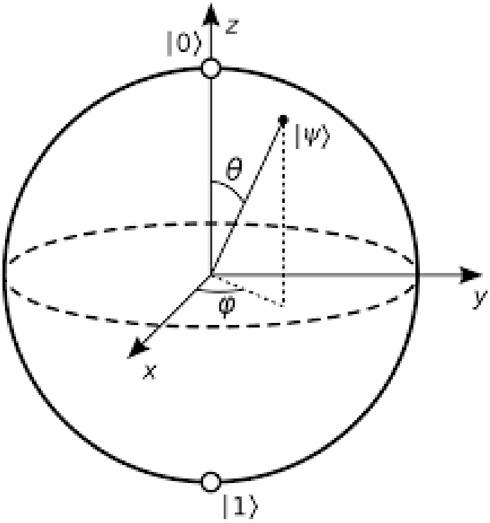
Shor's algorithm



Variational algorithms

- We can also apply paramterized gates
- Example: Rotate about the y-axis for some angle θ.

Bloch sphere again



Remember: Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle$$

H: energy operator. so:

$$\langle\psi|H|\psi\rangle$$

measures energy of a state.

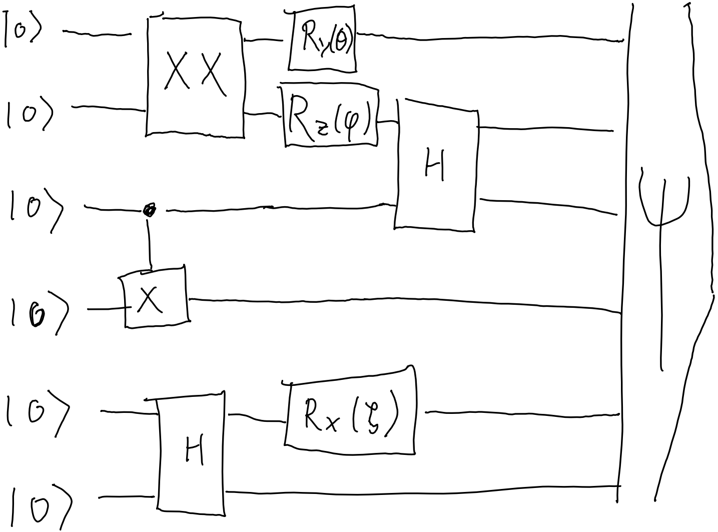
VQE - optimization

Look for a state with a low energy:

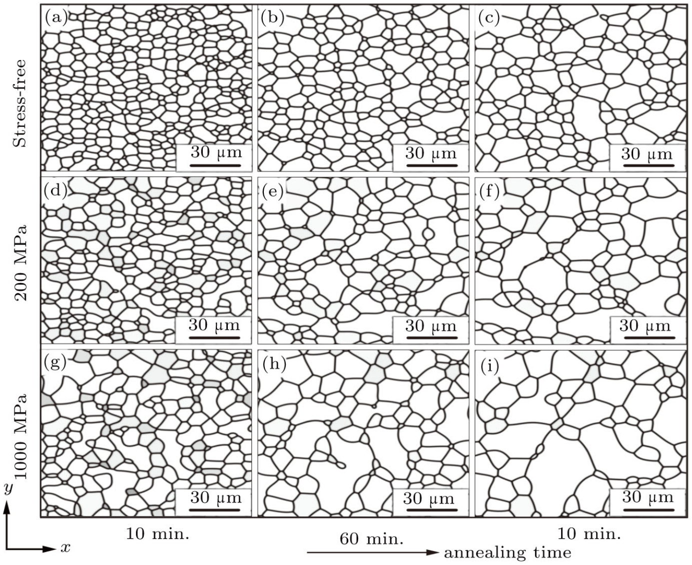
$$\min_{\theta} \langle \phi(\theta) | H | \phi(\theta) \rangle$$

Done with gradient descent.

Difficulties in gated QC

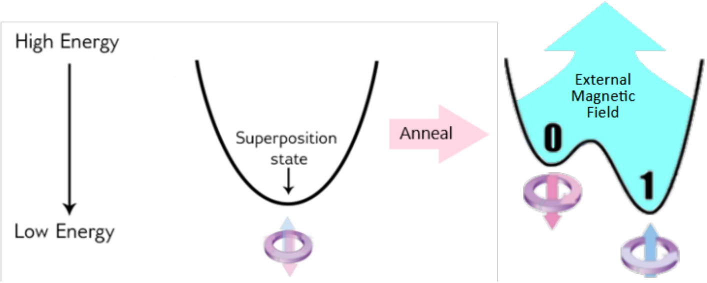


Annealing

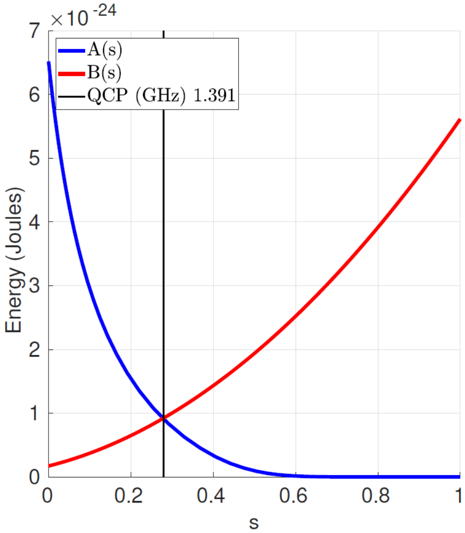


(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)
30 μm
Stress-free
200 MPa
1000 MPa
y
x
10 min.
60 min.
10 min.
annealing time

Quantum annealing



Annealing schedule



Classical problems

- Quantum annealing solves *classical* problems.

Examples

portfolio-optimization Public

Solve different formulations of the portfolio optimization problem.

Python · 42 · Apache-2.0 · 32 · 3 · 1 · Updated last week

flow-shop-scheduling Public

Flow Shop Scheduling example using the Quantum Hybrid NL Solver.

Python · 2 · Apache-2.0 · 5 · 0 · 0 · Updated 2 weeks ago

feature-selection-cqm Public

Use a hybrid solver to select features from two data sets

Python · 13 · Apache-2.0 · 10 · 1 · 2 · Updated last month

kibble-zurek Public

Simulate Kibble-Zurek mechanism on a quantum computer

Python · 2 · 5 · 0 · 0 · Updated on Sep 3

template-dash Public template

A template for creating visual examples using Plotly Dash.

Python · 0 · Apache-2.0 · 0 · 0 · 0 · Updated on Aug 13

mvrp Public

Capacitated Vehicle Routing Problem example on D-Wave's hybrid solvers.

Python · 3 · Apache-2.0 · 1 · 5 · 0 · Updated on Aug 3

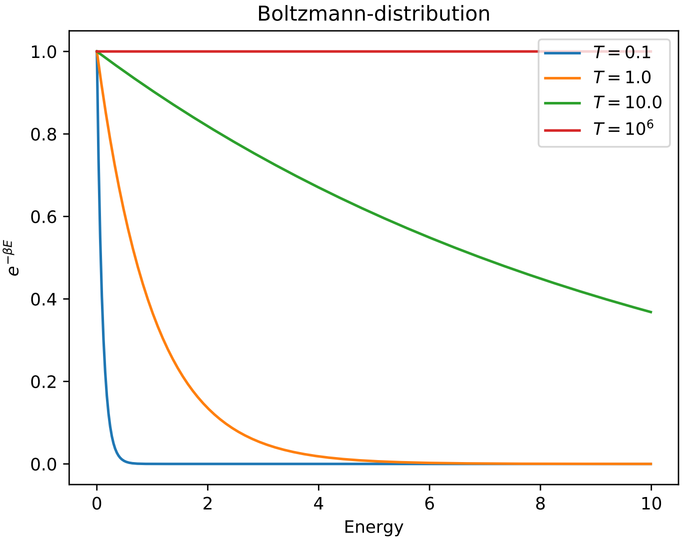
Nobel prize in Physics, 2024

Boltzmann distribution

$$p(s) = e^{-\frac{1}{T}E(s)} / \sum_{s'} e^{-\beta\frac{1}{T}E(s')}$$

where $E(s)$ is the energy function.

Boltzmann disribution

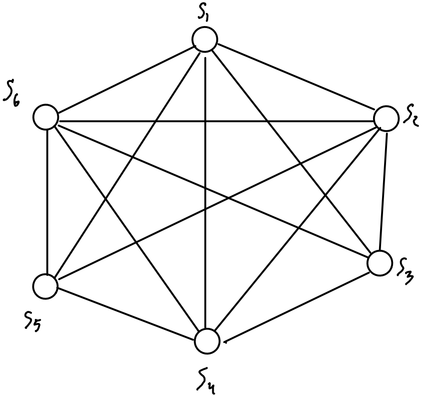


Connected BM

$$\mathbf{s} = \begin{pmatrix} s_0 \\ s_1 \\ \dots \\ s_n \end{pmatrix}$$

$$E(s) = \sum_{i,j} W_{i,j} s_i s_j + \sum_i h_i s_i$$

Boltzmann machine



$$H = \sum_{k=x,y,z} \left(\sum_{i<j} w_{ij}\, \sigma_i^k \sigma_j^k + \sum_{i=0}^{n-1} \tilde{w}_i\, \sigma_i \right)$$

Cost function

Classically:

$$\arg\min_{w} \sum_{i} q(s_i) \log q(s_i) - \sum_{i} q(s_i) \log p(s_i)$$

Quantum:

$$\arg\min_{w} \mathrm{Tr}\{\eta \log \eta\} - \mathrm{Tr}\{\eta \log \rho\}$$

where:

$$\eta = |q(s)\rangle\langle q(s)|$$

Complex numbers

$$
\begin{aligned}
z &= 10 + 3i \\
\bar{z} &= 10 - 3i \\
|z| &= z * \bar{z} = 10^2 + \cancel{10 * 3i} - \cancel{10 * 3i} - 3 * 3 * i^2 \\
&= 10^2 + 3^2
\end{aligned}
$$

Spin operators

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

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

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

Measurements

$$\langle \sigma_z \rangle = \langle \psi | \sigma_z | \psi \rangle$$

Possible outcomes are given by eigenvectors of operators:

$$\sigma_z \left|\downarrow\right\rangle = -1 * \left|\downarrow\right\rangle \tag{5}$$

Measurements 2

For those that did linear algebra:

$$\sigma_z = 1 * |\uparrow\rangle \langle\uparrow| - 1 * |\downarrow\rangle \langle\downarrow|$$

show all possible outcomes when measuring σ_z

Born's rule

$$\sigma_z \left(\frac{1}{\sqrt{2}} \left|\uparrow\right\rangle + \frac{1}{\sqrt{2}} \left|\downarrow\right\rangle \right) = \begin{cases} 1 * \left|\uparrow\right\rangle & \text{with } p = \frac{1}{2} \\ -1 * \left|\uparrow\right\rangle & \text{with } p = \frac{1}{2} \end{cases}$$

Measuring the state destroys the state! Also,

$$\left(\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}}\right)^2 = 1$$

Two particles

So far, we have dealt with one particle or qubit. Multiple qubits?

$$|{\uparrow\uparrow}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Four possibilities:

$$|{\uparrow\uparrow}\rangle , |{\uparrow\downarrow}\rangle , |{\downarrow\uparrow}\rangle , |{\downarrow\downarrow}\rangle$$

entanglement

Suppose we have a superposition state:

$$\frac{1}{\sqrt{2}} \left|\uparrow\uparrow\right\rangle + \frac{1}{\sqrt{2}} \left|\downarrow\downarrow\right\rangle \tag{6}$$

And we measure the first particle to be $\left|\uparrow\right\rangle$. What do we know about the second particle?

entanglement

Suppose we have a superposition state:

$$\frac{1}{\sqrt{2}} \left|\uparrow\uparrow\right\rangle + \frac{1}{\sqrt{2}} \left|\downarrow\downarrow\right\rangle \tag{6}$$

And we measure the first particle to be $\left|\uparrow\right\rangle$. What do we know about the second particle? Measuring the first particle **changed** the second particle

Python environment

Need:

- Python ≥ 3.8
- numpy
- scipy

Assignment 1

- states: `up = np.array([[1], [0]])`
- Transpose: `up.T`
- Operators: `sigma_x = np.array([[0, 1], [1, 0]])`
- Matrix product: `sigma_x @ up`
- Expectation value: `up.T @ \sigma_x @ up`

Running code on a QPU

Download qiskit SDK:

- `pip install qiskit`
- `pip install qiskit-ibm-runtime`
- Create account on `https://quantum.ibm.com/`

qiskit tutorial

Follow the qiskit tutorial at `https://github.com/Qiskit/qiskit-tutorials/blob/2fc7ed53fcc7bb3bff4855e400d00ee050a82b81//tutorials/circuits/01_circuit_basics.ipynb`