

Variational Quantum Algorithms

or Quantum Machine Learning!

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THOMAS JEFFERSON NATIONAL ACCELERATOR
FACILITY

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REYES Summer Program



U.S. DEPARTMENT OF
ENERGY

Office of
Science



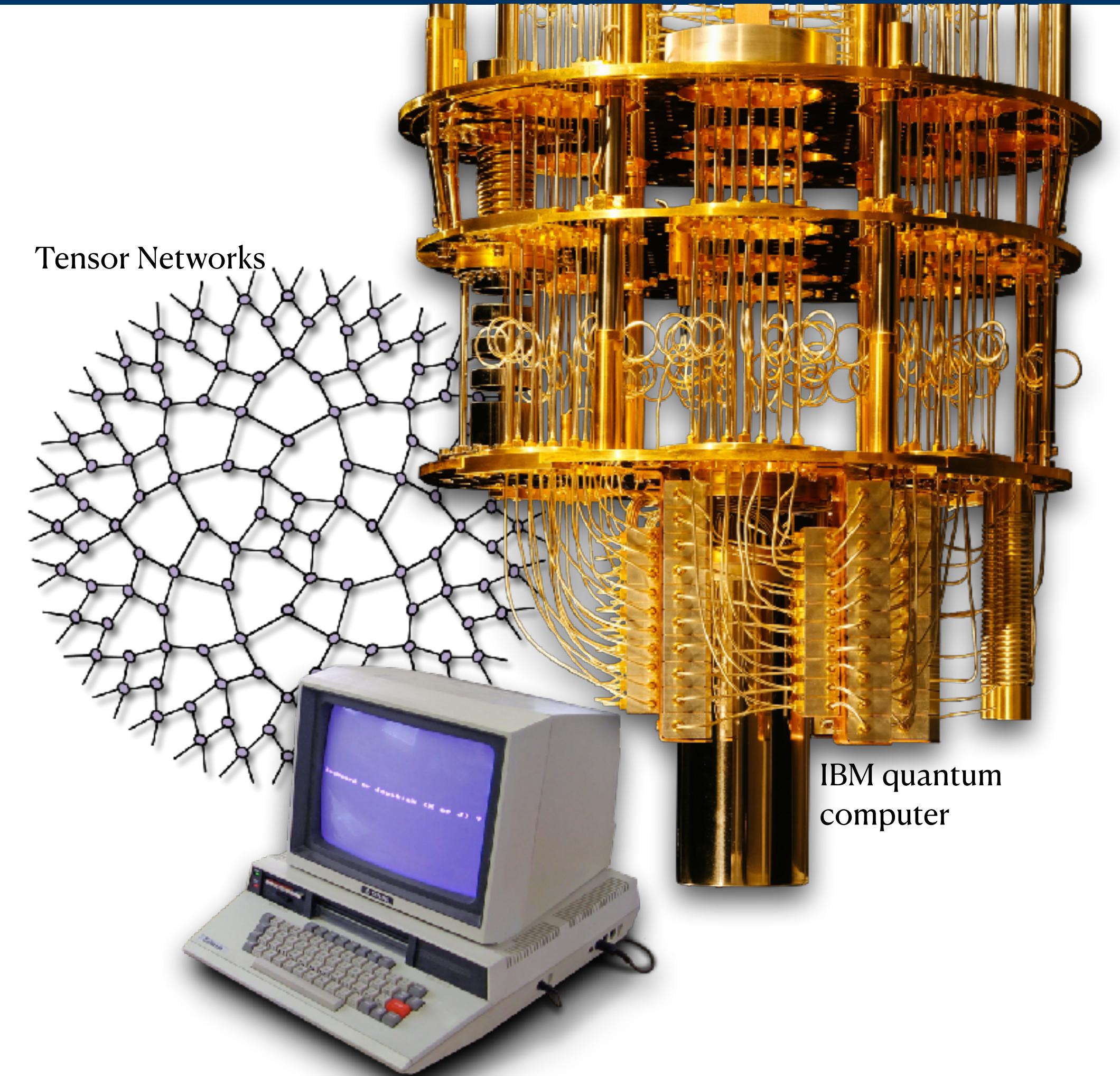
Outline

(Recap)

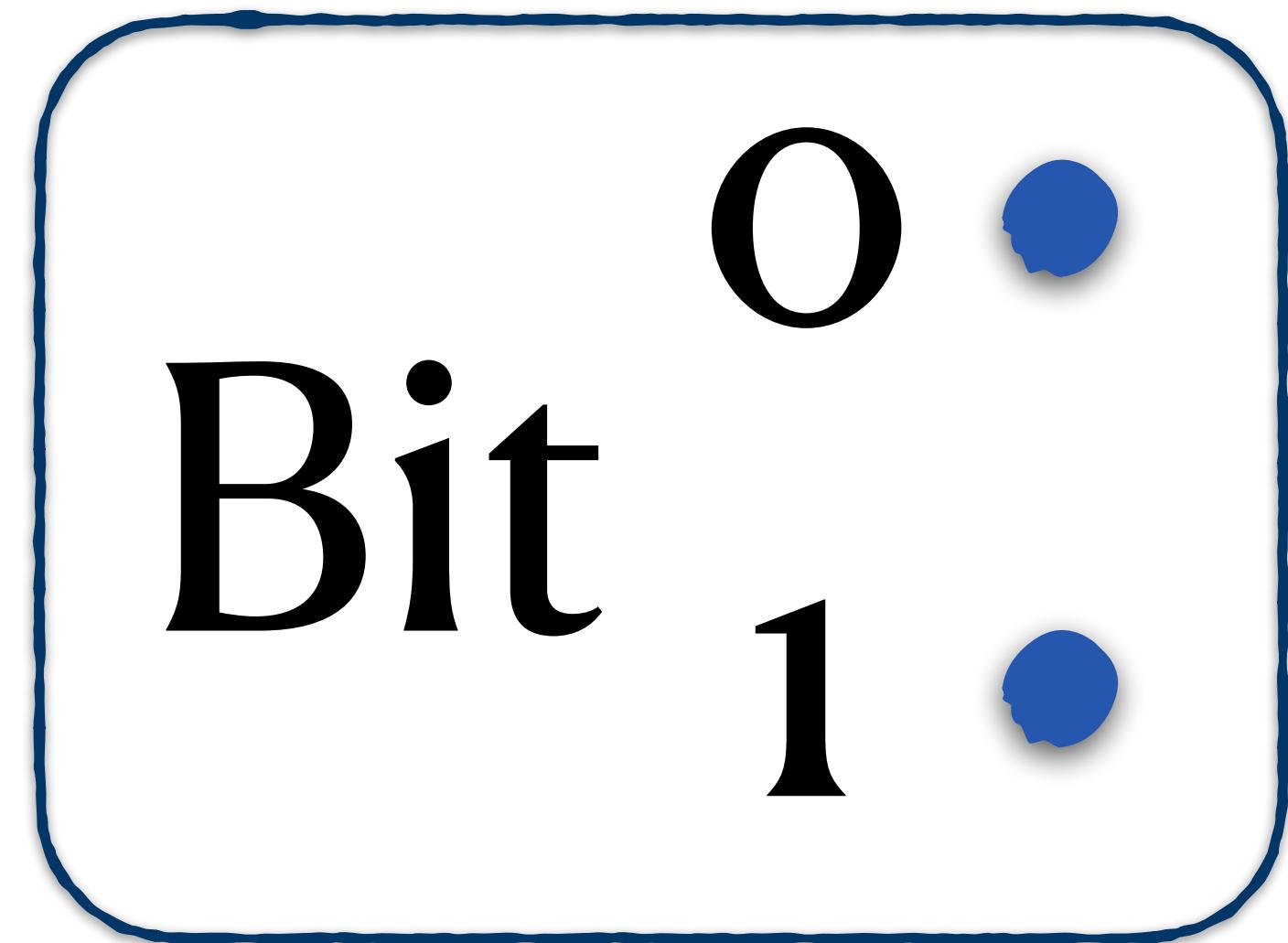
Quantum Computing

Simulating the
Quantum Nature

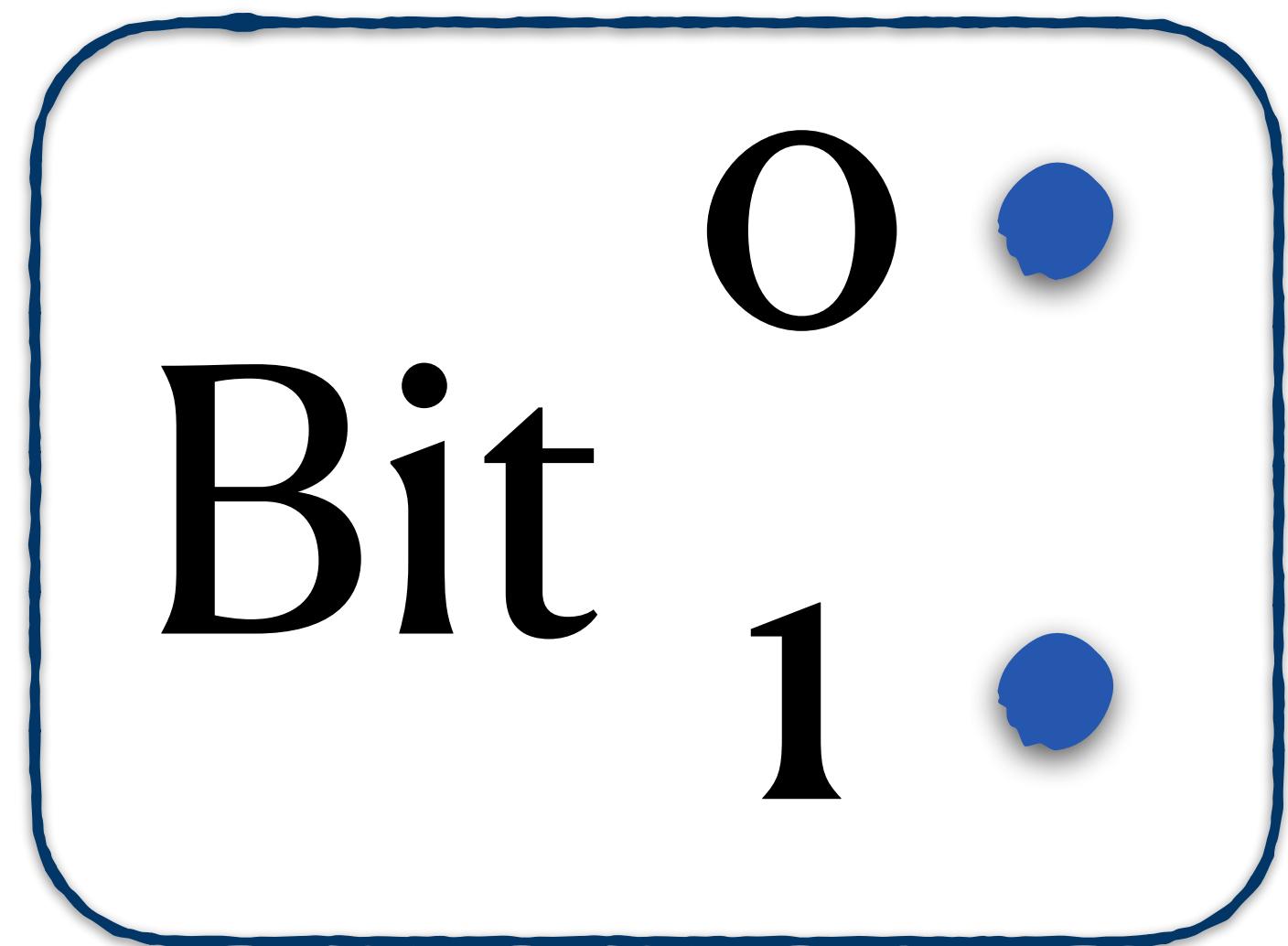
Machine Learning



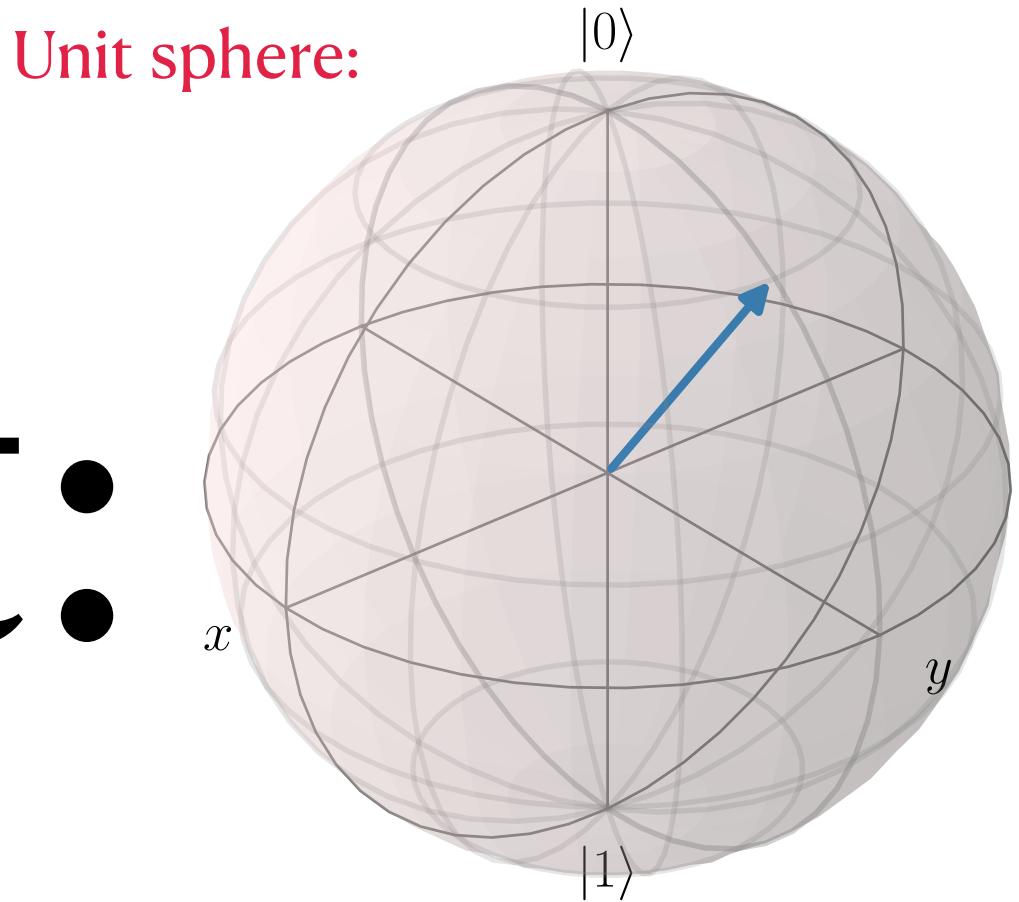
What's wrong with my good old computer?



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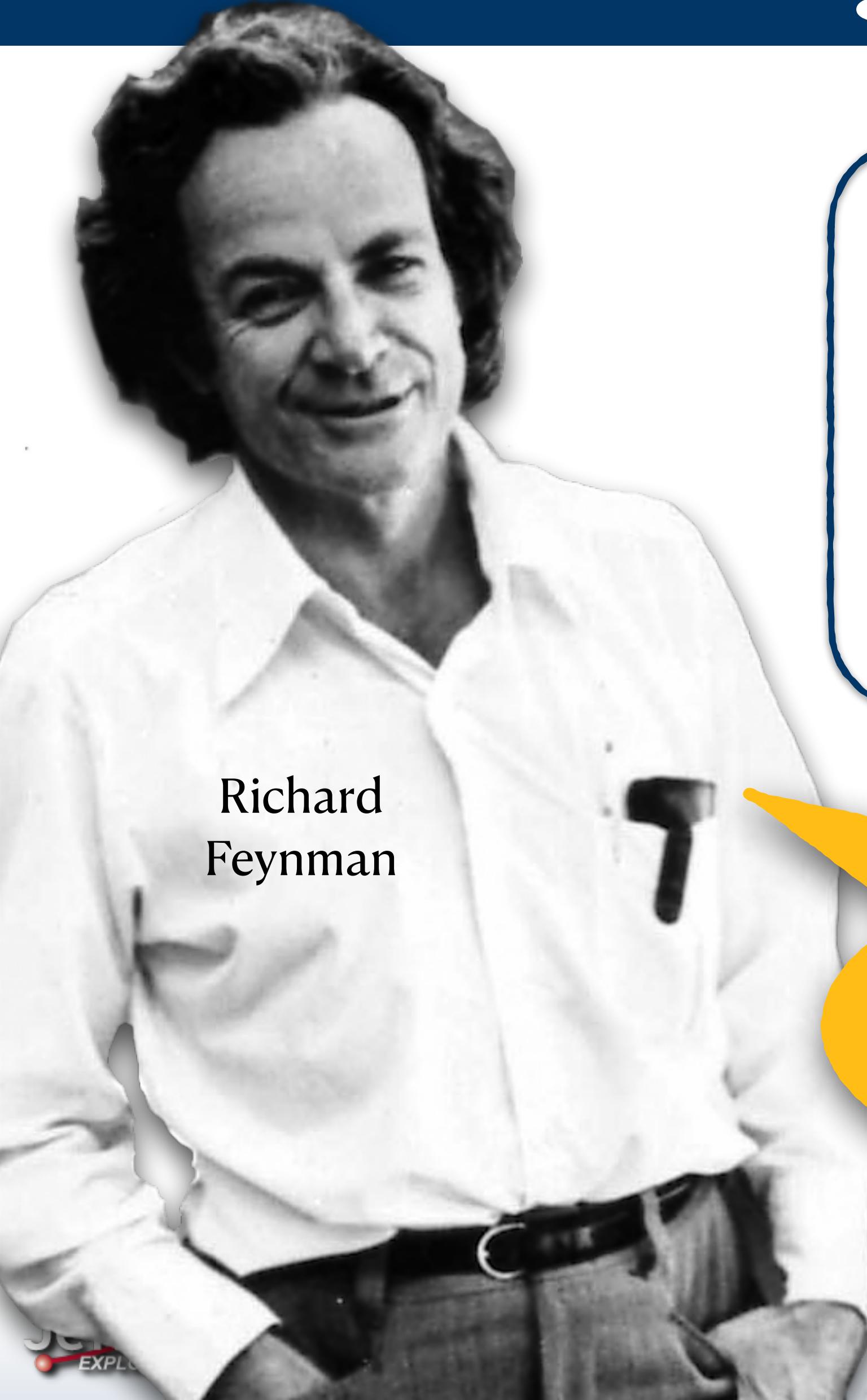


QuBit:

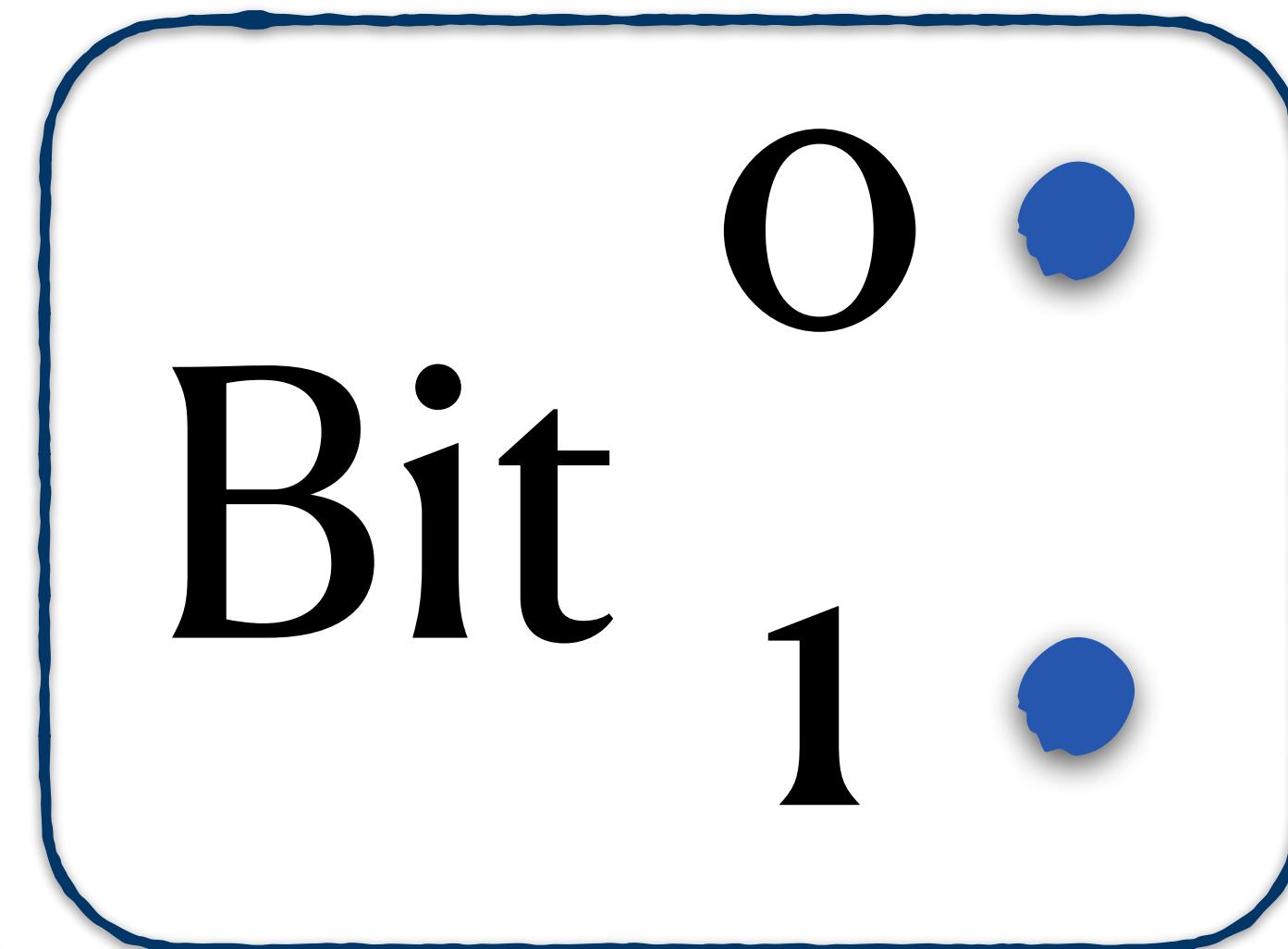


Superposition
Entanglement

What's wrong with my good old computer?



Richard
Feynman



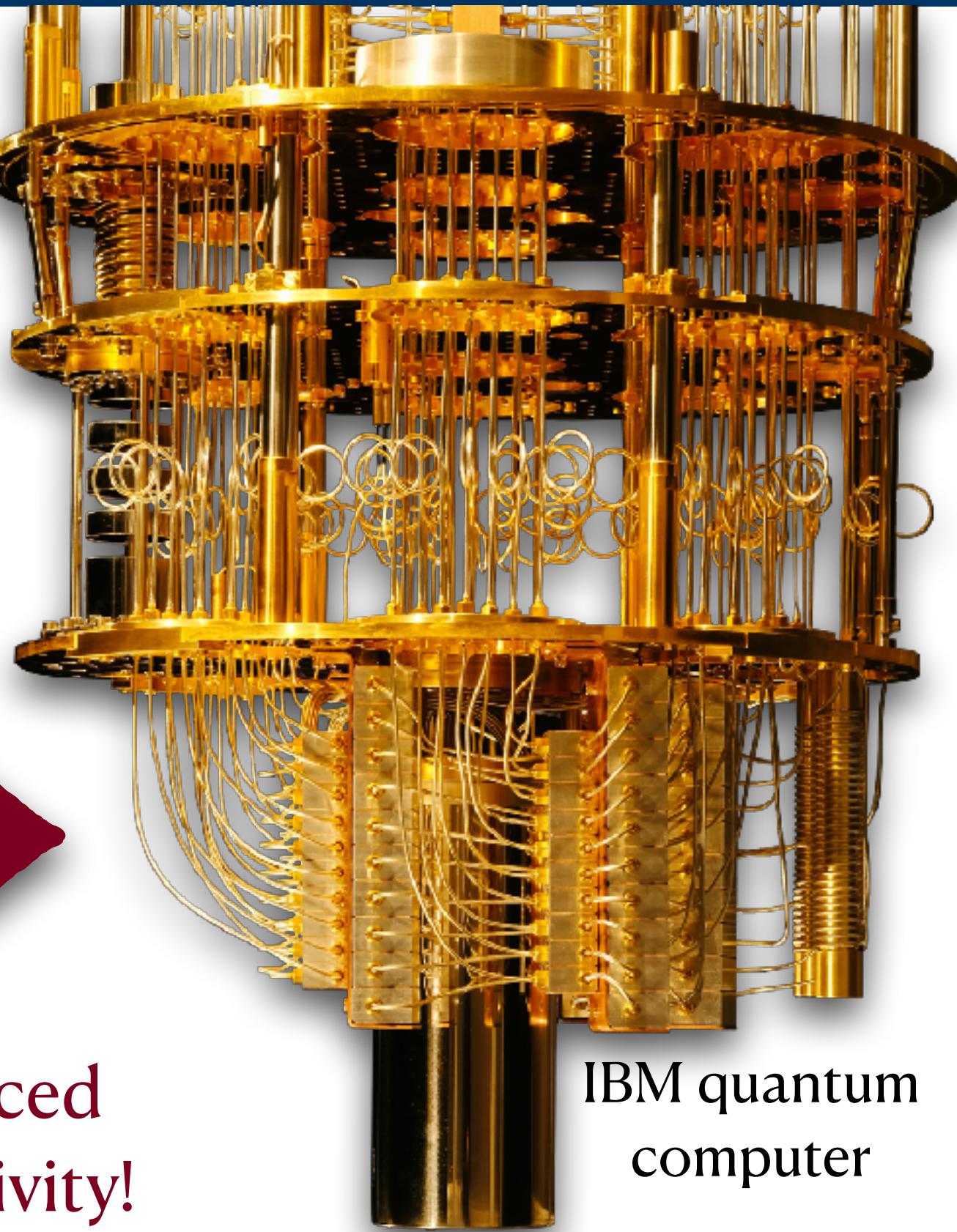
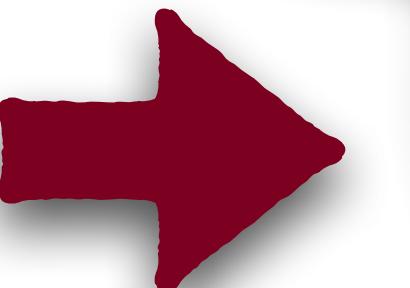
Unit sphere:

Superposition
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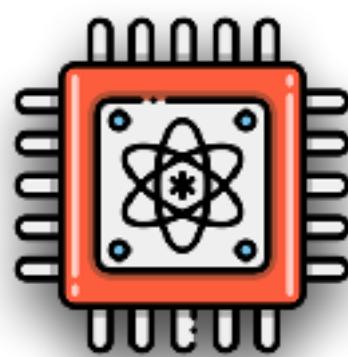
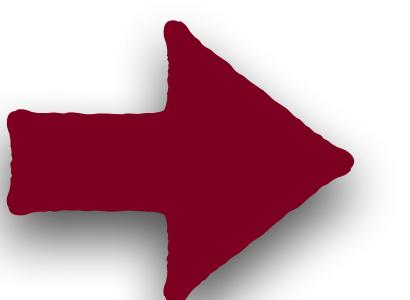
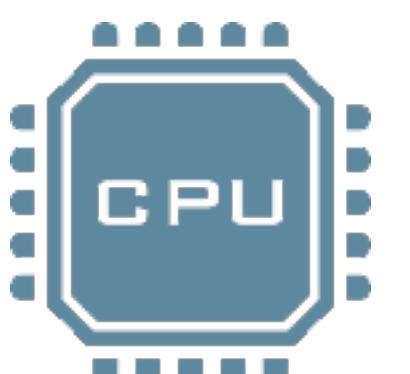
Nature isn't
classical, dammit!

Why is this interesting? Why now?

- ❖ Quantum computing may make “impossible” possible!
- ❖ Quantum computing might solve the world’s biggest challenges!
- ❖ Building a Knowledge Foundation
- ❖ Preparing for Future Applications
- ❖ Now Quantum Computers are noisy; time to prepare them for the future!



Enhanced expressivity!

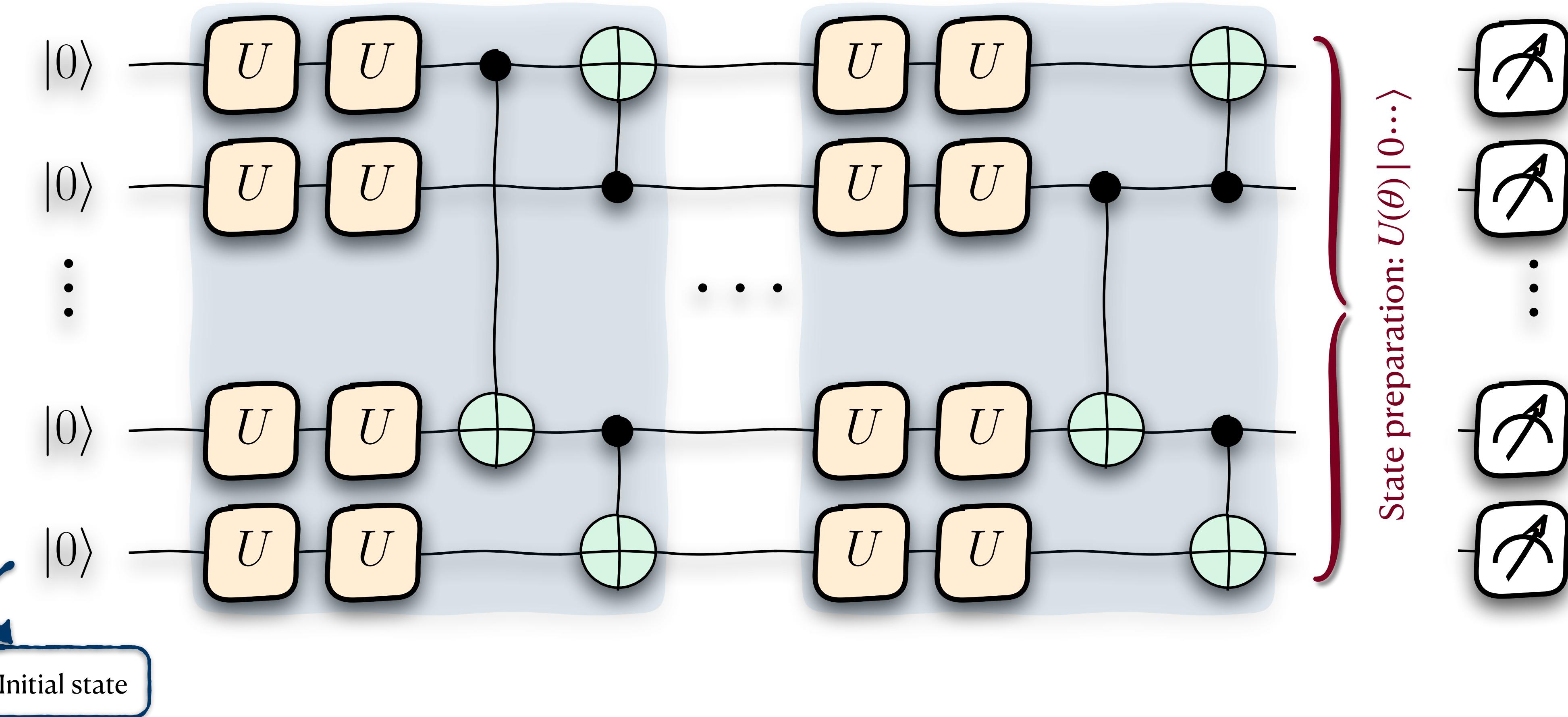


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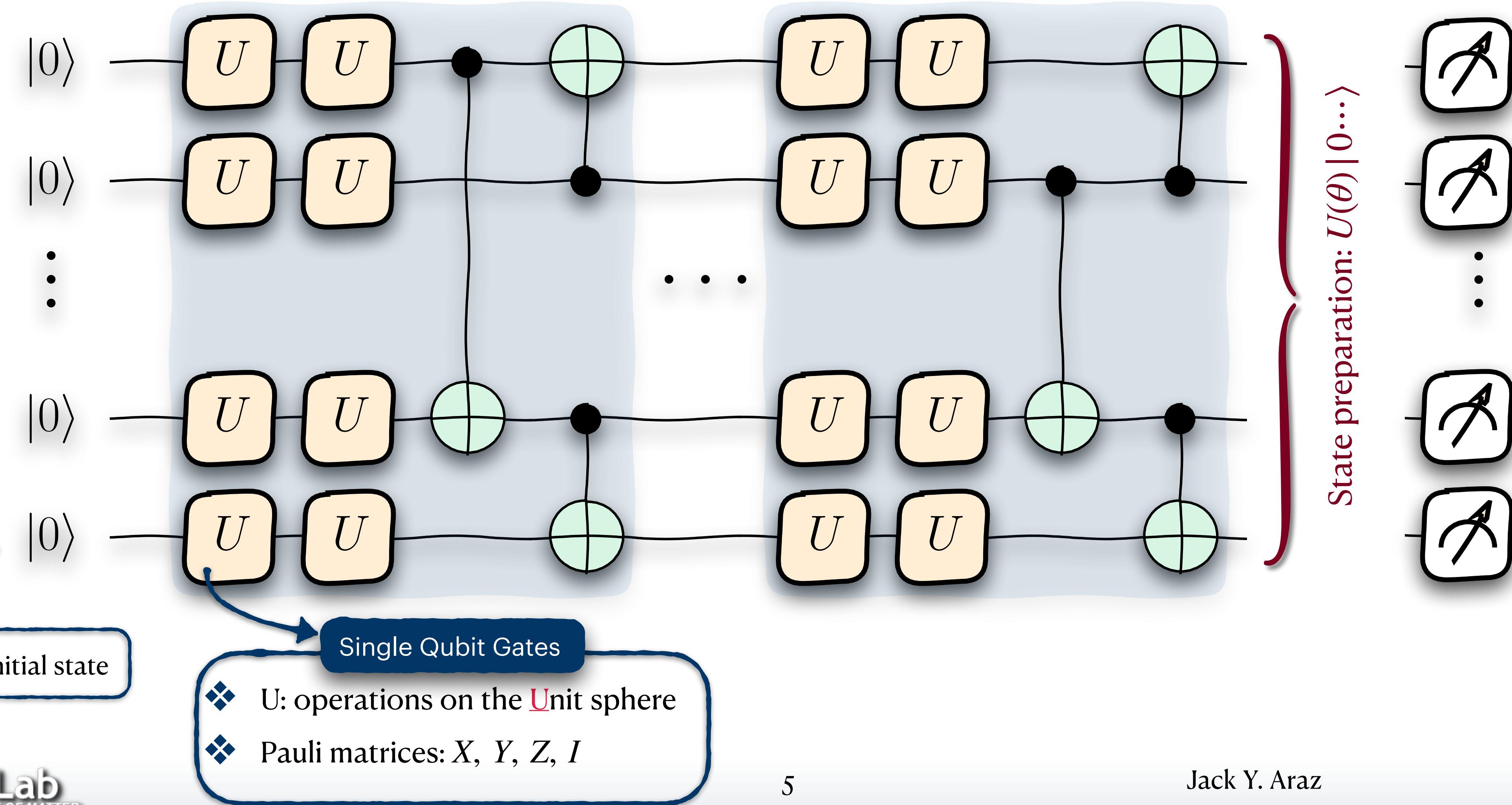
How does the Quantum Computer work (theoretically)?

Read from left to right!

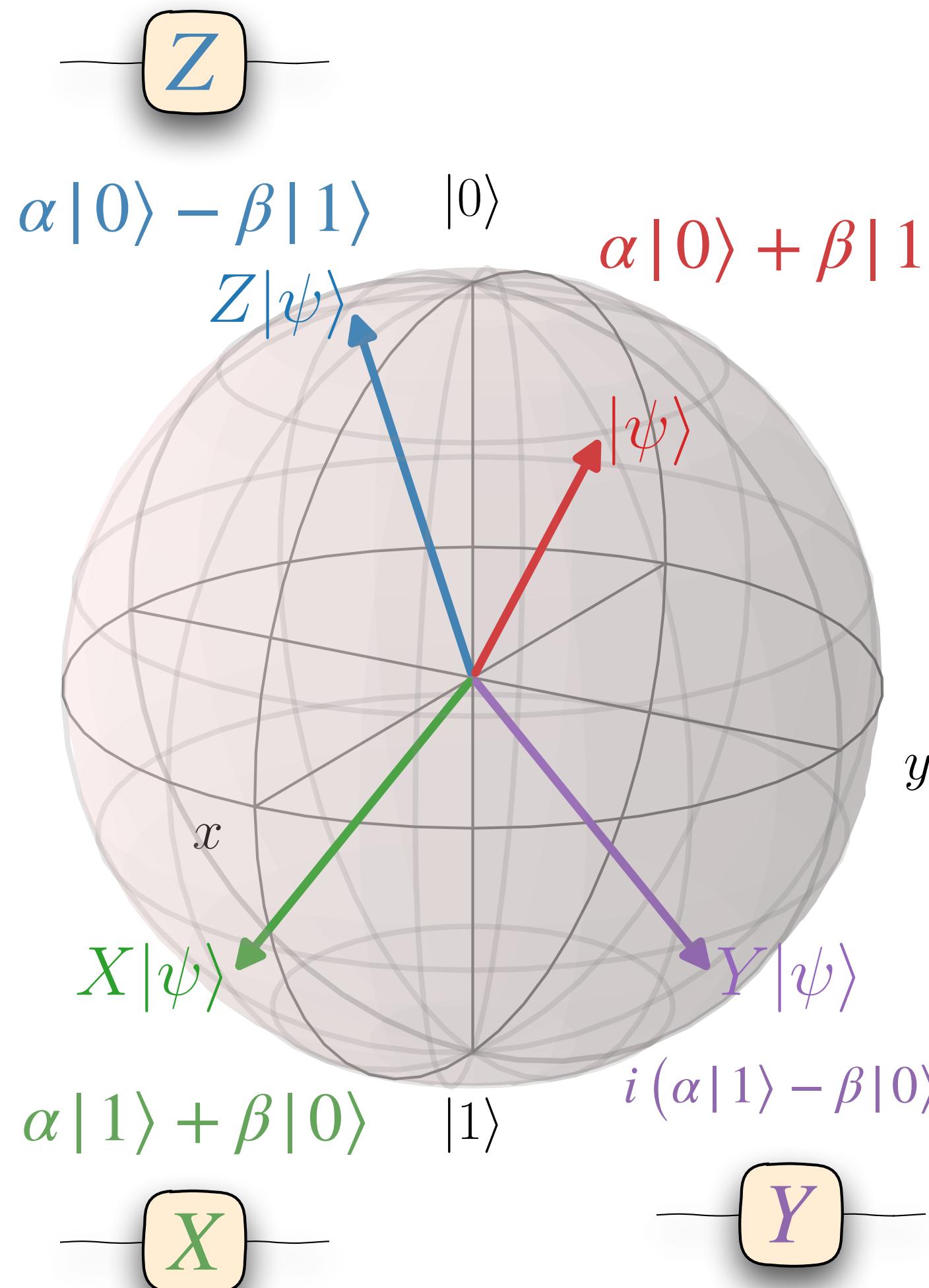


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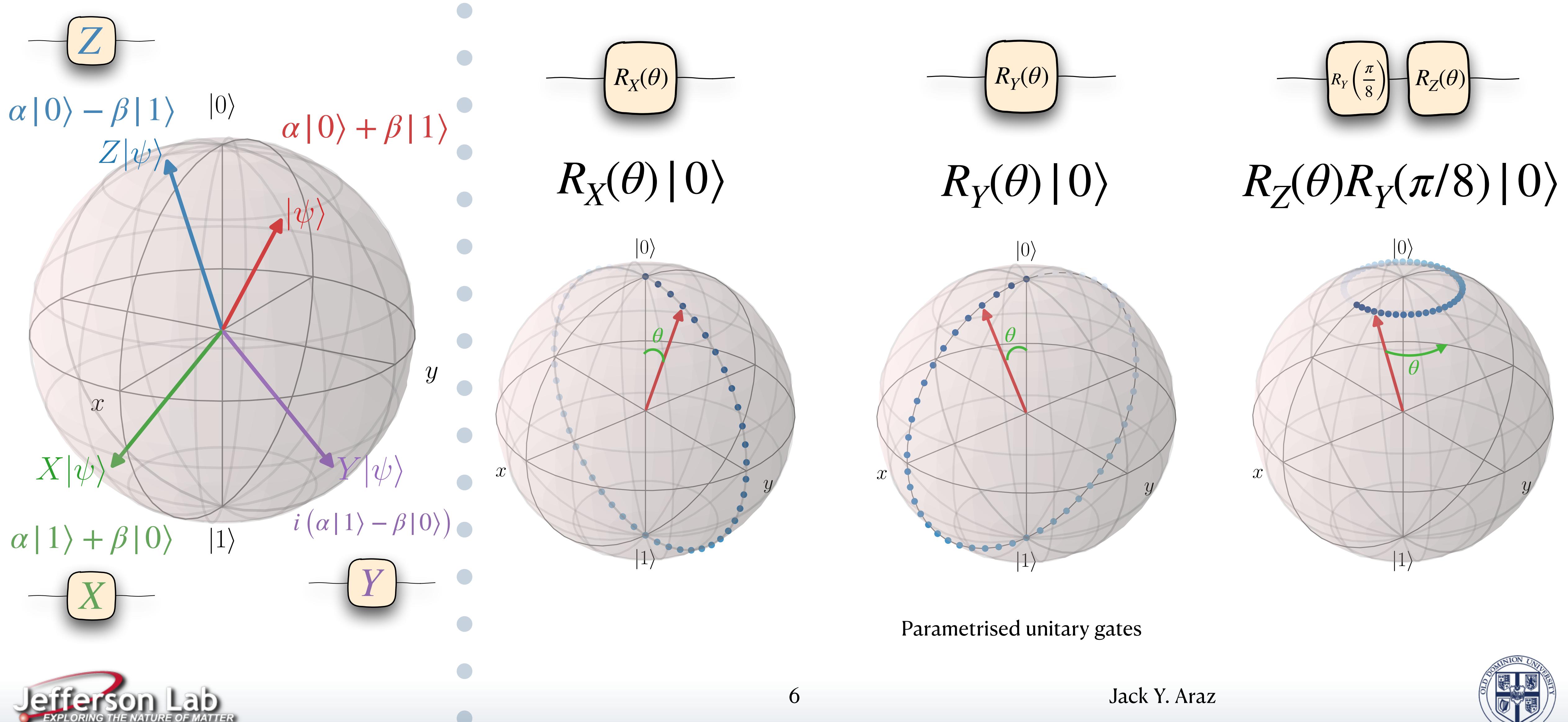
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Pauli matrices are the letters of our alphabet

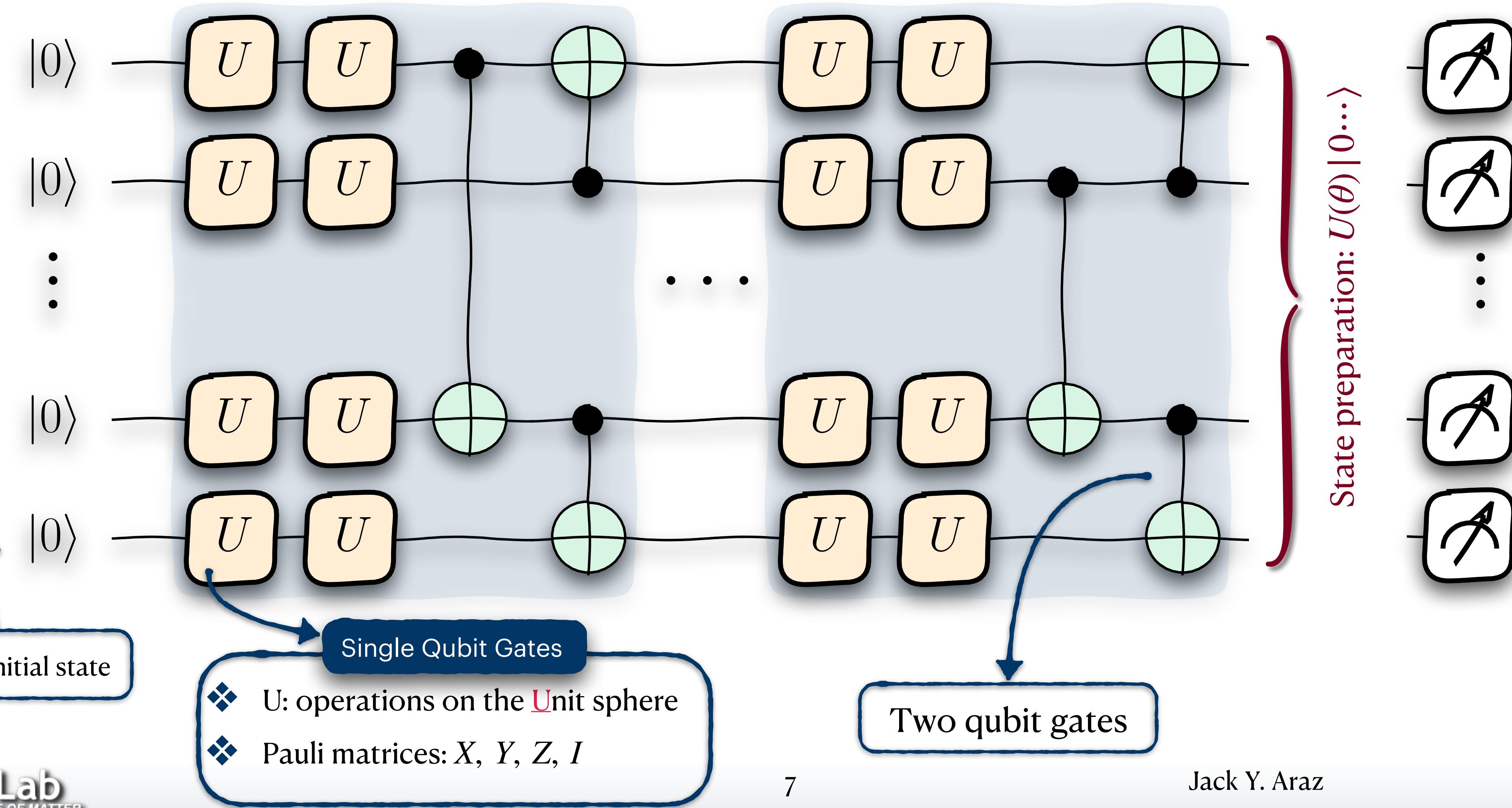


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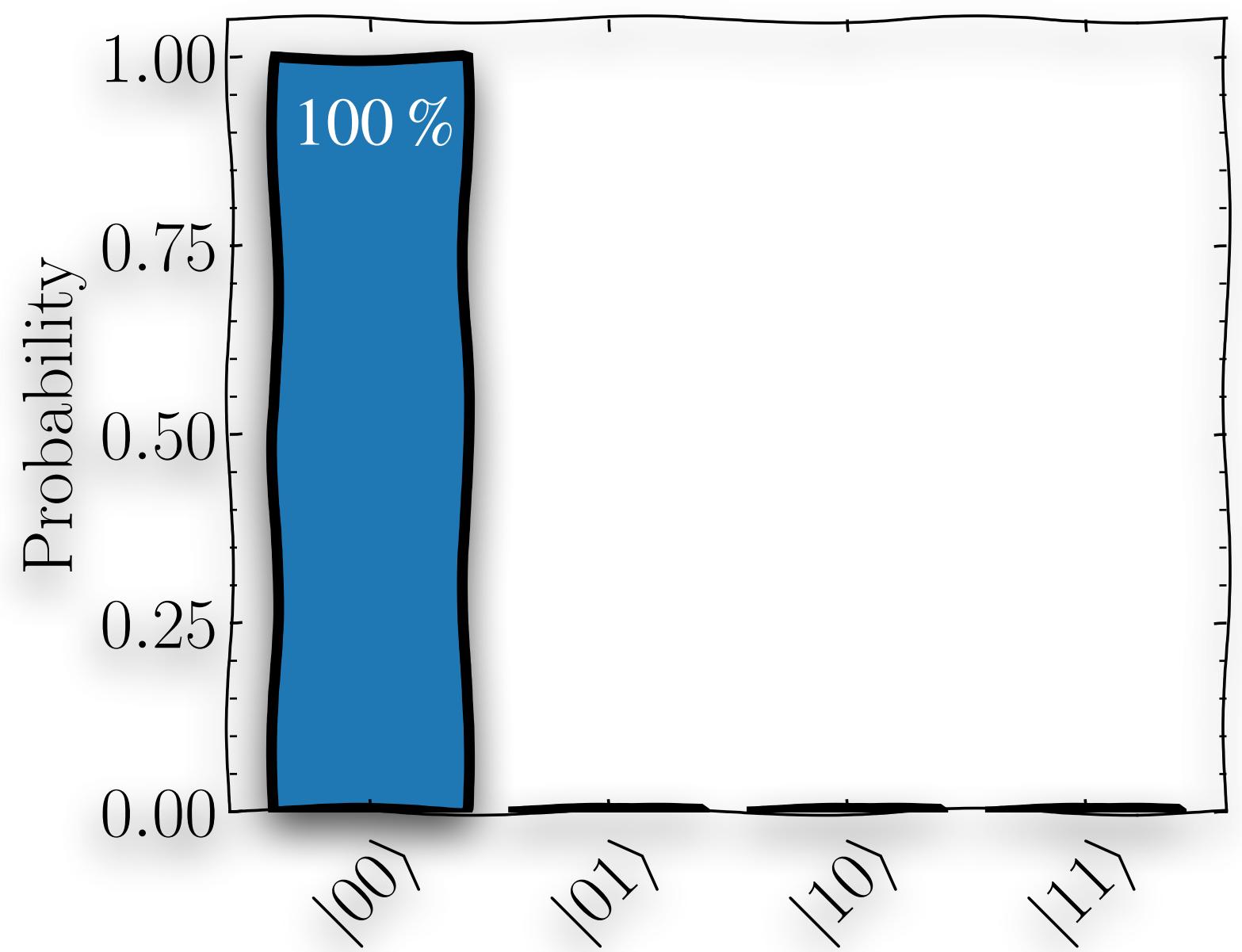
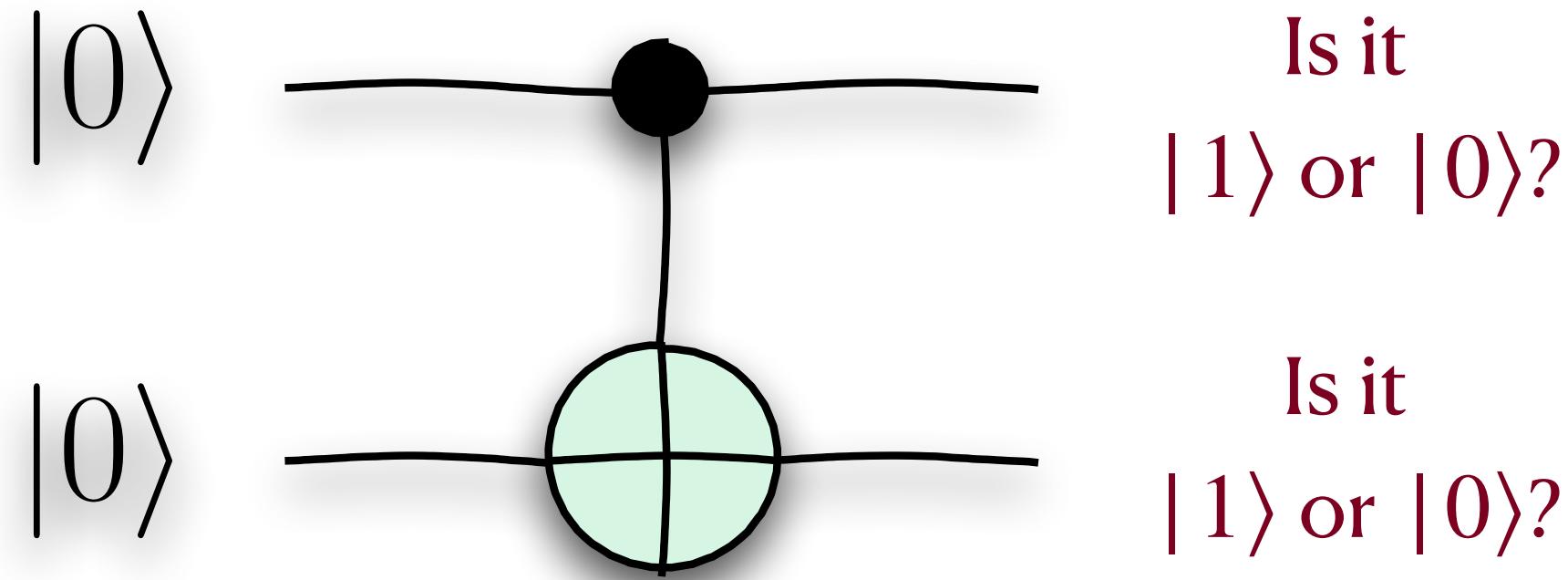


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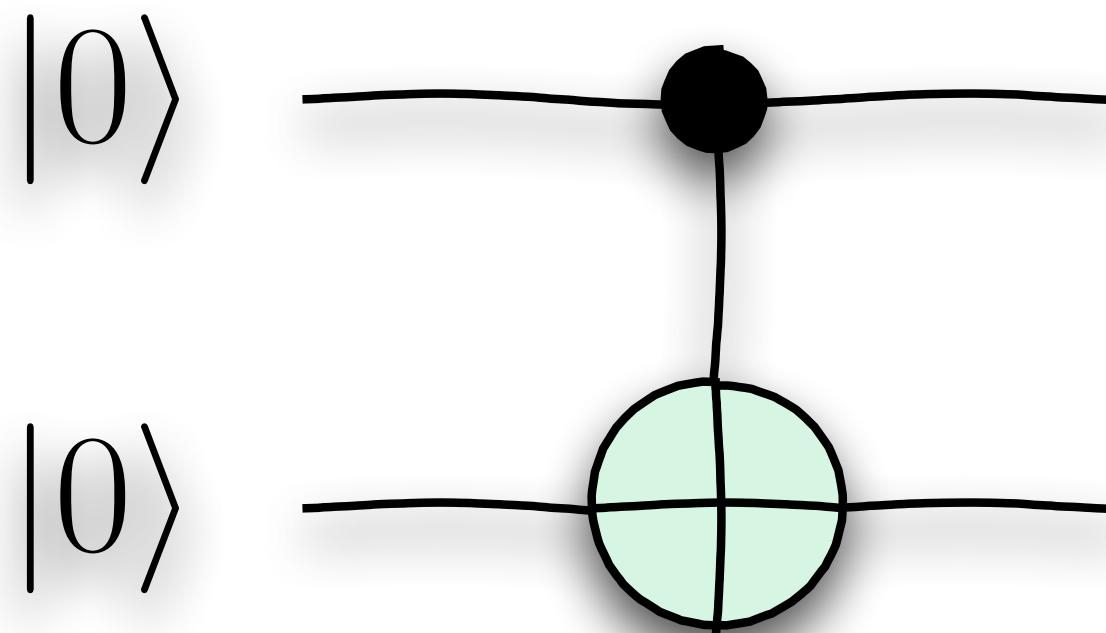
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Two qubit gates

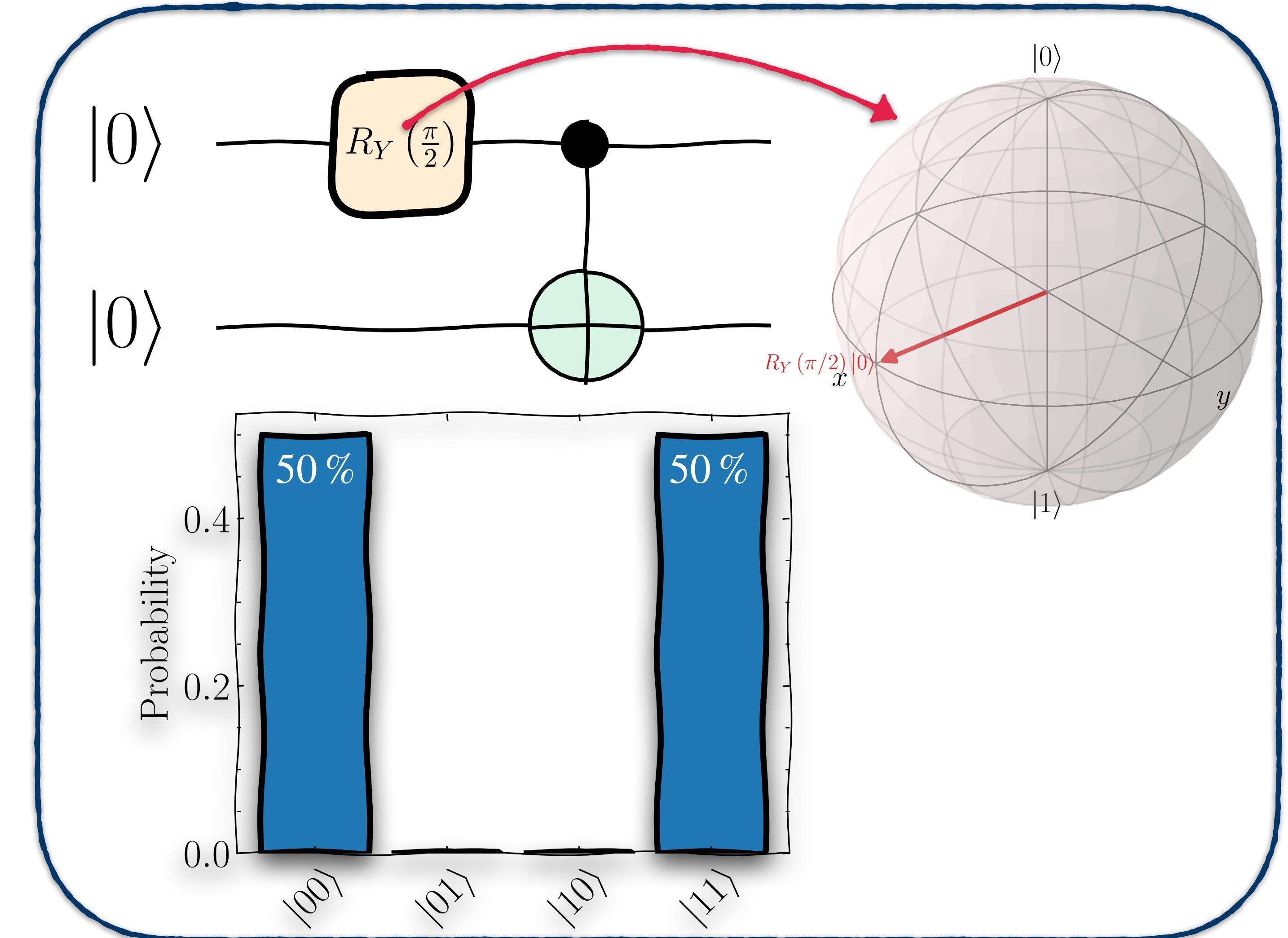
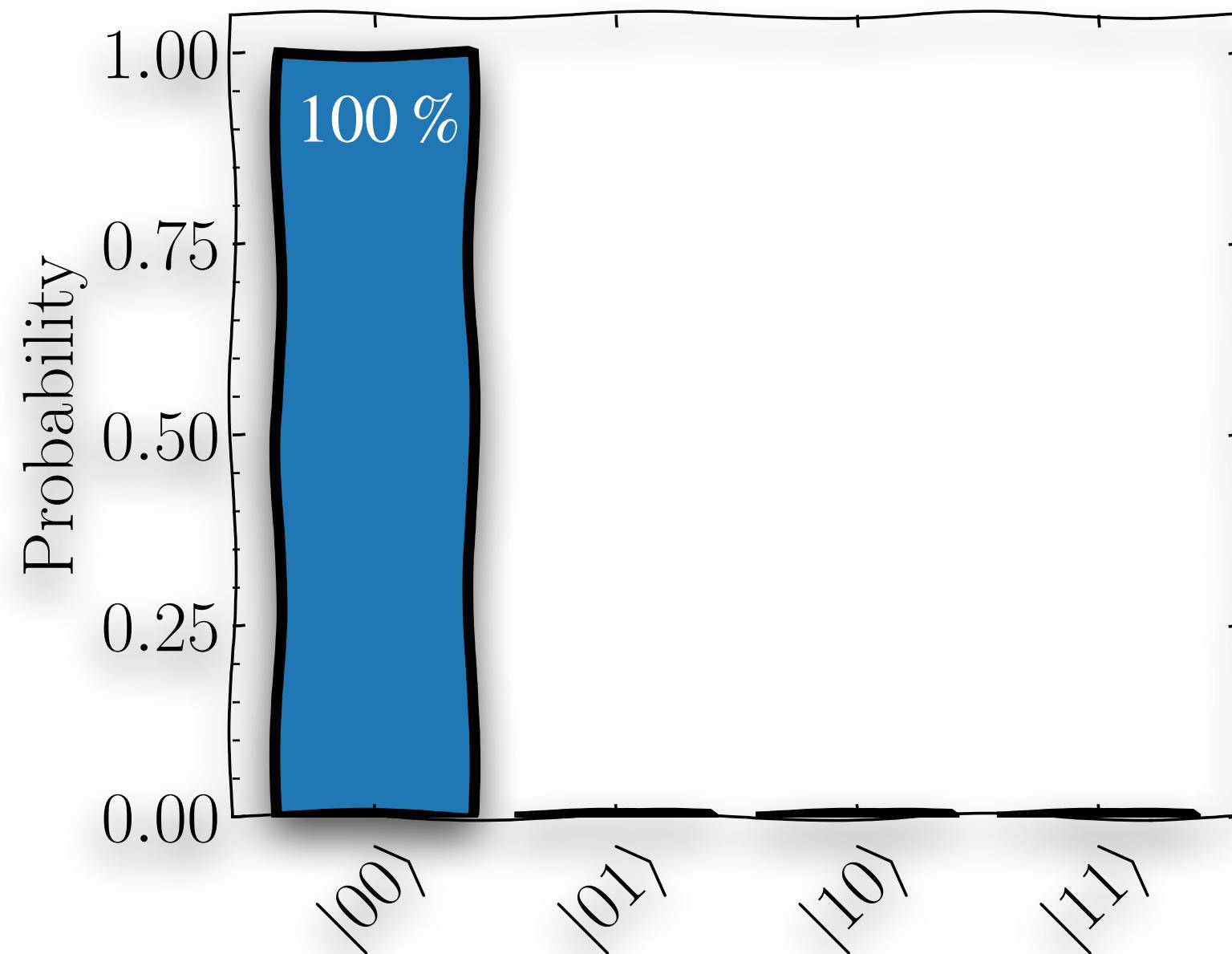


Two qubit gates

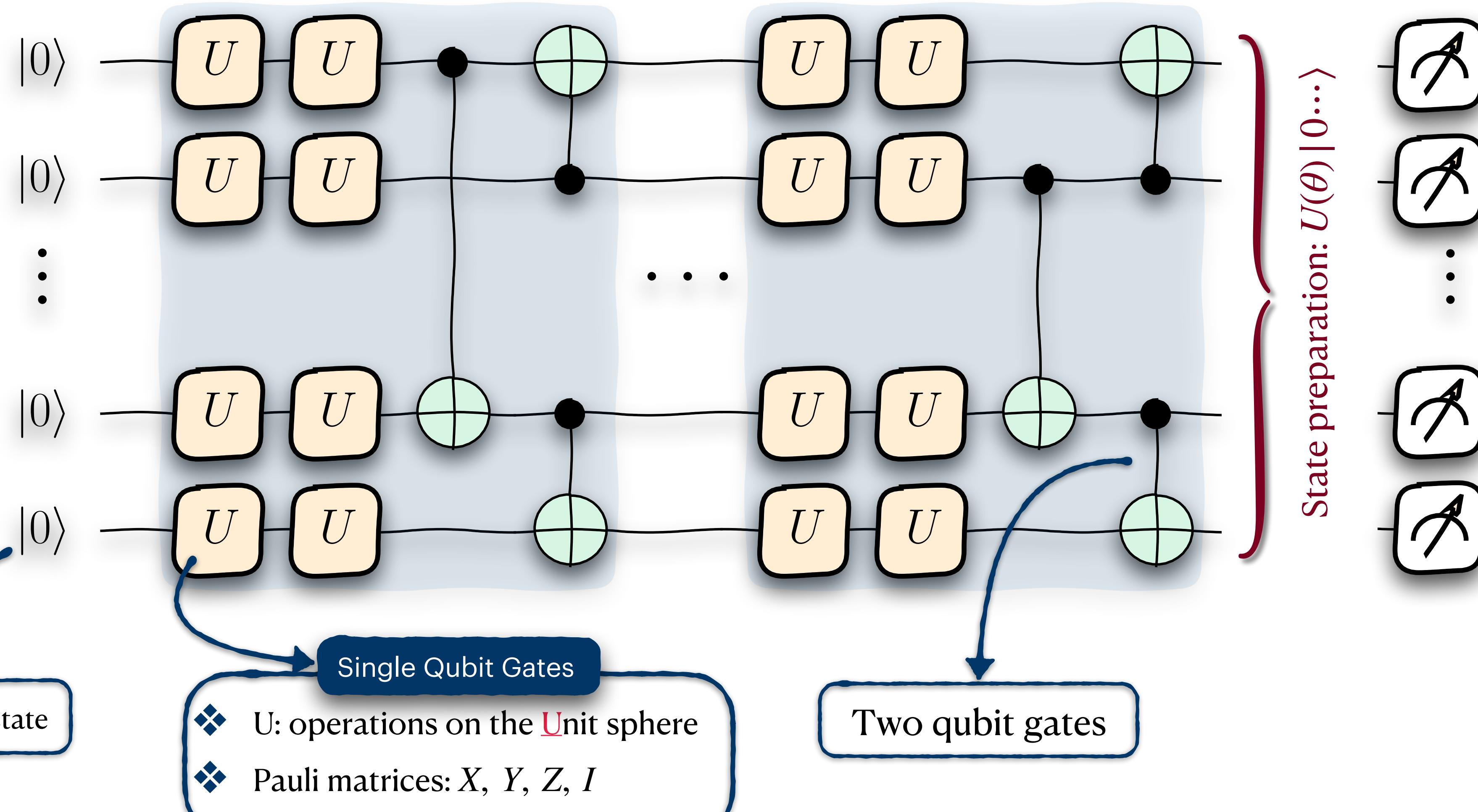


Is it
 $|1\rangle$ or $|0\rangle$?

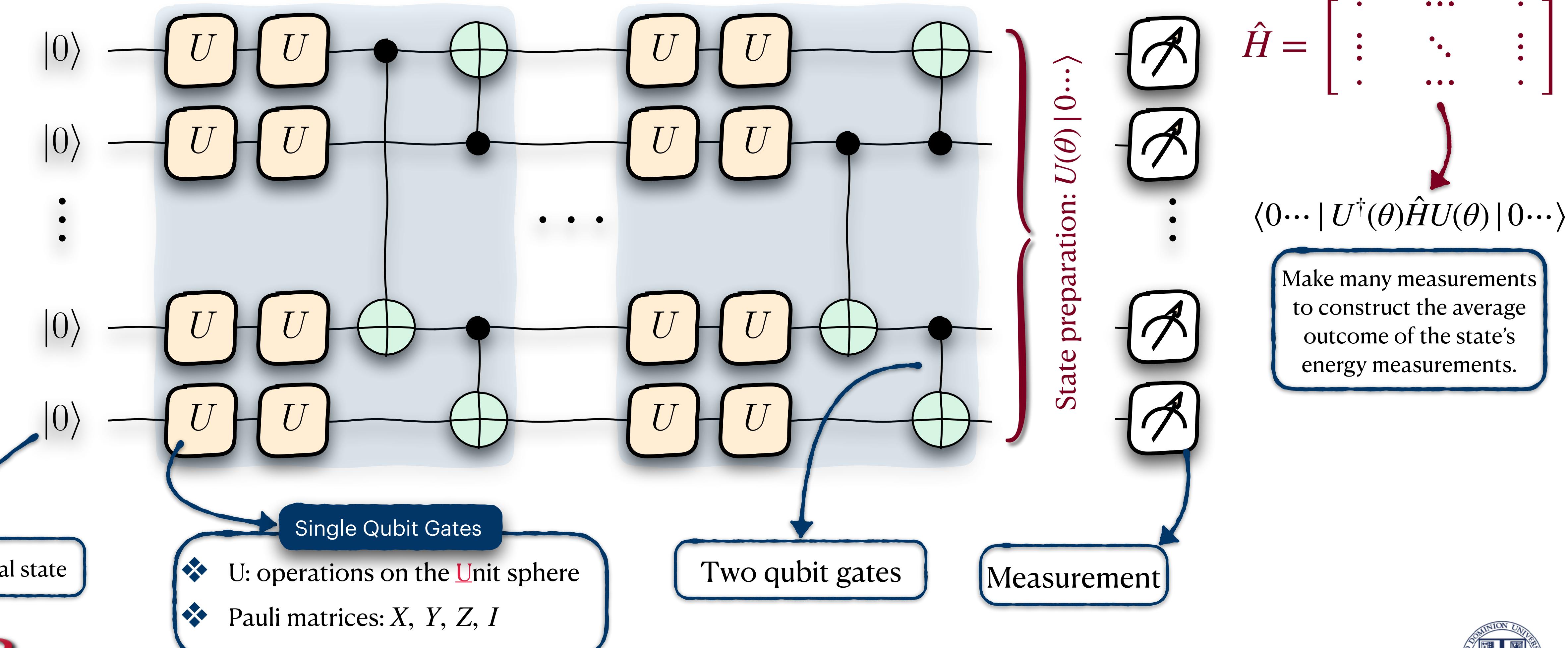
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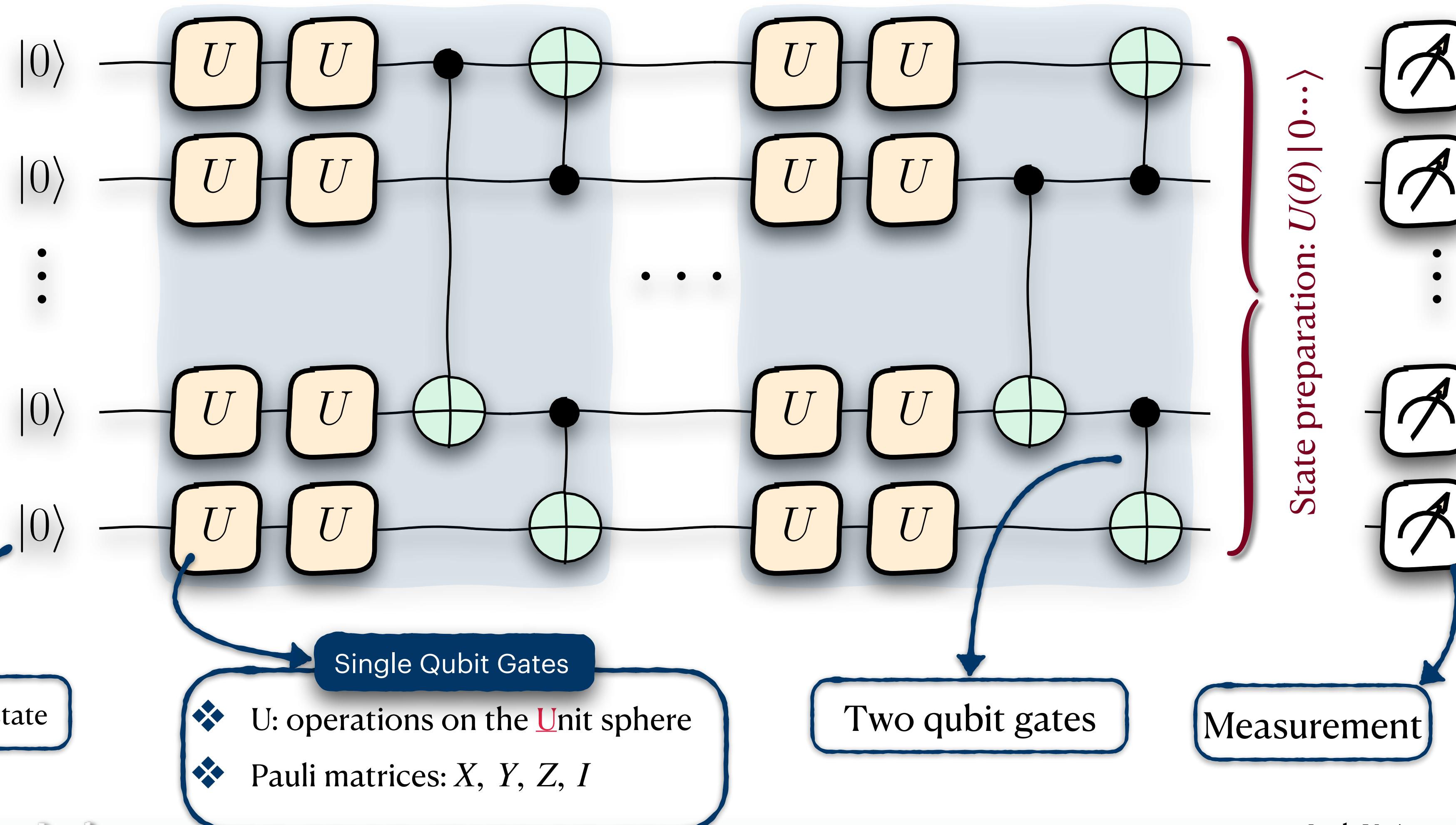
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$$\hat{H} = \begin{bmatrix} \cdot & & & \\ \cdot & \ddots & & \\ \vdots & & \ddots & \\ & & & \ddots \end{bmatrix}$$

$\langle 0\dots | U^\dagger(\theta) \hat{H} U(\theta) | 0\dots \rangle$

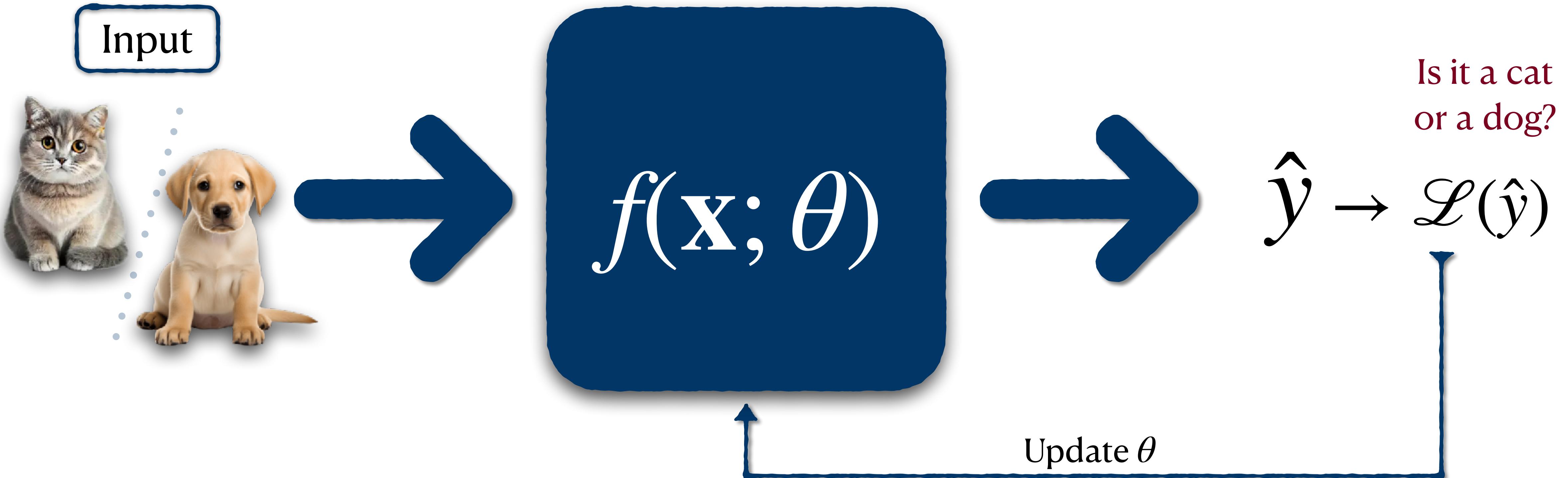
Make many measurements to construct the average outcome of the state's energy measurements.

Further reading:
Nielsen & Chuang;
Quantum Computation & Quantum Information

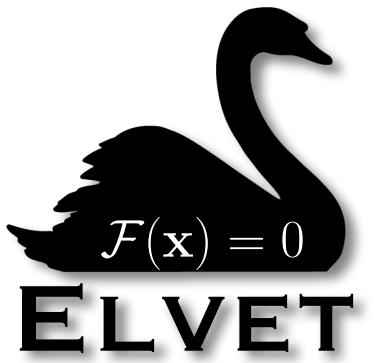
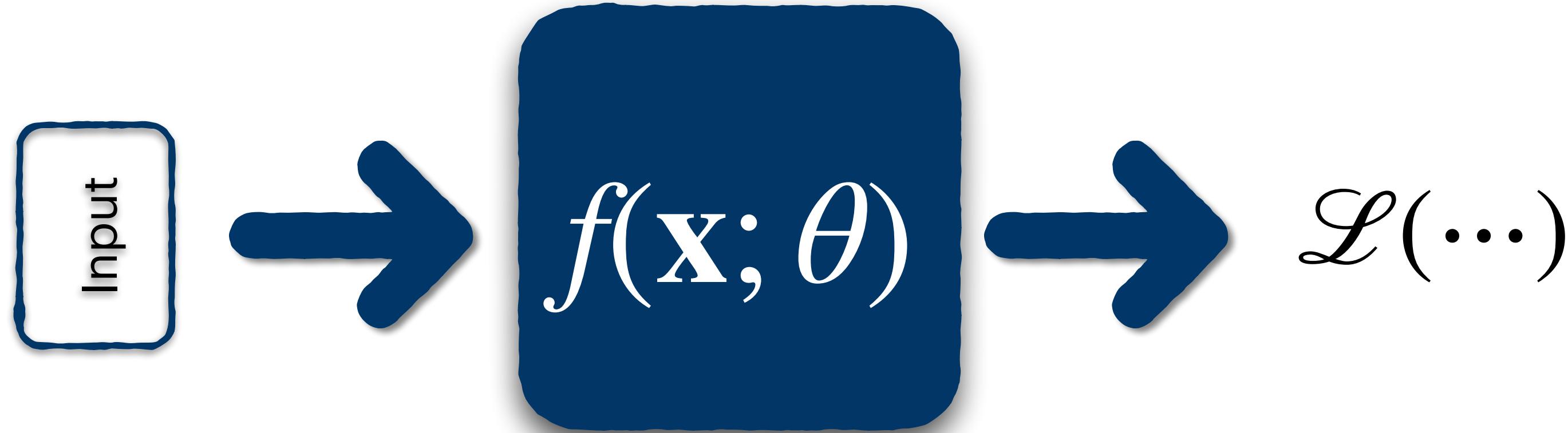
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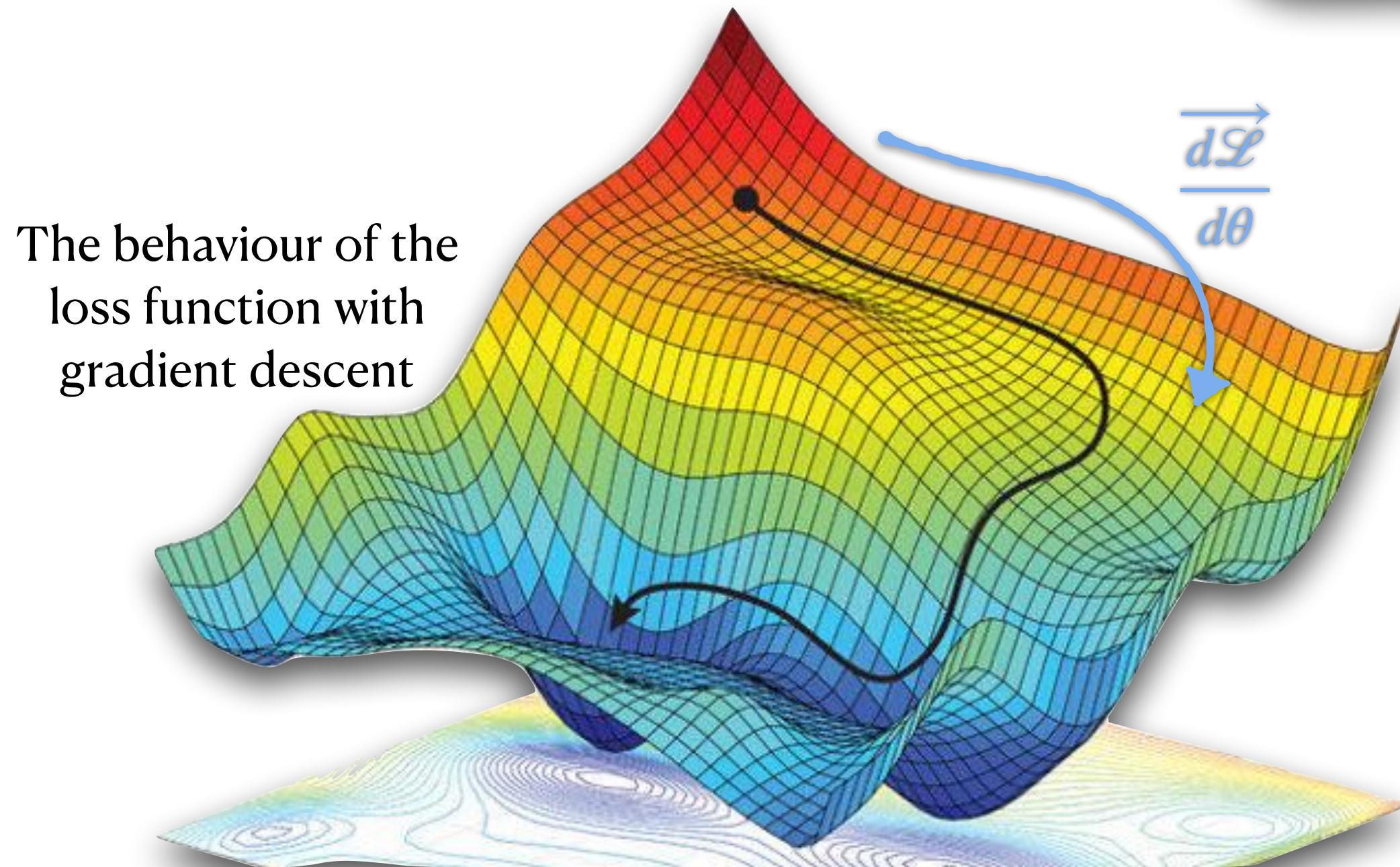
The name of the game is “optimisation”



What is machine learning?



JYA, et al; arXiv: 2103.14575



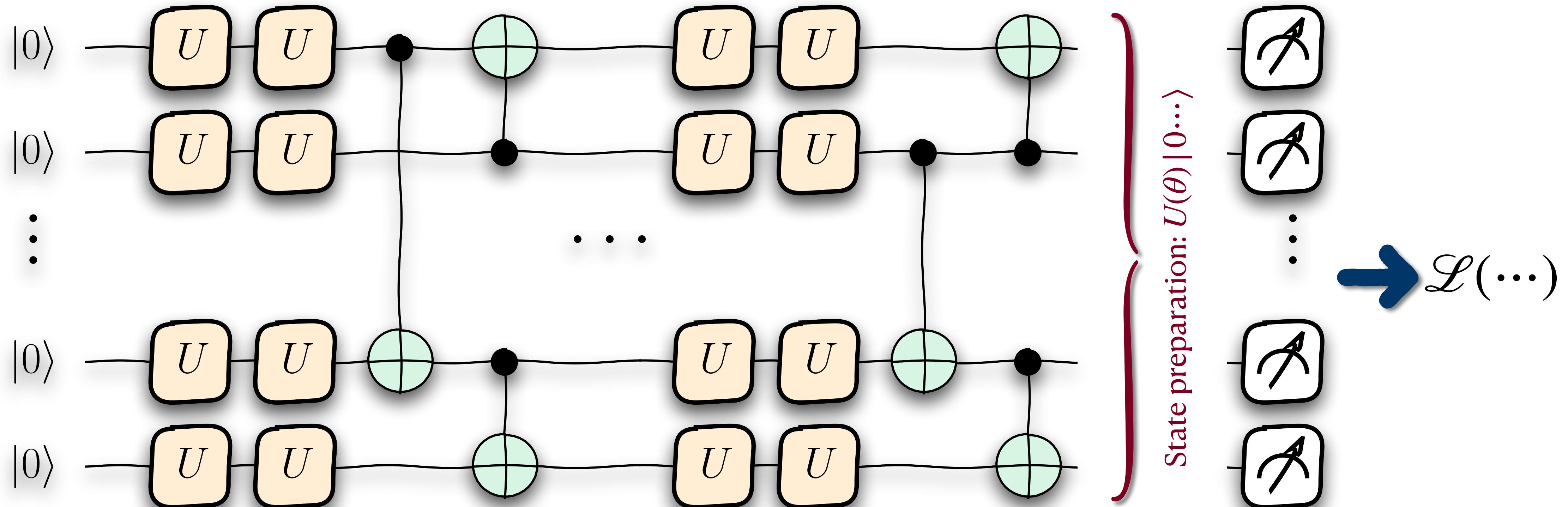
The behaviour of the loss function with gradient descent

Image credit: Francisco Lima

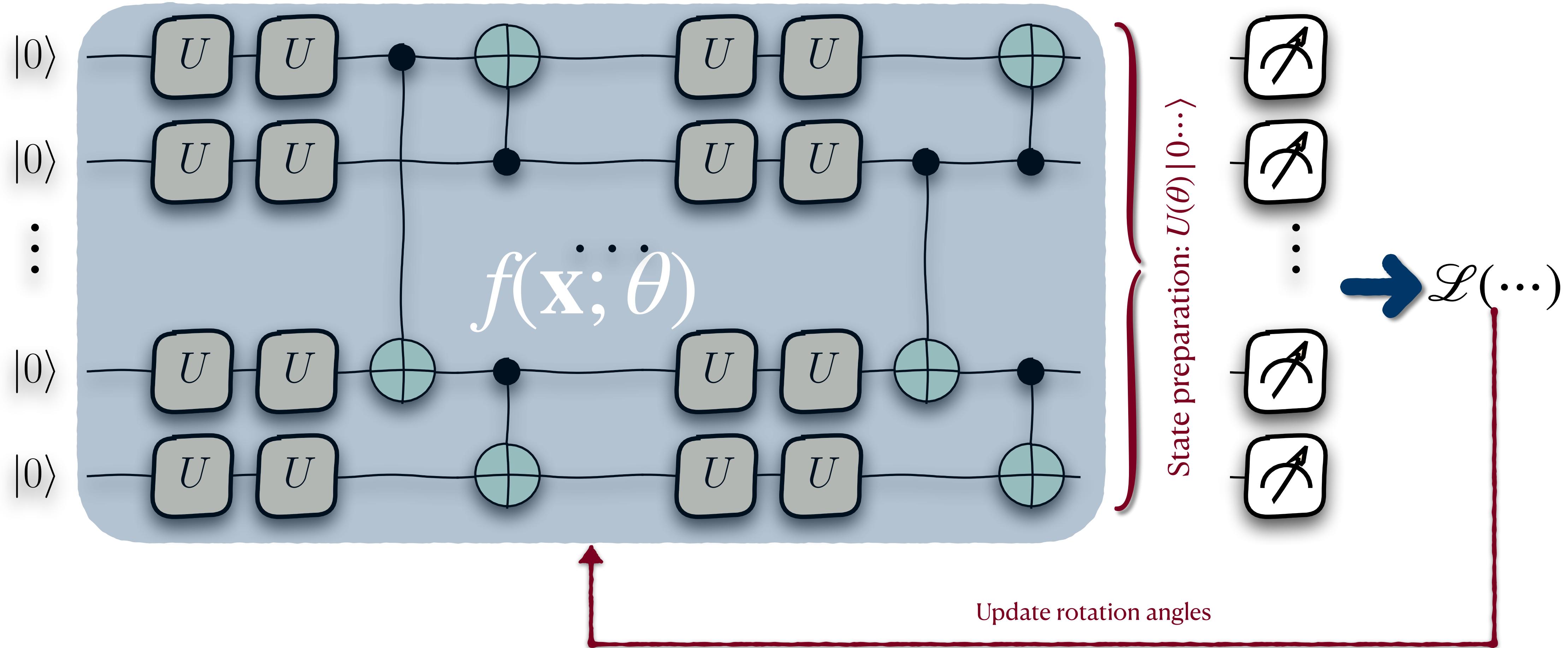
Problem definition
❖ Loss function: cross-entropy, mean squared error or a differential equation.

$$\min_{\theta} \mathcal{L}(\dots)$$

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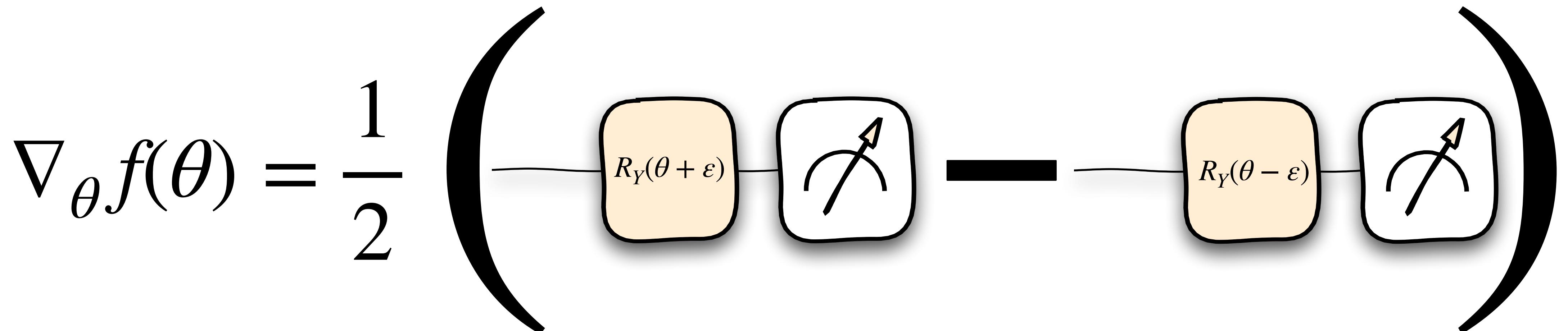


What is the gradient of a quantum circuit?

Quantum computer can not compute gradients!

Parameter Shift

$$\nabla_{\theta} f(\theta) = \frac{1}{2} [f(\theta + \varepsilon) - f(\theta - \varepsilon)]$$



Simulating the Quantum Nature

Simulating the Quantum Nature

- ❖ Condensed matter & quantum many-body systems
 - ❖ Simulating atomic/molecular structure (chemistry)
 - ❖ Understanding the structure of proton (nuclear physics)
- And many more...

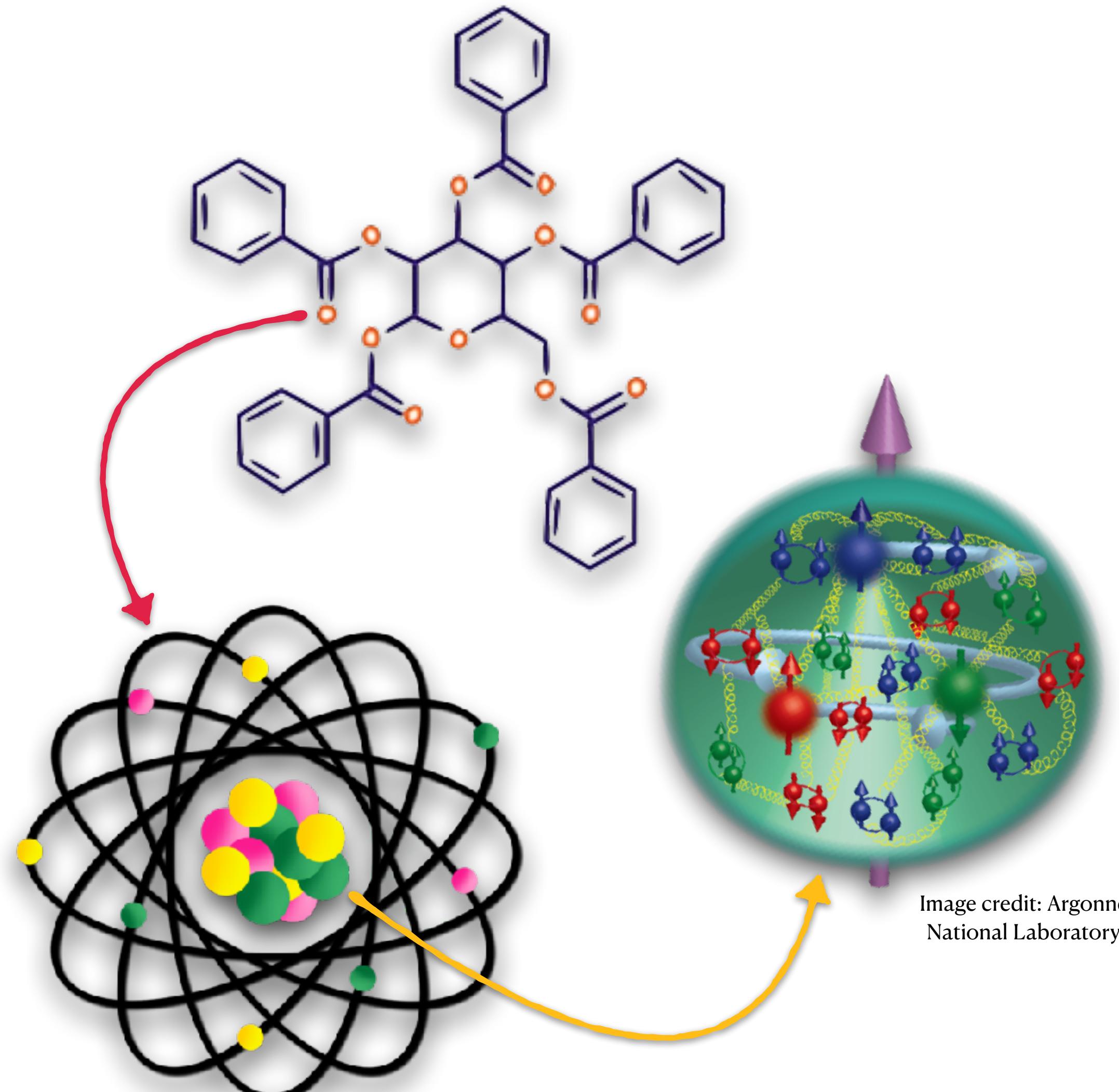


Image credit: Argonne National Laboratory

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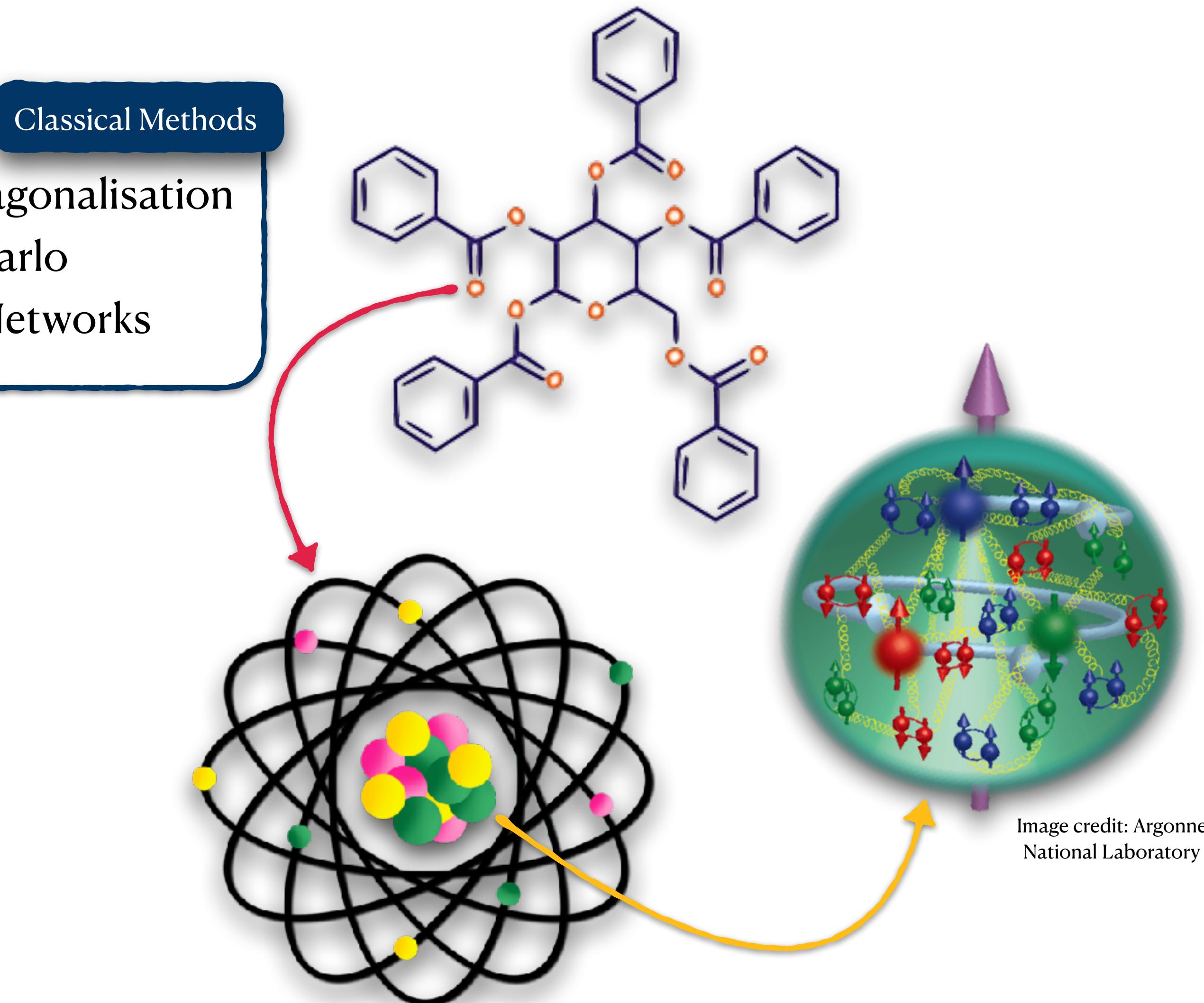
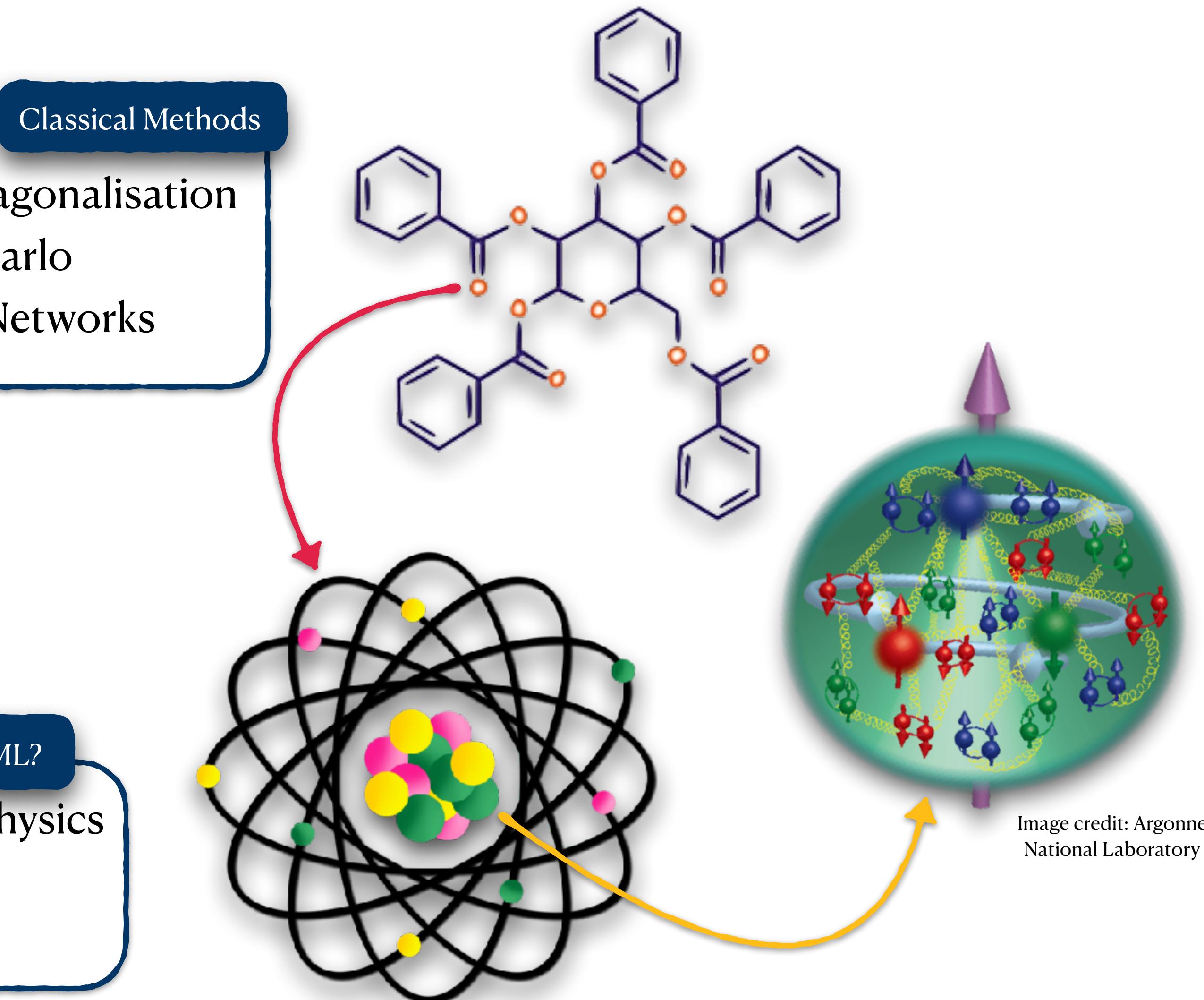


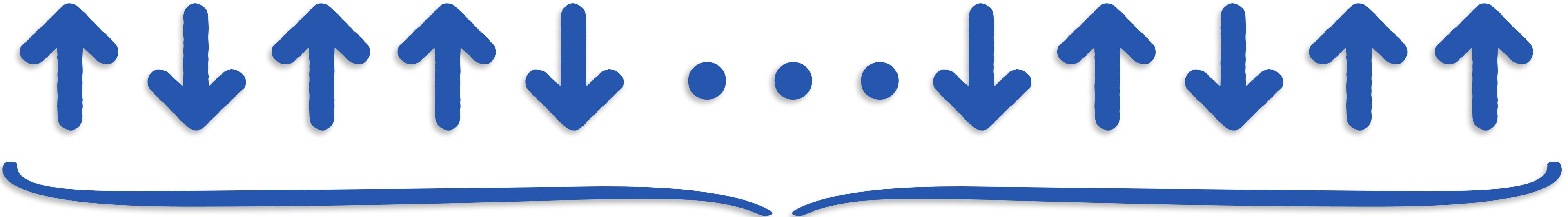
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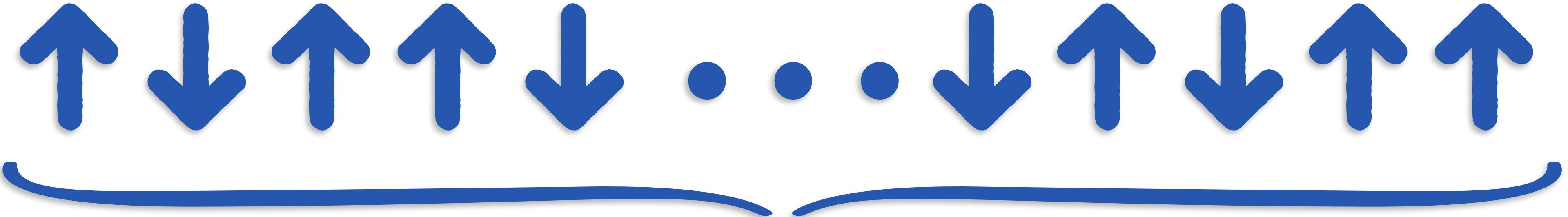
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System of electrons with
spin up or down
What's its natural form?

We can only simulate
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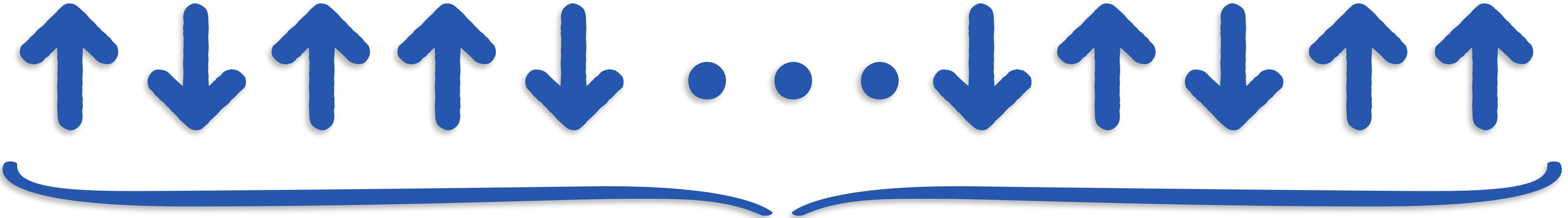
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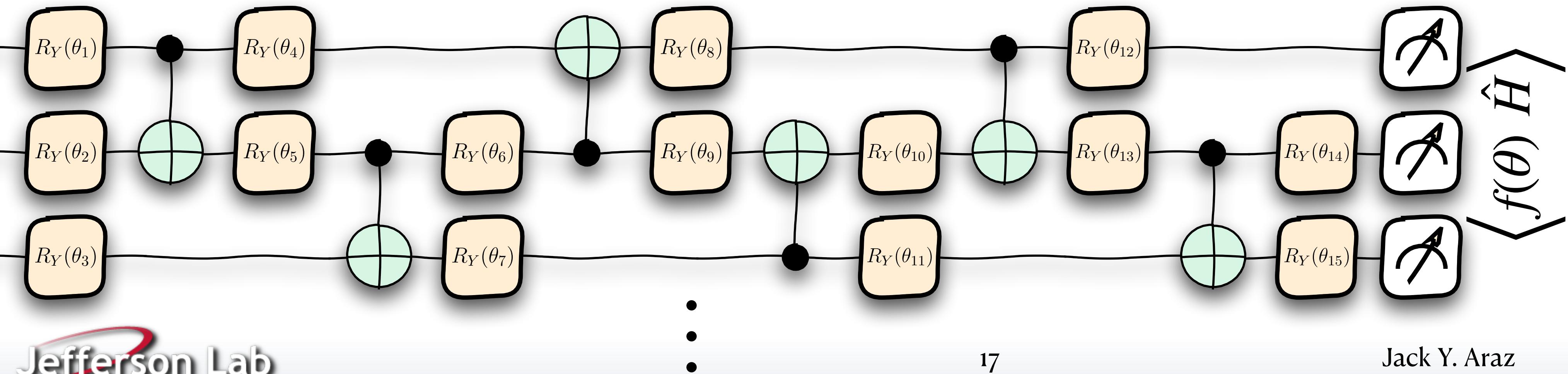
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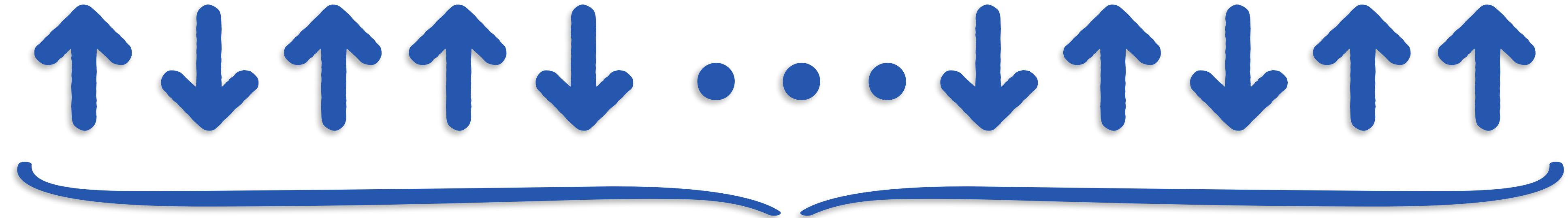
$$\begin{aligned} | \uparrow \rangle &\rightarrow | 1 \rangle \\ | \downarrow \rangle &\rightarrow | 0 \rangle \end{aligned}$$



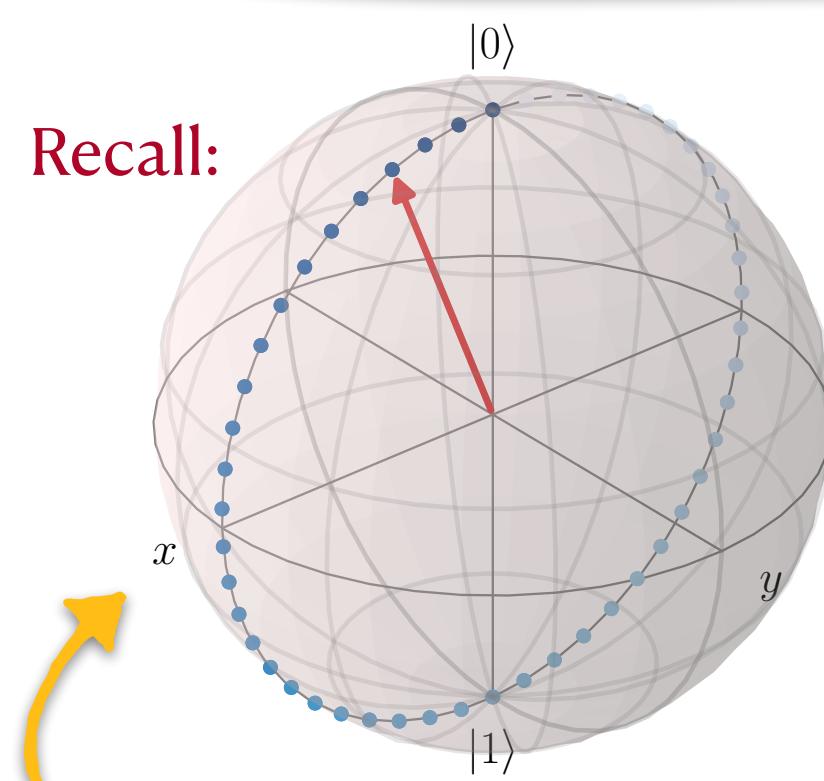
$$\rightarrow \min_{\theta} \langle f(\theta) \hat{H} \rangle$$

The “Hamiltonian”, \hat{H} , describes the dynamics of a quantum system

Simulating the Quantum Nature



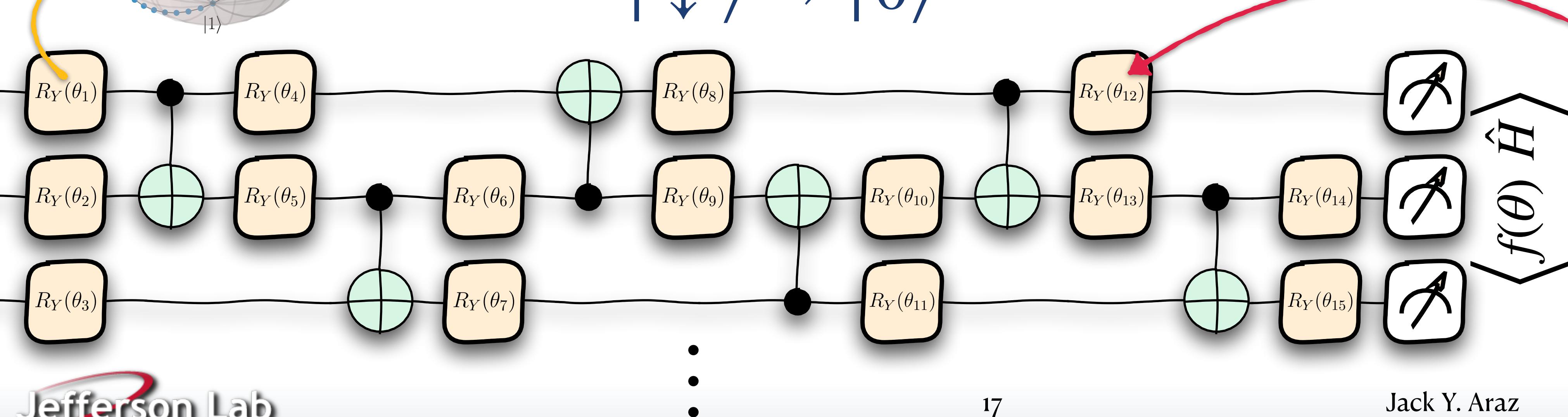
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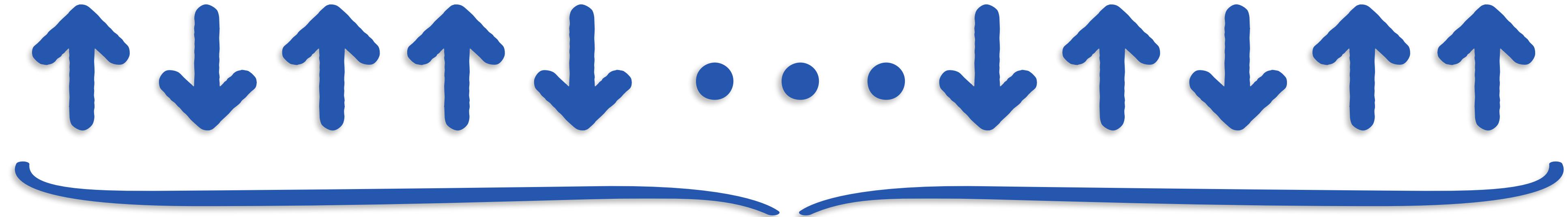
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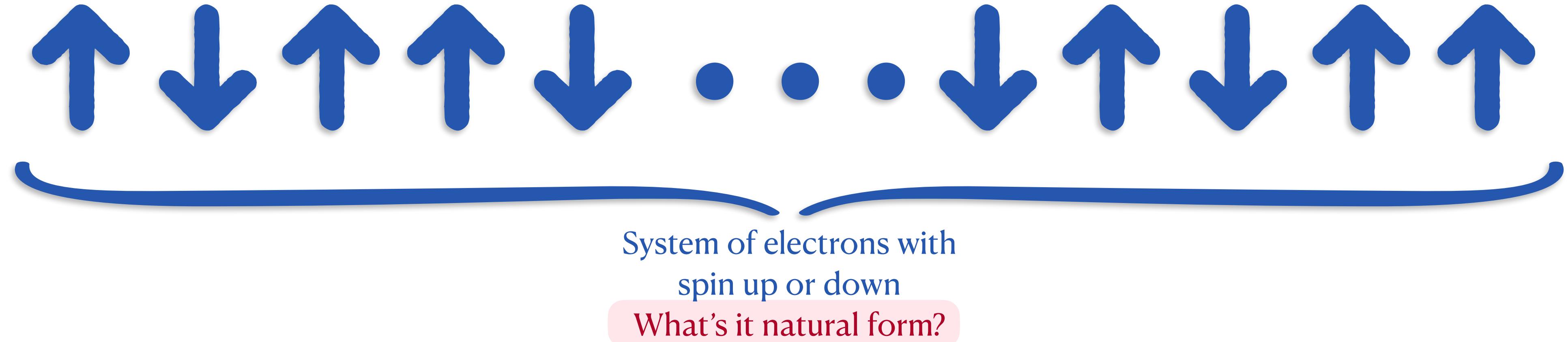
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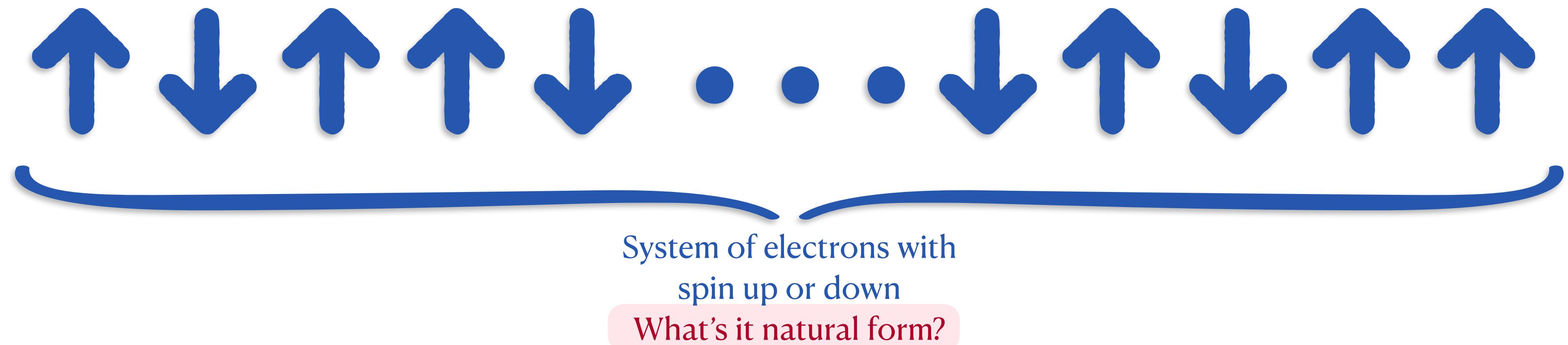
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$$\hat{U}(\theta)|0\rangle = |\psi(\theta)\rangle \rightarrow \langle\psi(\theta)|\hat{H}|\psi(\theta)\rangle \geq \langle\text{gs}|\hat{H}|\text{gs}\rangle$$

Hands-on time!