# Quantum Computation for Nuclear Physics

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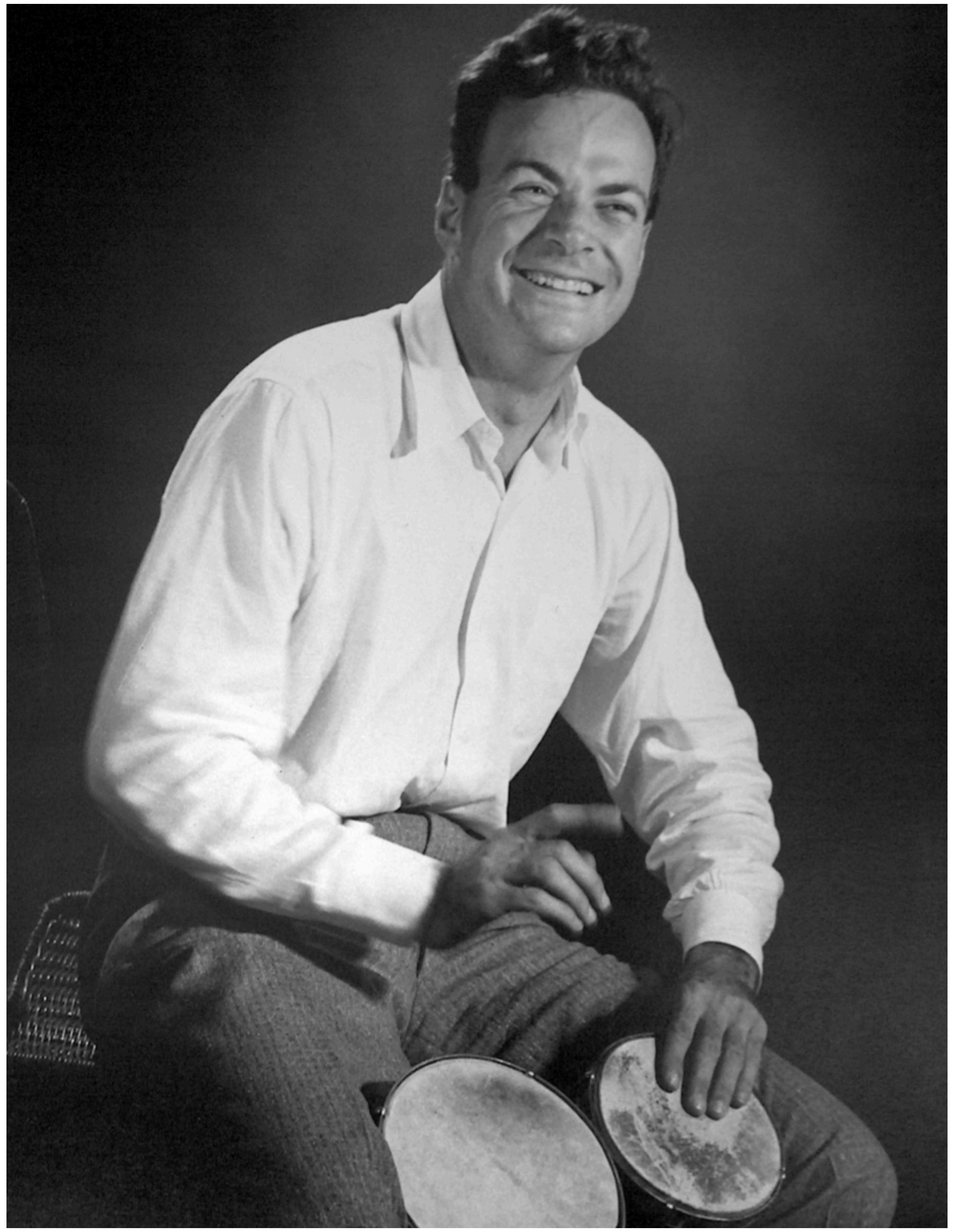
BNL Physics Department Summer Lectures 2020

# What is quantum computation?



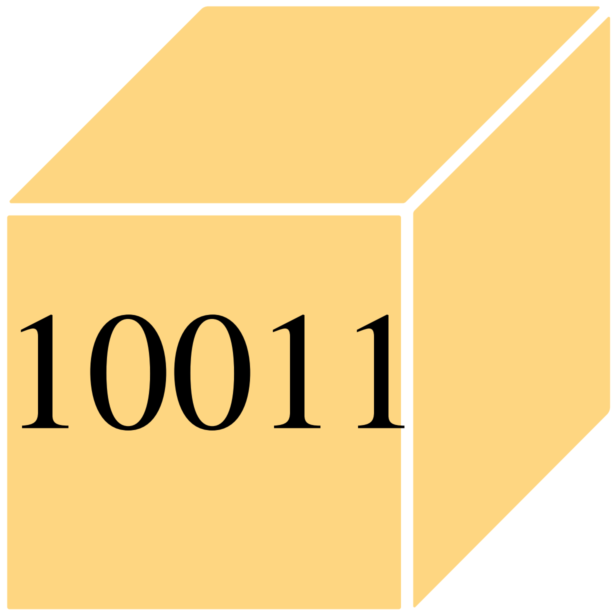
**Richard Feynman (1981)**
"Simulating Physics with Computers"

*"Nature isn't classical*
*... and if you want to make a simulation of Nature,*
*you'd better make it quantum mechanical,*
*and by golly it's a wonderful problem,*
*because it doesn't look so easy."*

*"…What I hoped to do was to design a computer*
*in which I knew how every part worked with everything*
*specified down to the atomic level. In other words I wanted*
*to write down a Hamiltonian for a system that could*
*make a calculation. "*

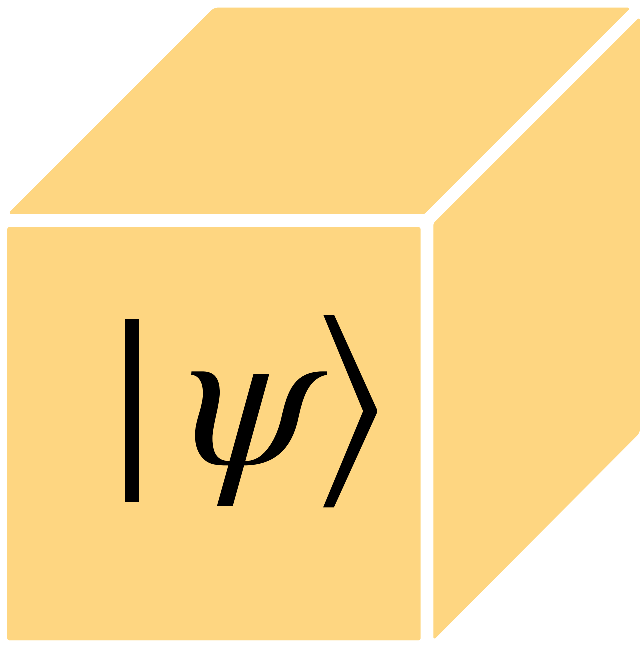
# What is quantum computation?

- **Classical Computers** can efficiently simulate statistical processes, *but not quantum mechanical ones* **— exponential resources!**




$\$ \sim \exp(V)$

- **Unlike Quantum Computers**
  **= Universal Quantum Simulators**

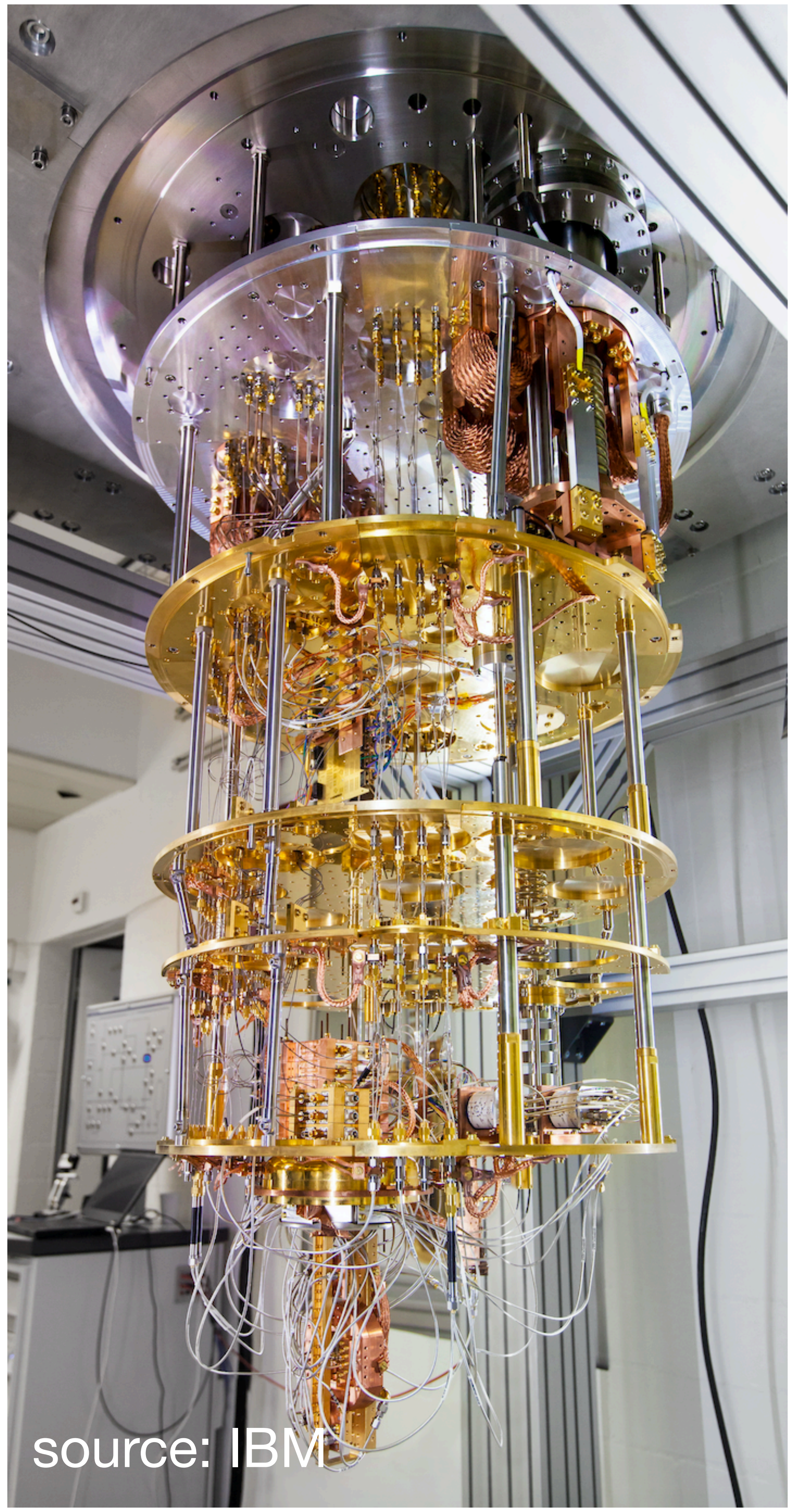


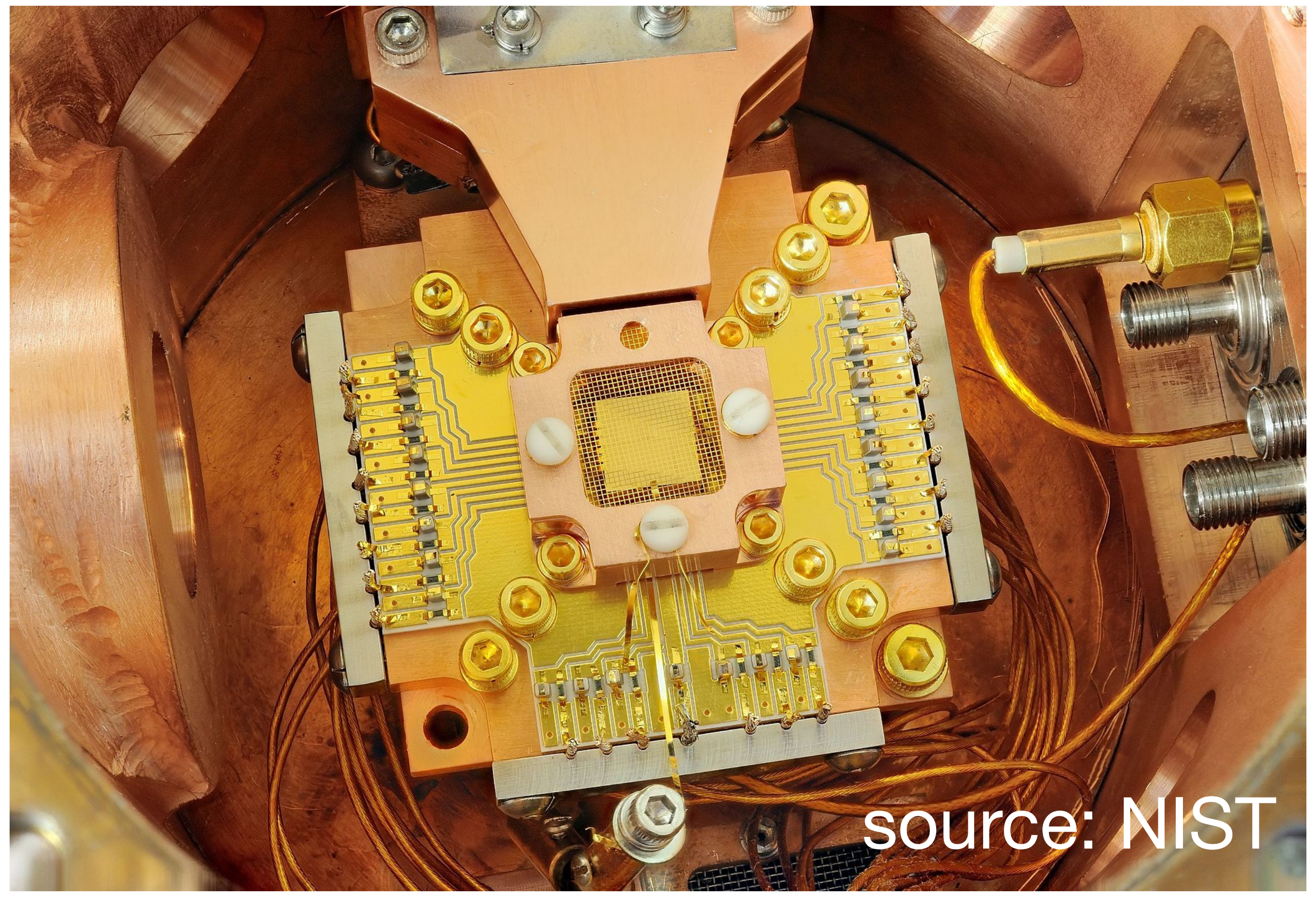

$\$ \sim V$

## Today: A (nuclear) theorists perspective

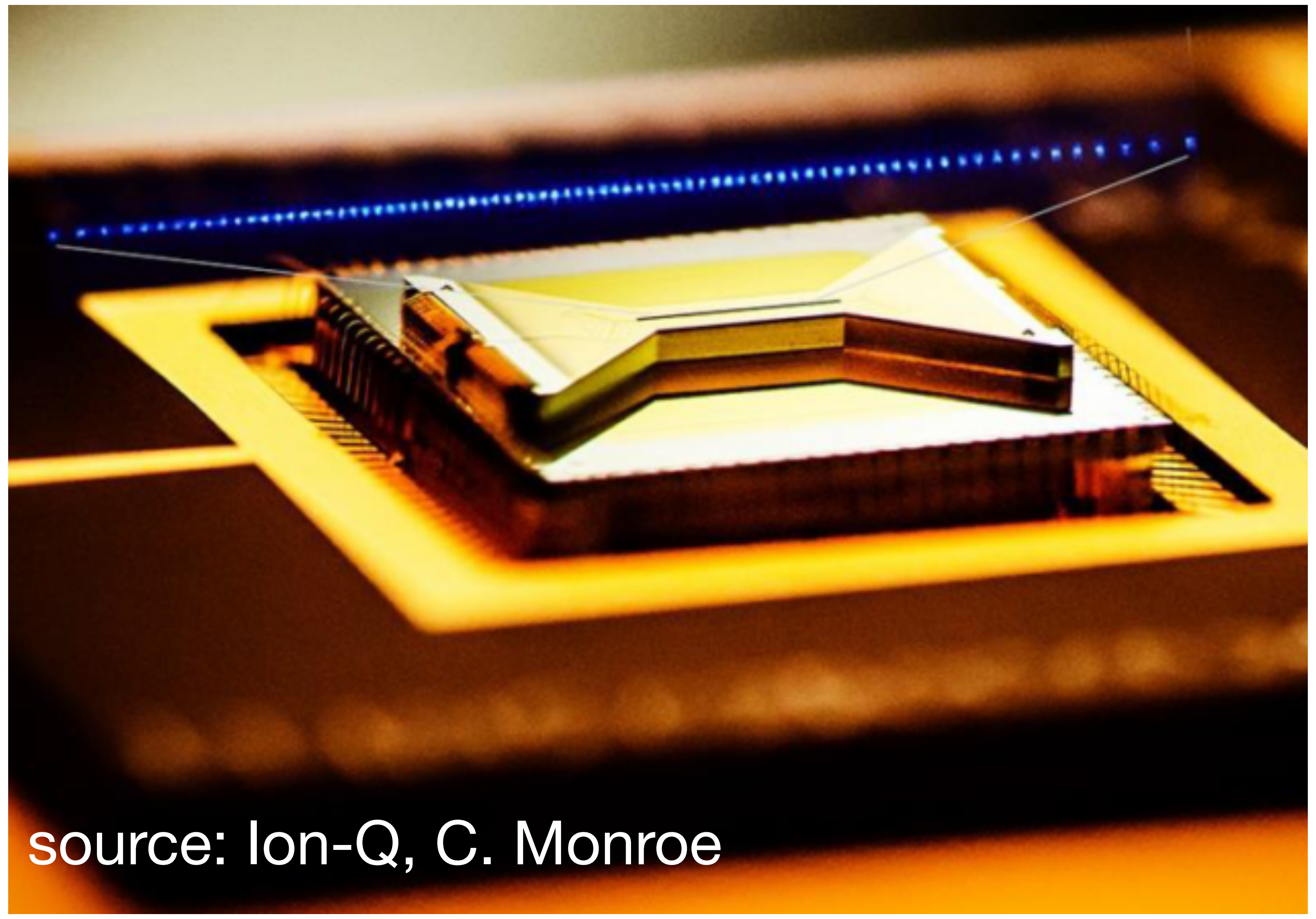
# What is quantum computation?

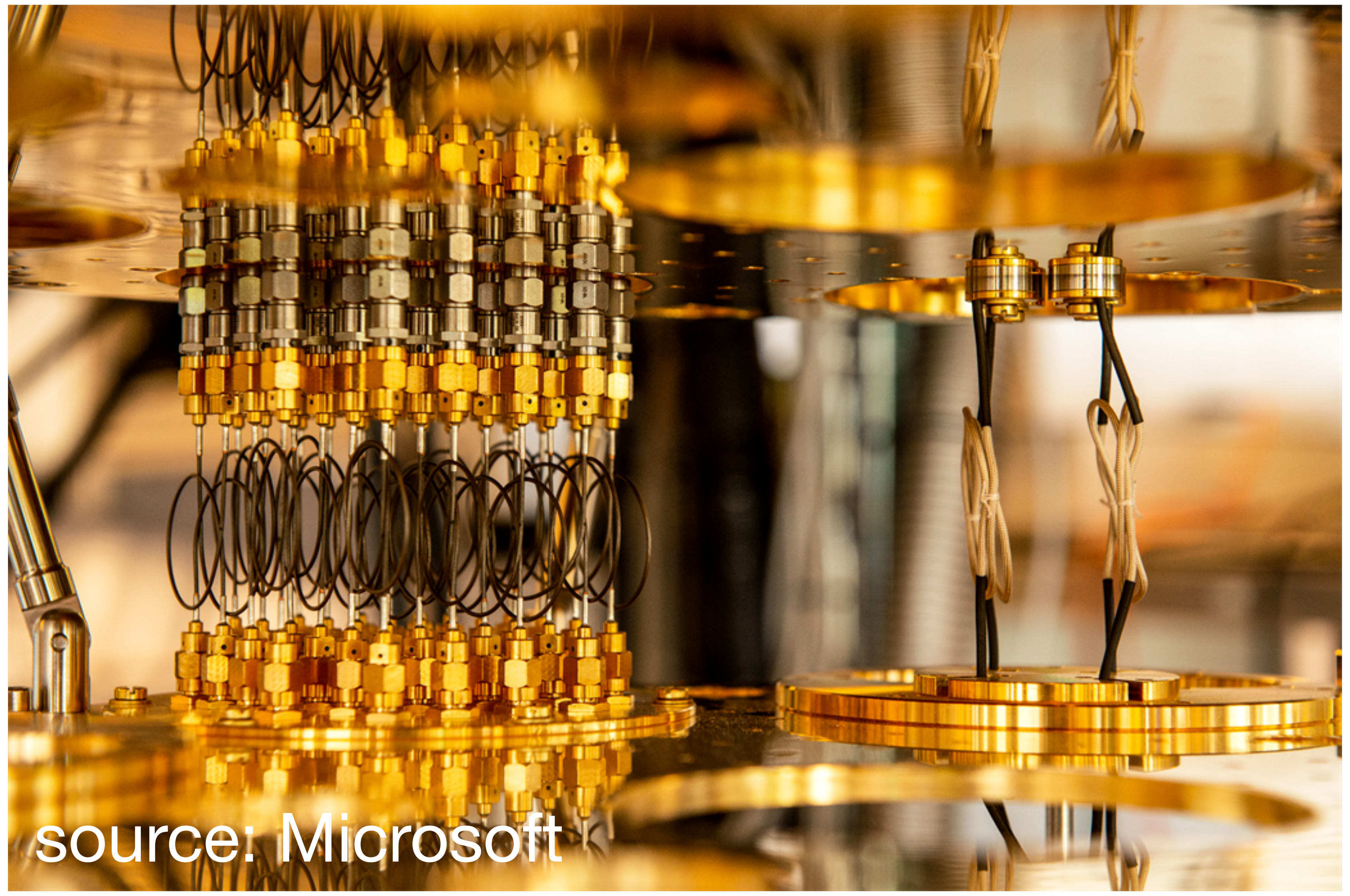
## Digital (universal) Quantum Computers



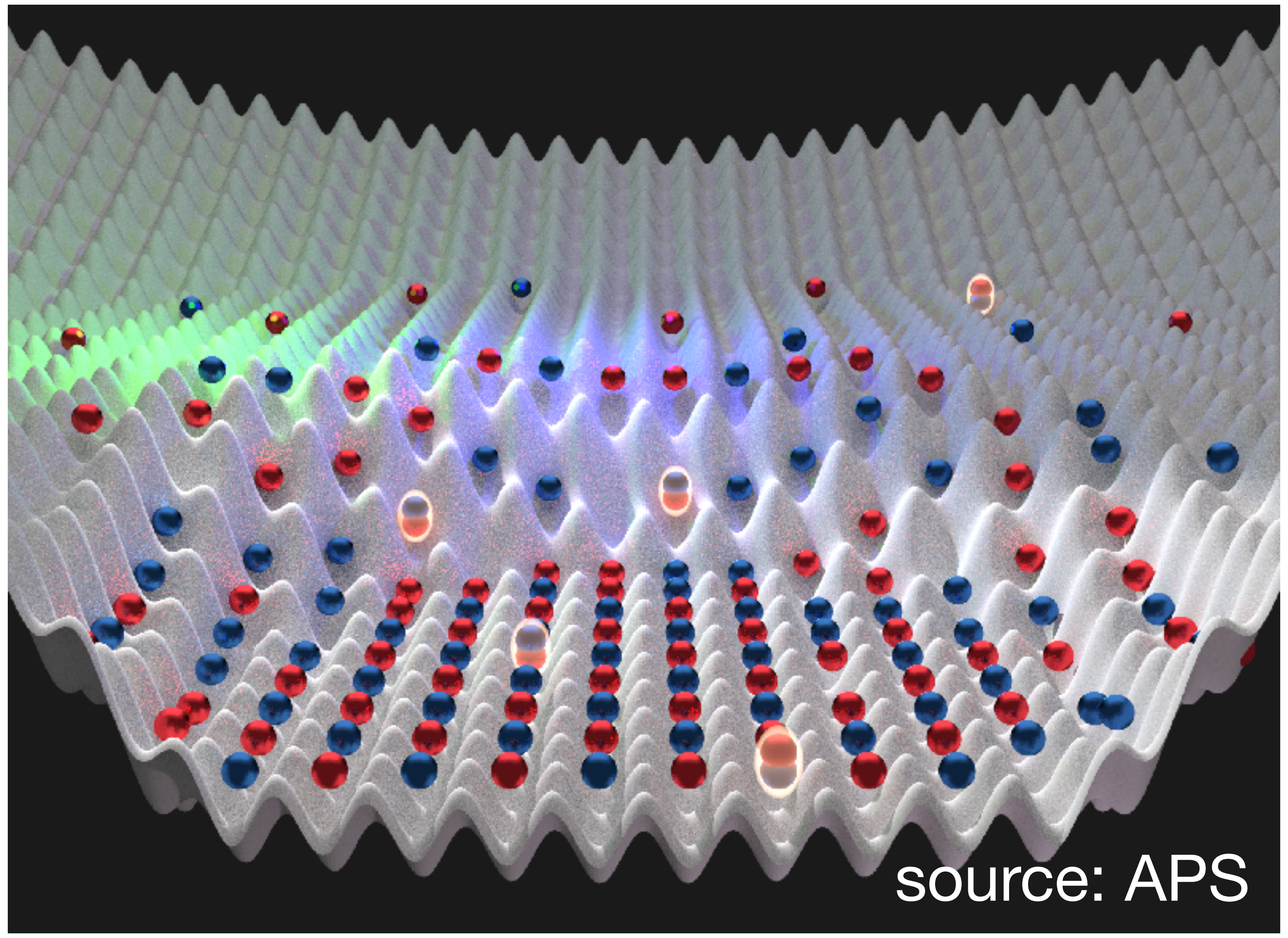




# What is quantum computation?

## Analog (non-universal) Quantum Simulators



source: APS

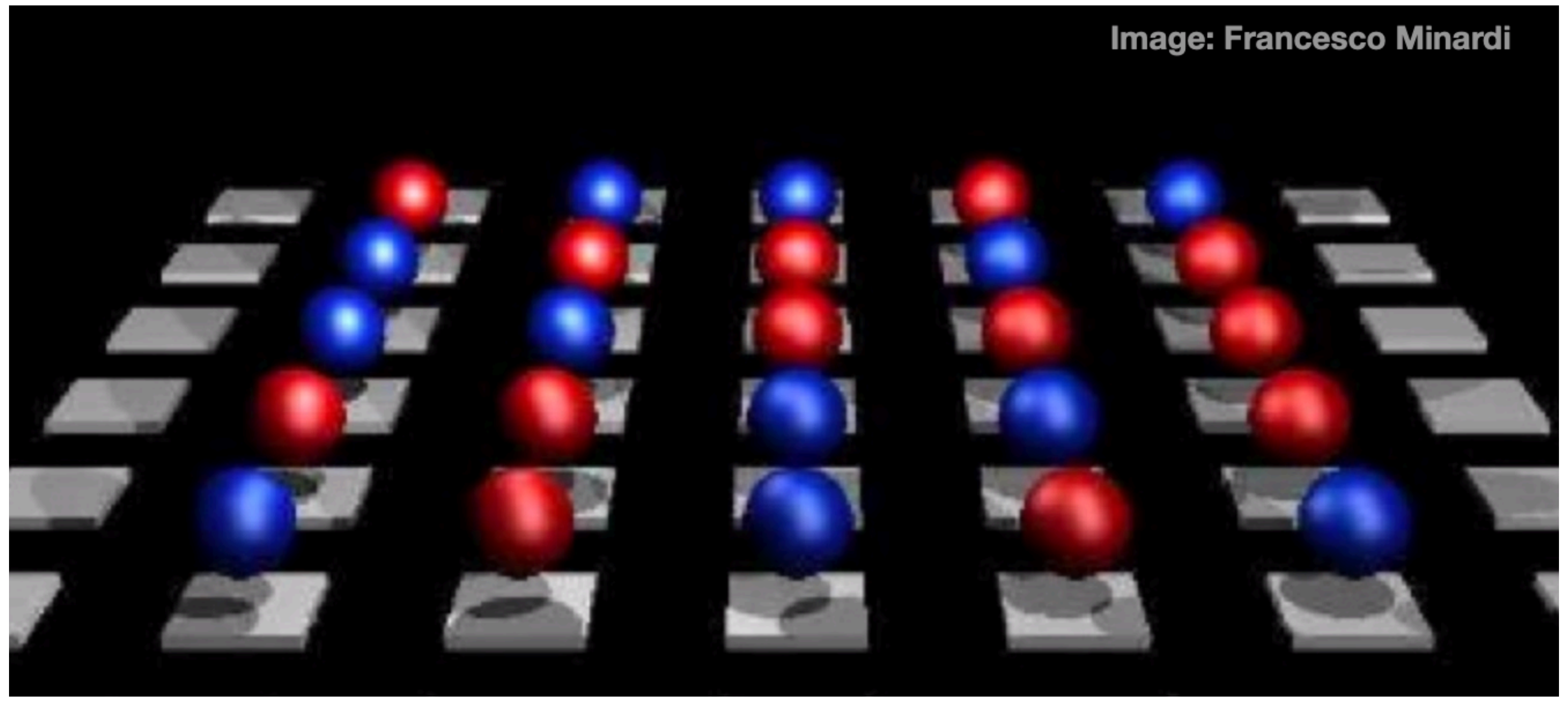
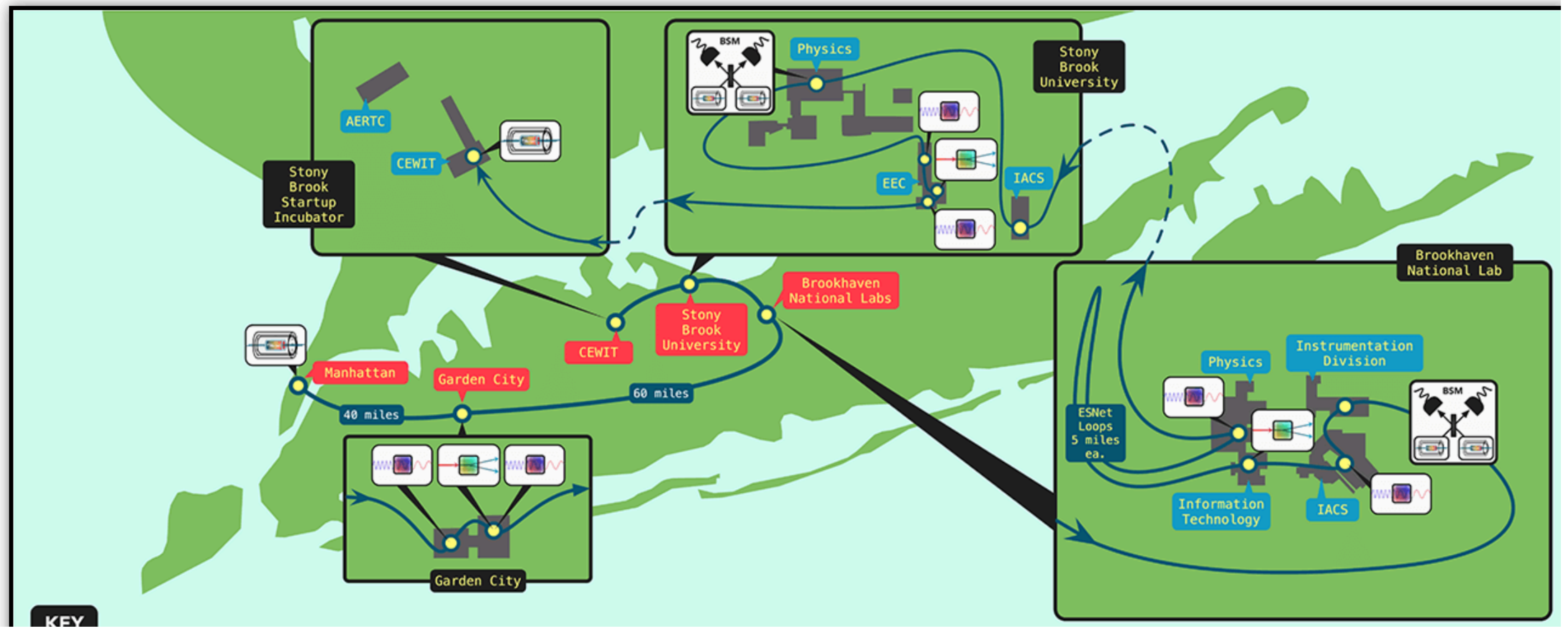


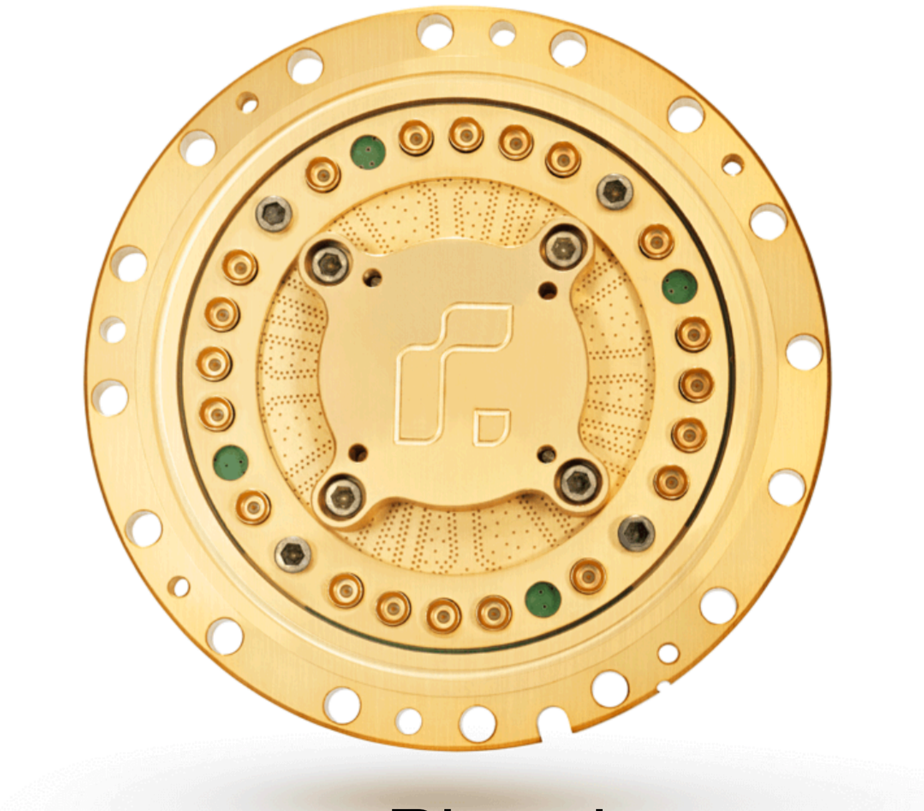
Image: Francesco Minardi

## Quantum Communication and Cryptography




source: Figuera group, BNL

## Quantum Annealing



source: Rigetti

+ much more!

# Current Status

Quantum Computers just learned to walk



*Scott Adams/Dilbert*

Noisy Intermediate-Scale Quantum (NISQ) technology

Impressive Progress in recent years!

# Resources

- https://www.bnl.gov/science/quantum.php

BROOKHAVEN NATIONAL LABORATORY Quantum Information Science and Technology

- https://www.bnl.gov/physics/NTG/

BROOKHAVEN NATIONAL LABORATORY *Nuclear Theory Group*

- https://www.bnl.gov/compsci/quantum/

BROOKHAVEN NATIONAL LABORATORY *Computational Science Initiative*

- Books, e.g. *“Quantum Computation and Quantum Information”*, Nielsen & Chuang

- Webpages of the big players, e.g. Department of Energy, Google, IBM, Ion-Q, Microsoft, NIST, Rigetti etc.

email me: **nmueller@bnl.gov**
visit: **https://www.bnl.gov/physics/NTG/people/mueller.php**

# Outline of this lecture

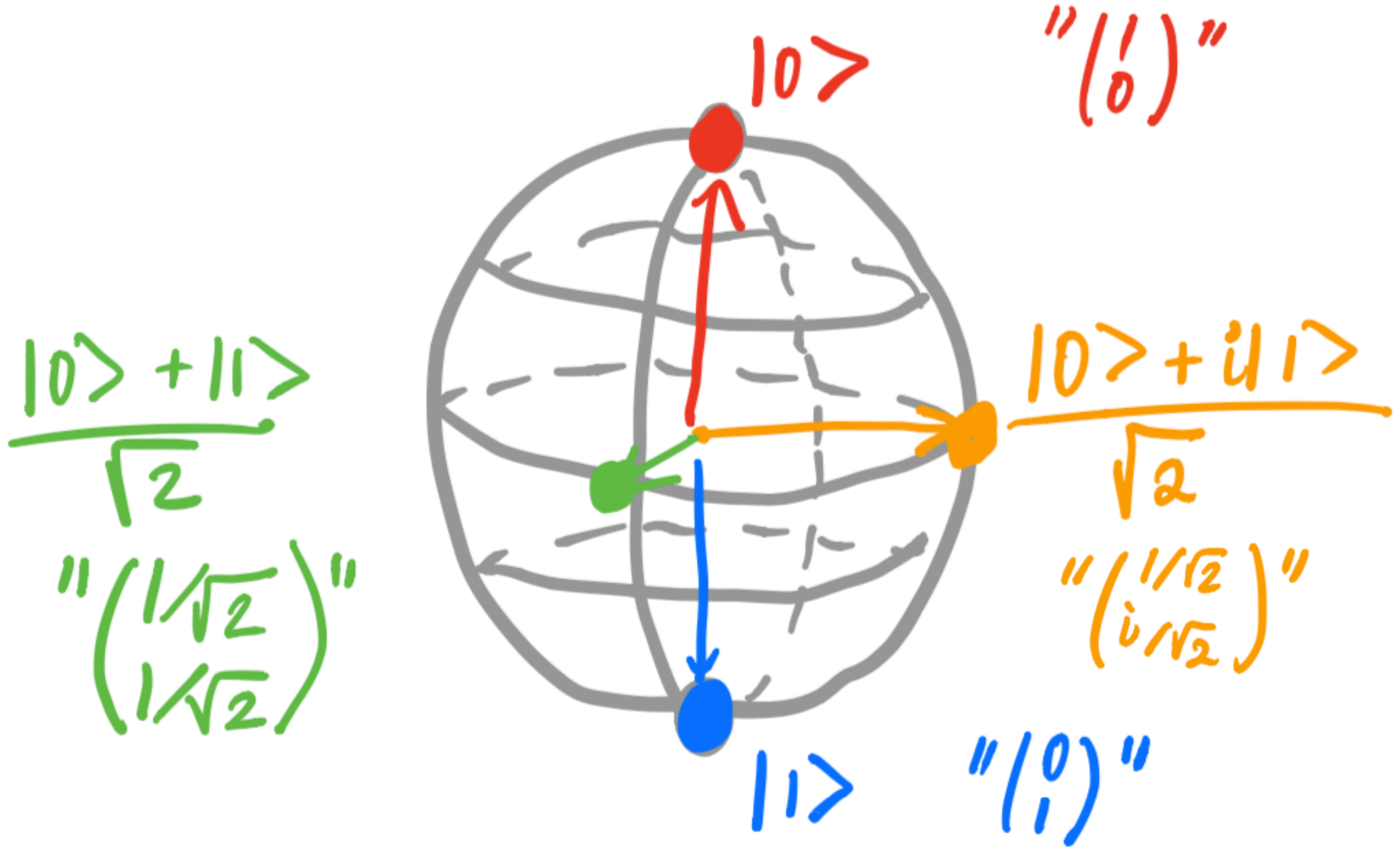
1. Basics - Quantum 101
2. Quantum Computing (Nuclear) Physics
3. How to do it?
4. New Ideas

# Basics - Quantum 101

- **Qubit = spin 1/2**


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

$a\,|\,0\rangle + b\,|\,1\rangle$




- **Hilbert space** $\mathscr{H} = \text{span}(\,|\,0\rangle, |\,1\rangle)$

- **Many qubits, big Hilbert space** $\mathscr{H}' = \mathscr{H} \otimes \mathscr{H} \ldots \otimes \mathscr{H}$

$$\big(a_0\,|\,0\rangle + b_0\,|\,1\rangle\big) \otimes \big(a_1\,|\,0\rangle + b_1\,|\,1\rangle\big) = a_0a_1\,|\,00\rangle + a_0b_1\,|\,01\rangle + b_0a_1\,|\,10\rangle + b_0b_1\,|\,11\rangle$$

$$\begin{pmatrix}a_0\\b_0\end{pmatrix} \otimes \begin{pmatrix}a_1\\b_1\end{pmatrix} = \begin{pmatrix}a_0a_1\\a_0b_1\\b_0a_1\\b_1a_1\end{pmatrix}$$

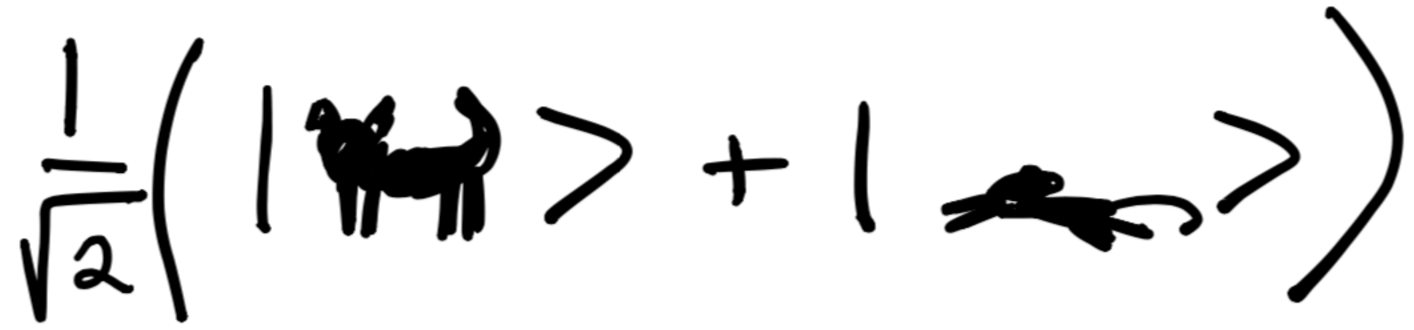
Size of this vector grows exponentially $2^N$
with quantum mechanical degrees of freedom

# Basics - Quantum 101

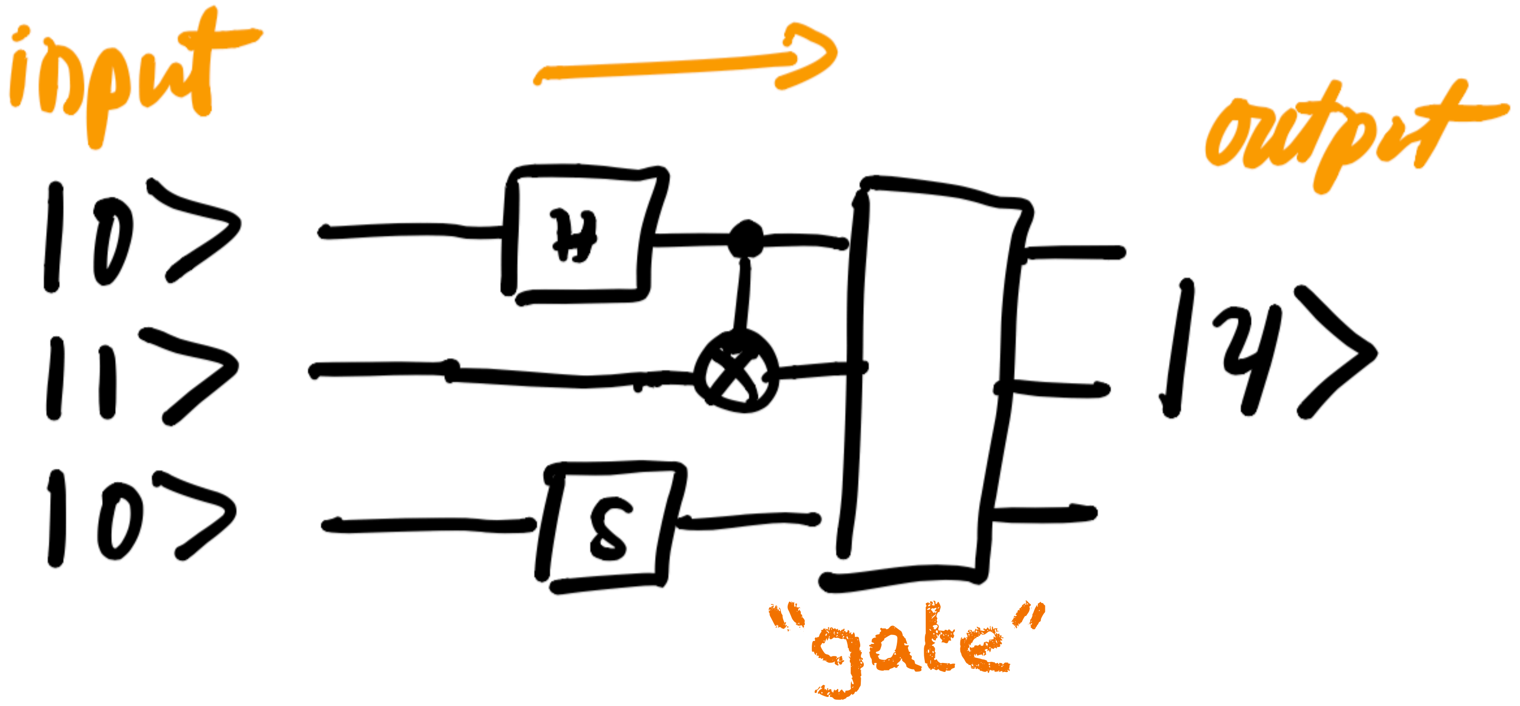
- **Information can be encoded** $|001001110\rangle$

- **Power of quantum: superposition of information**

$$\frac{1}{\sqrt{2}}\Big(|001001110\rangle + |110001111\rangle\Big)$$



- **Information processing via quantum circuit** $|001001110\rangle \to |111101110\rangle$




classically, think "matrix multiplication"
(matrix size grows exponential)

$$\begin{pmatrix}0\\1\end{pmatrix} = M\begin{pmatrix}1\\0\end{pmatrix}$$ (M unitary)

- **Quantum parallelism** $x = 001001110, \quad f(x)?$

$$\frac{1}{\sqrt{2}}\Big(|001001110\rangle + |111001111\rangle\Big) \to \frac{1}{\sqrt{2}}\Big(|101110010\rangle + |000110001\rangle\Big)$$

# Basics - Quantum 101

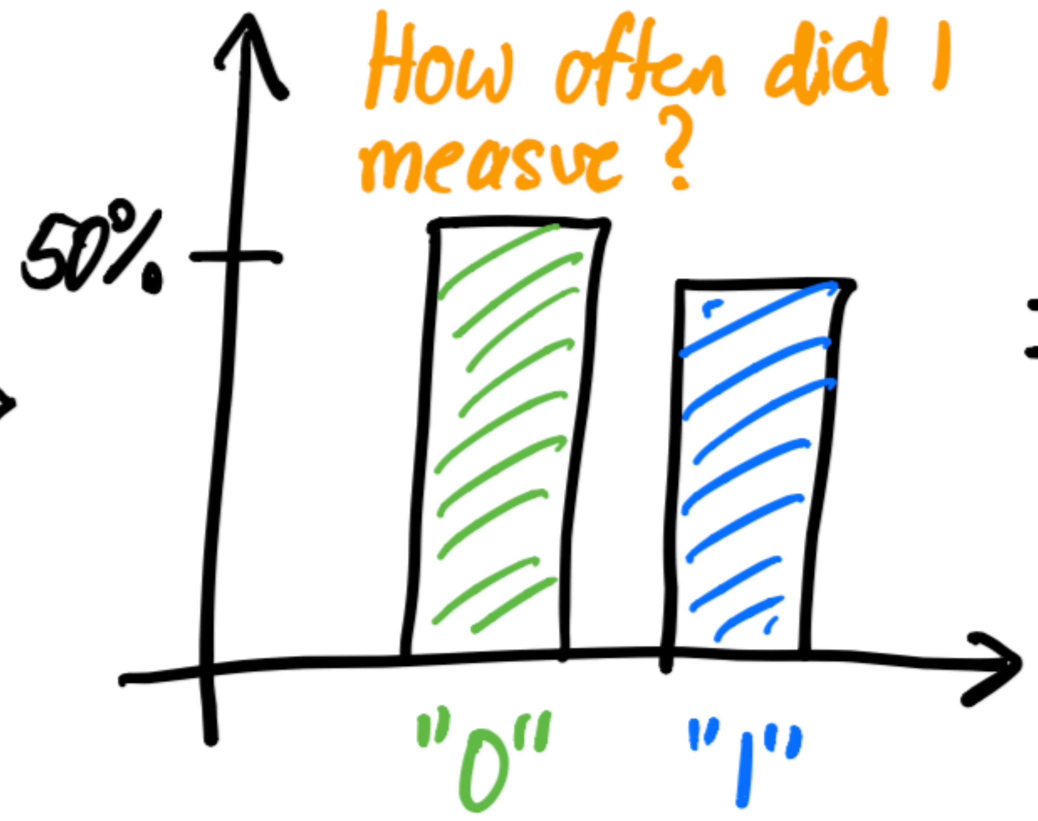
- Information can be **entangled** $$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(\,|01\rangle + |10\rangle\Big)$$

- **Entanglement** is a resource in Quantum Information Science!

- Quantum Mechanics: Extract Information via **Measurement**

Compute

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




$\Rightarrow$ we loose information

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

or $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ ?

- **Extracting** answer from Quantum Computer: subtile issue

# Quantum Computation for Physics

## Challenges

- **Quantum-Many Body systems**

$= |\psi\rangle = |p\rangle \otimes |n\rangle \otimes |p\rangle \cdots |p\rangle$

size of Hilbert space $s^N$ (Gold $N = 197$)

- **Many degrees of freedom, exponentially large Hilbert space**

$$i\hbar\partial_t |\psi\rangle = H|\psi\rangle \qquad H = \sum_i \frac{\hat{p}^2}{2m} + \sum_{ij} V_{ij} + \sum_{ijk} V_{ijk} + \ldots$$

(Hamiltonian operator)

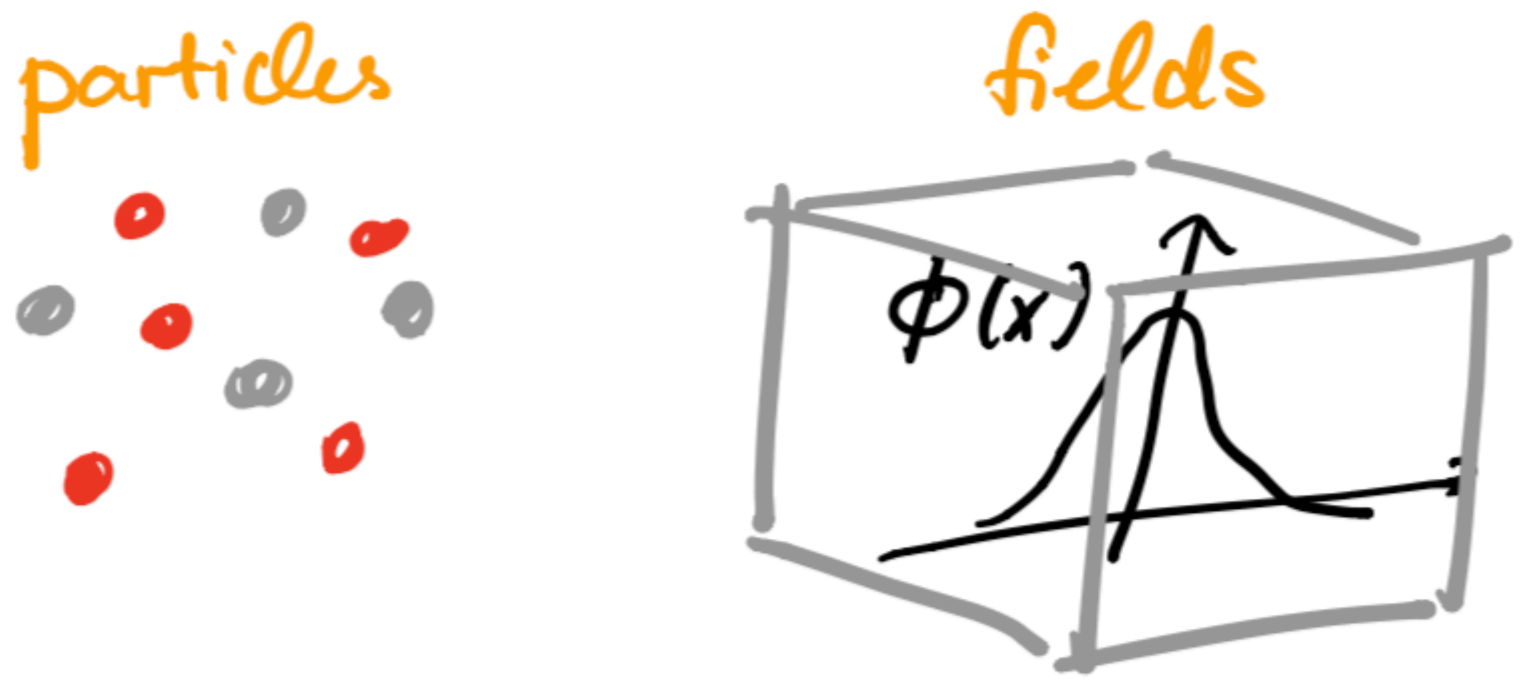
- Assuming $|n\rangle$ and $|p\rangle$ each had 2 states, **Schroedinger equation for Gold = matrix equation of size** $2^{197} \sim 10^{59}$

  (earth consists of ~ $10^{50}$ atoms, yet only 197 qubits enough to represent Hilbert space of Gold)

# Quantum Computation for Physics

## Challenges

- **Quantum Many-Body Theory → Quantum Field Theory**

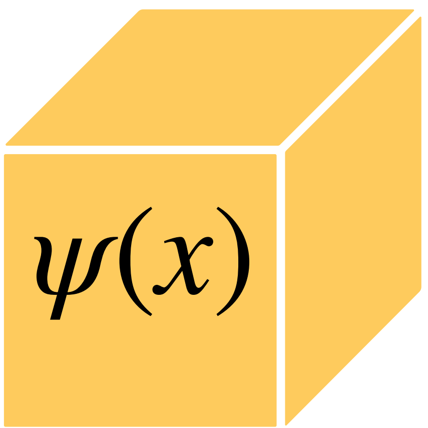



- **Example (Quantum) Electrodynamics**

$$H = \int d^3x \left\{ \frac{E^2(x)}{2} + \frac{B(x)^2}{2} + \psi^\dagger(x)\gamma^0(i\gamma \cdot \nabla + m)\psi(x) \right\}$$

- **Every $x$ labels one quantum mechanical degree of freedom.**

Infinitely many dof's in any volume V!

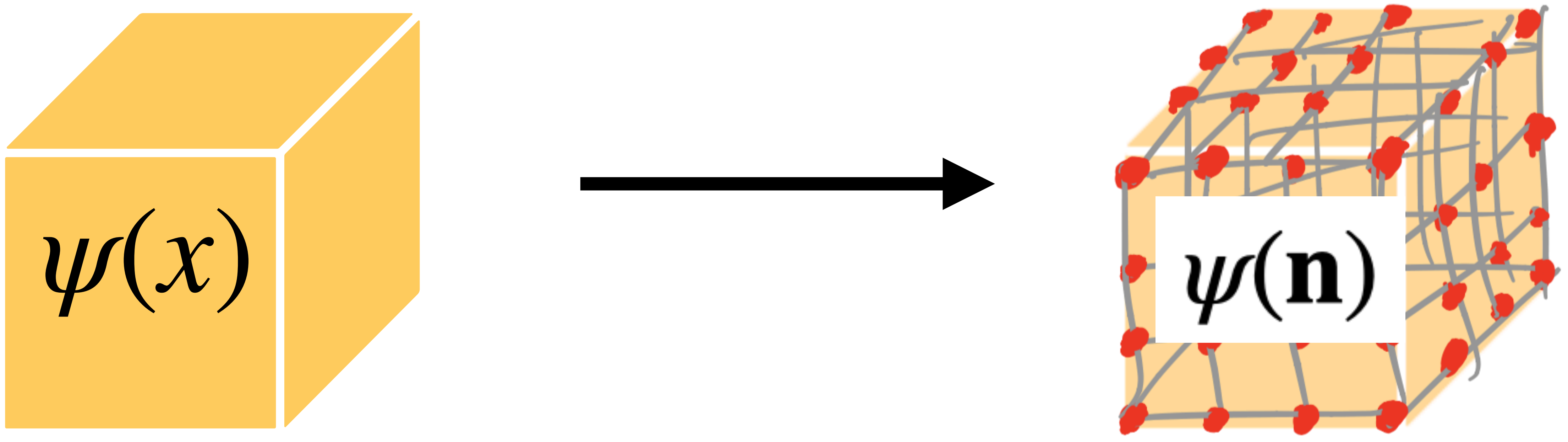



$\Psi$ "Heisenberg field operator"

# Quantum Computation for Physics

## Challenges

- **Quantum Field Theory→ <u>Lattice</u> Quantum Field Theory**




$$\mathbf{x} = \mathbf{n}a_s \qquad \mathbf{n} = (n_x, n_y, n_y)$$

- **Lattice Quantum Field Theory ~ Quantum Many Body Theory**

# Quantum Computation for Physics

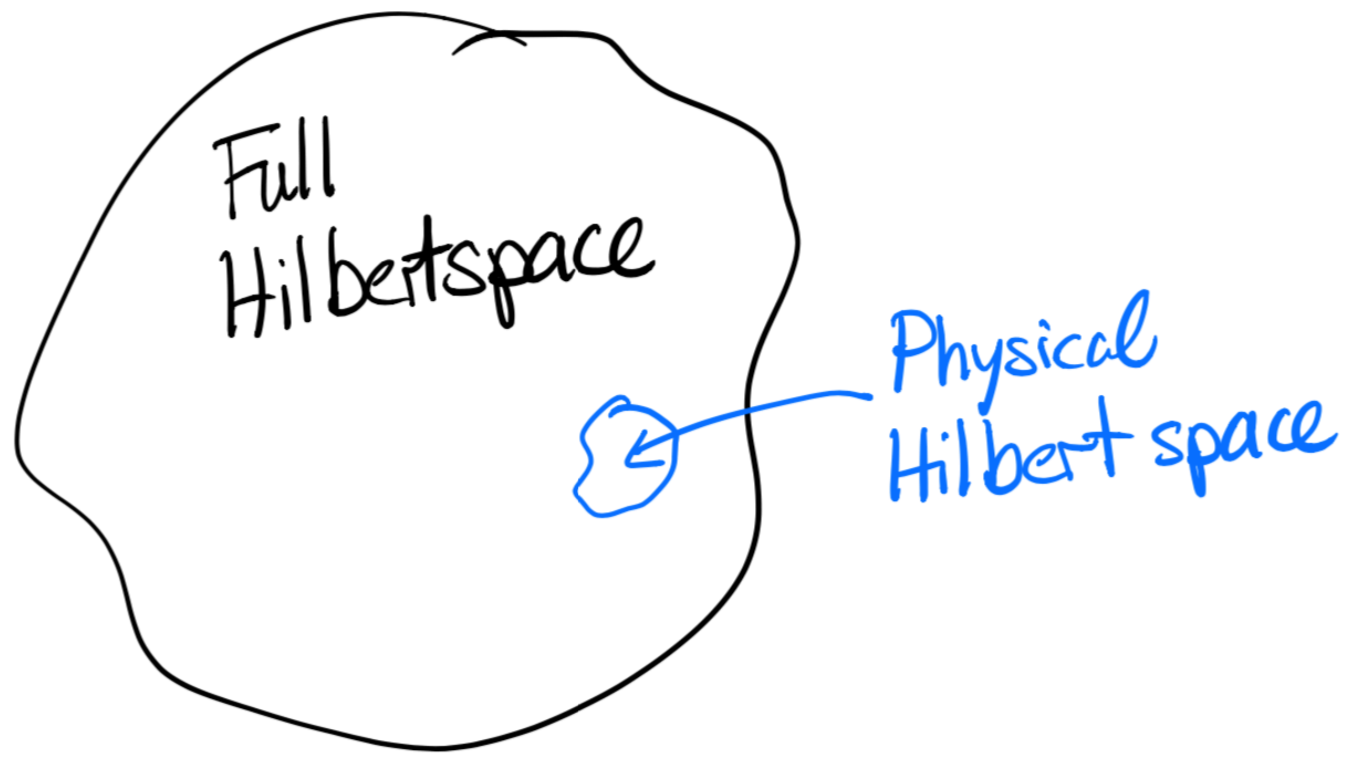
## Challenges

- Gauge Theories (e.g. QED)

$$H = \int d^3x \left\{ \frac{E^2(x)}{2} + \frac{B(x)^2}{2} + \psi^\dagger(x)\gamma^0(i\gamma \cdot \nabla + m)\psi(x) \right\}$$

- Electroweak Force — Gauge Theory!
- Strong Force — Gauge Theory!
- Gravity — Gauge Theory!

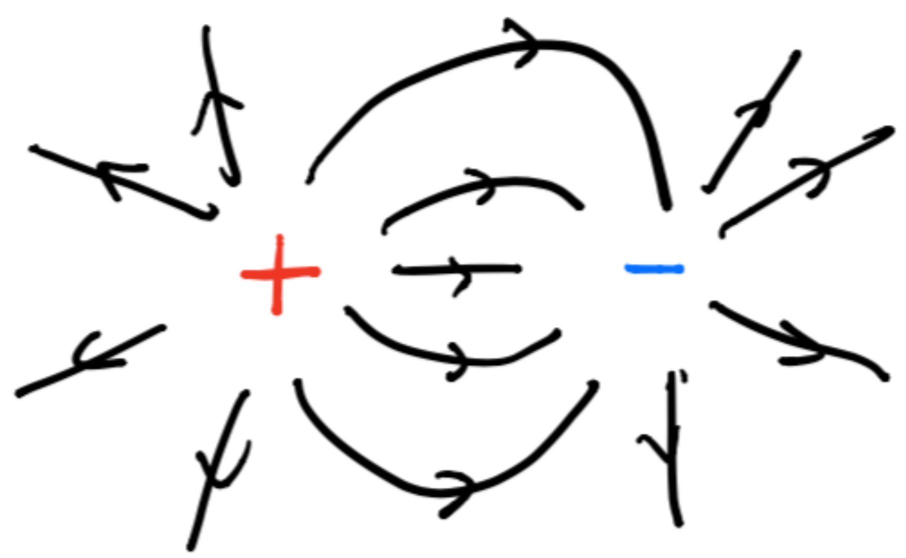
- **Redundancy**, not all dofs are physical!




- Gauss law (operator) defines physical sector

$$e^{iG(\mathbf{x})} |\psi^{\text{phys}}\rangle = |\psi^{\text{phys}}\rangle$$

$$G(\mathbf{x}) = \nabla_{\mathbf{x}} E(\mathbf{x}) - J(\mathbf{x})$$

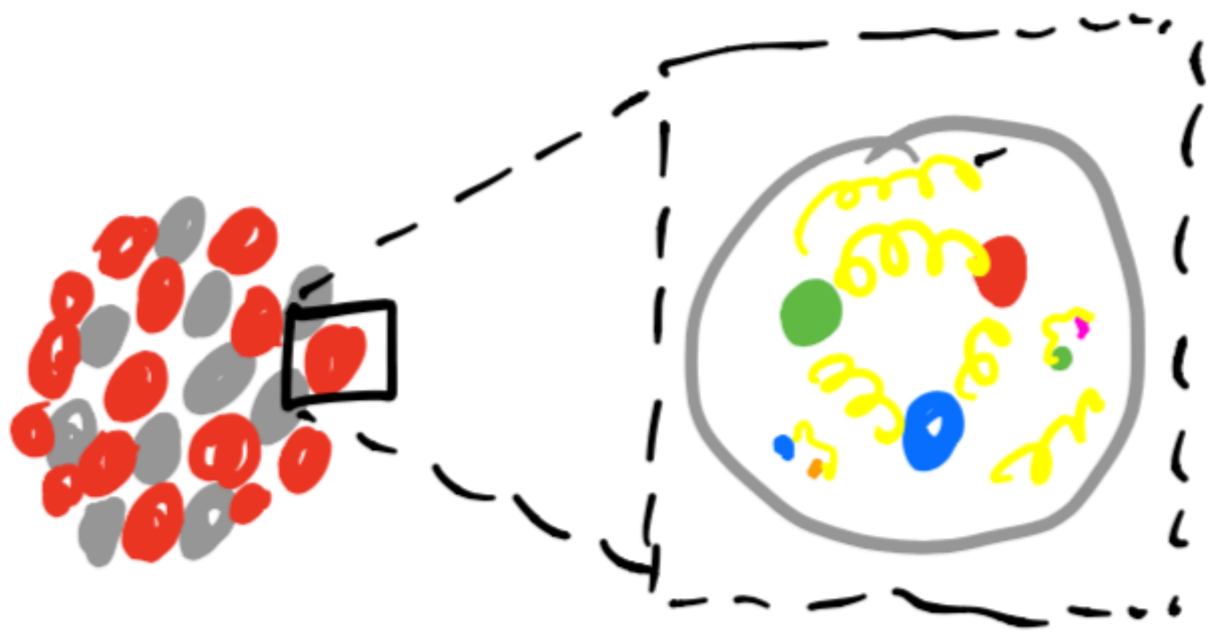


# How to compute something?

# Quantum Computation for Nuclear Physics

## Lattice QCD simulations

Quantum Chromodynamics (QCD)

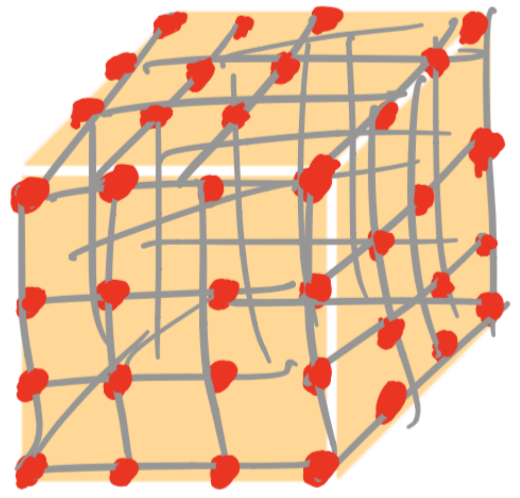


- **From Hamiltonian to Lagrangian**

$$\mathcal{L}_{\mathrm{QCD}} = \bar{\psi}_i \left(i(\gamma^\mu D_\mu)_{ij} - m\,\delta_{ij}\right)\psi_j - \frac{1}{4}G^a_{\mu\nu}G^{\mu\nu}_a$$

$$(G^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu - igf^{abc}A^b_\mu A^c_\nu)$$

- **… to path integral** $Z = \int dA\, e^{iS_{\mathrm{QCD}}[A]}$



$$(S_{\mathrm{QCD}} = \int d^4x \mathscr{L}_{\mathrm{QCD}} \to a_S^3 \sum_{\mathbf{n}} \mathscr{L}^{\mathrm{lattice}}_{\mathrm{QCD}})$$

$$dA \equiv \prod_{\mathbf{x}} dA(\mathbf{x}) \to \prod_{\mathbf{n}} dA(\mathbf{n})$$

- **In Euclidean Spacetime: statistical mechanics problem**

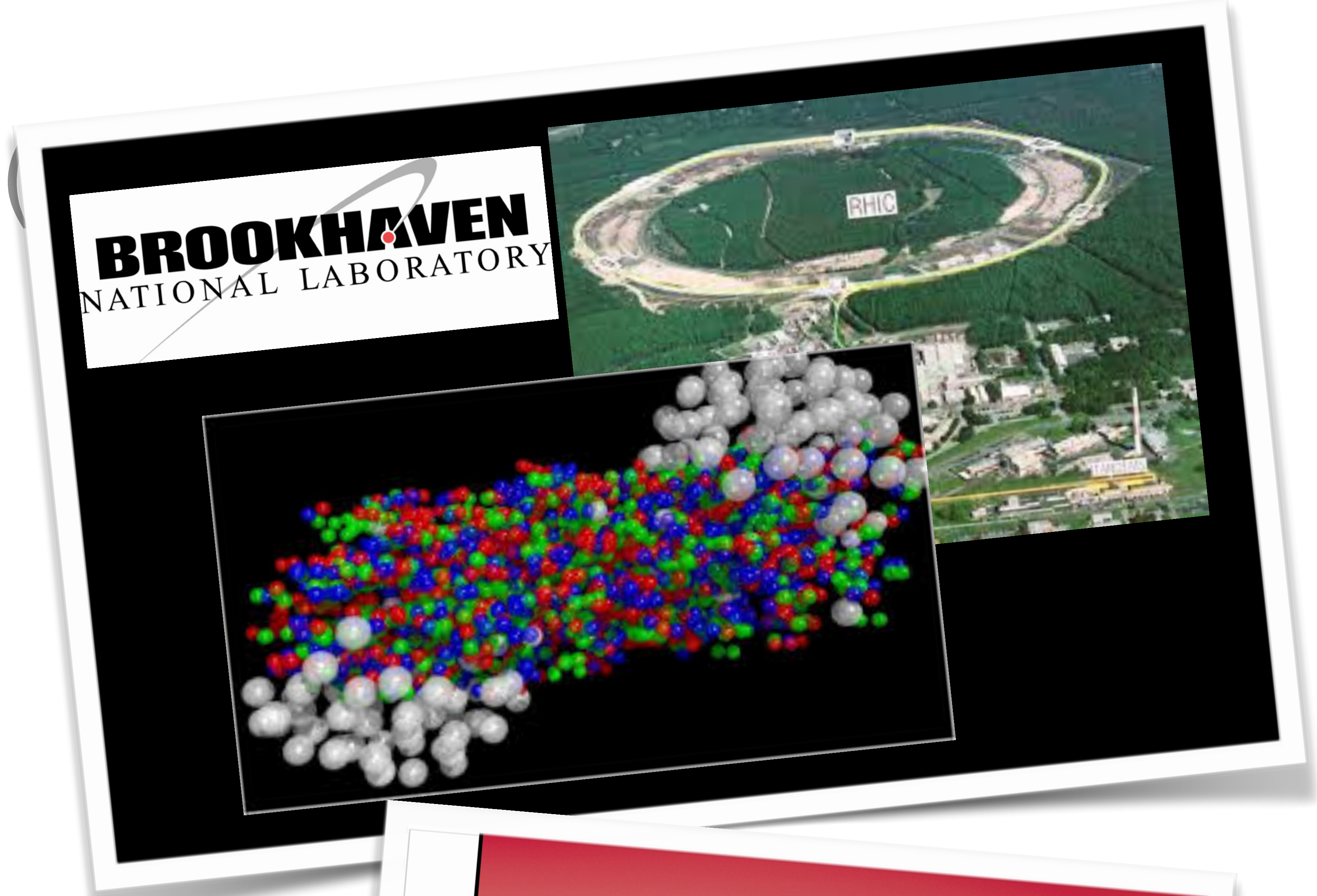
$$Z_E = \int dA\, e^{-S_{\mathrm{E}}[A]}$$

Lattice Monte-Carlo simulations work in many dimensions!

# Quantum Computation for Nuclear Physics

## Lattice QCD simulations

- Very expensive
- Do not work for various interesting problems (

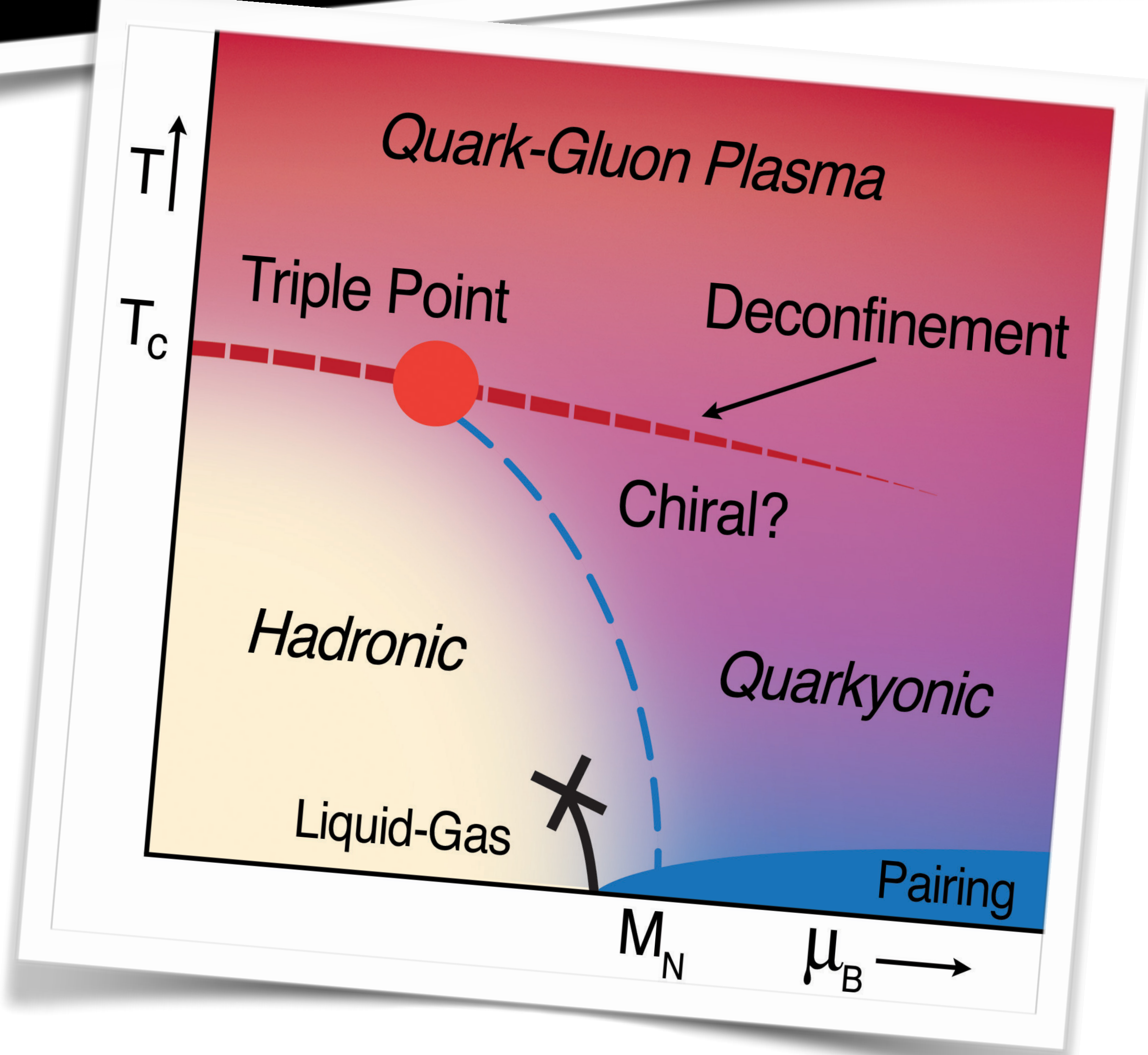



- ~~Real-time physics, systems out of Equilibrium~~ Nope, euclidean space time remember?

- ~~Systems at high density~~ Nope, "sign problem"

$$Z_E = \int dA\, e^{-S_E[A;\mu]}$$

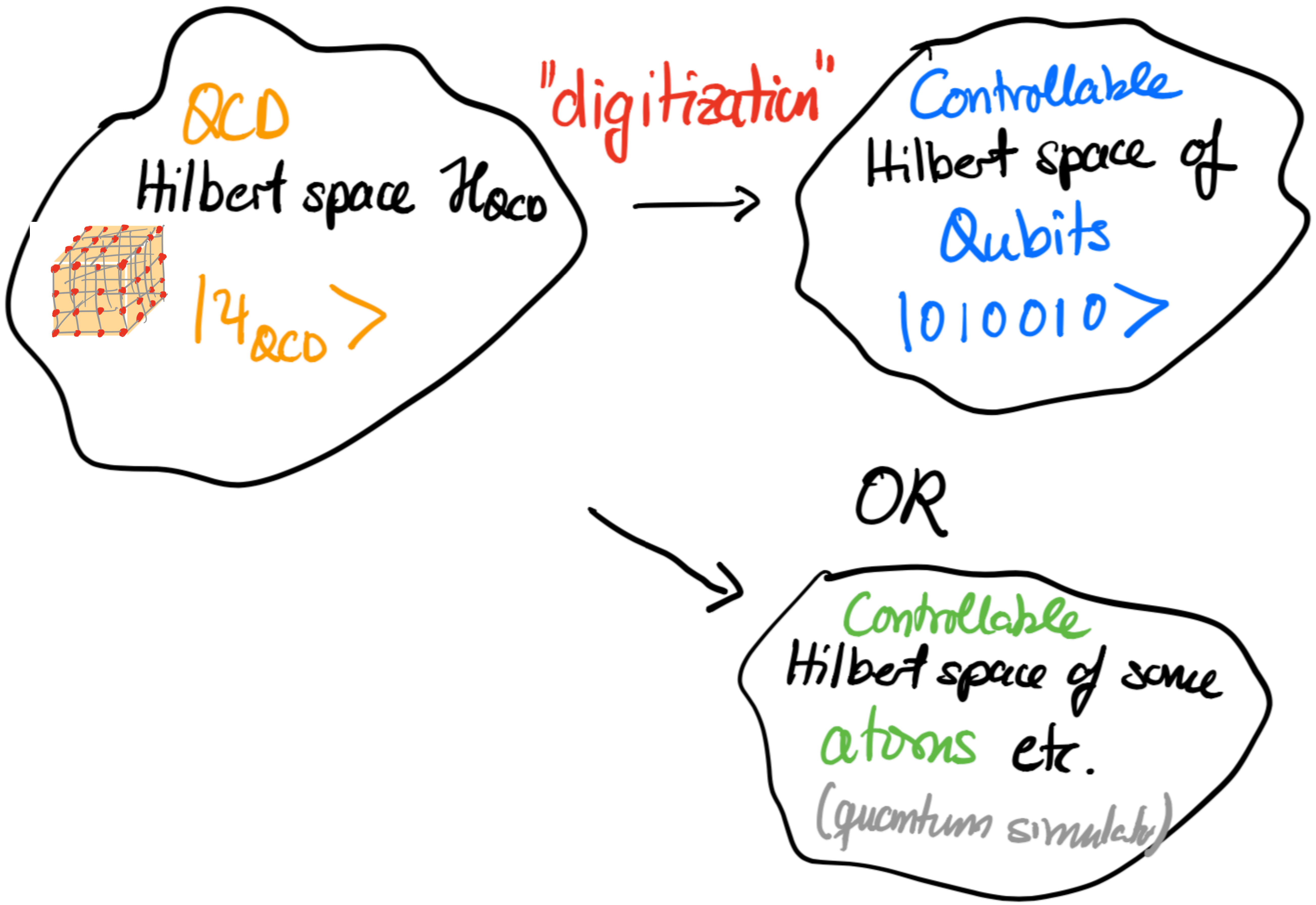
imaginary!



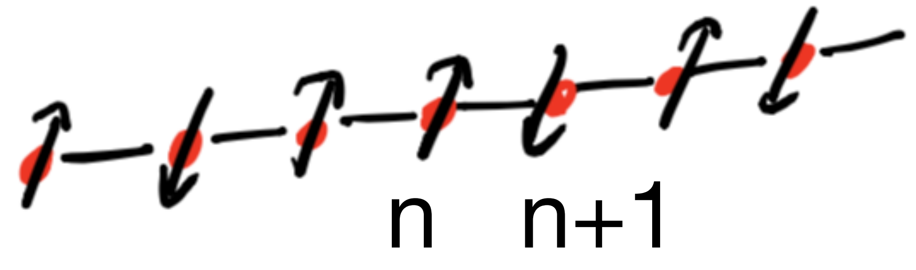

(*) over-simplfication. Please don't be mad, lattice practitioners

# How to do it?

## Step 1: Digitization




- Example 1D: fermions




$$H = -t \sum_n c_n^\dagger c_{n+1} + h.c.$$
$$+ m \sum_n (-1)^n c_n^\dagger c_n + \text{interactions}$$

- Local Hilbert space $\mathscr{H} = \otimes_n \mathscr{H}_n$
  - Fermion = 2 states

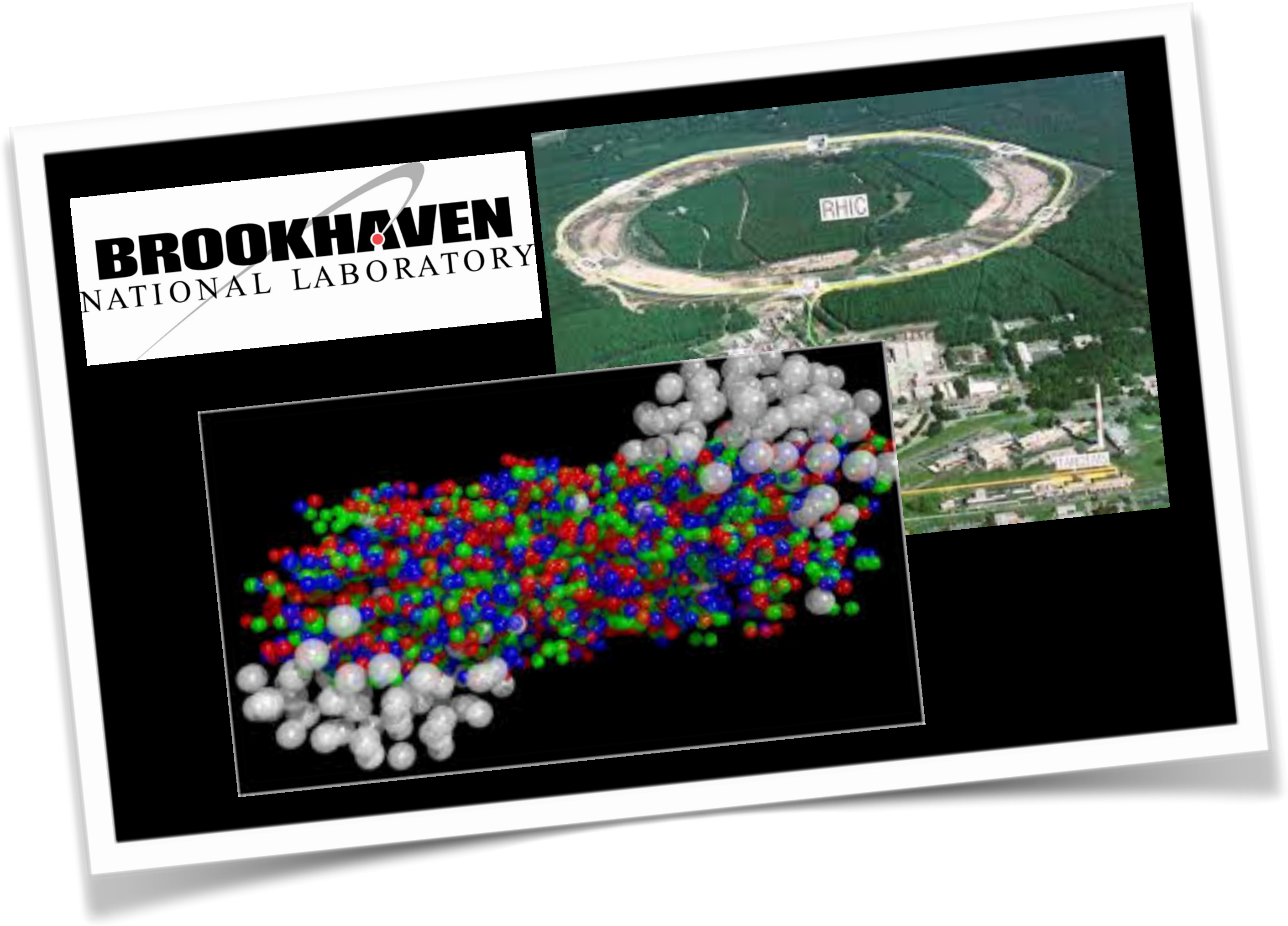
    (occupied/unoccupied)
  - qubit = 2 states

    $(|1\rangle, |0\rangle)$

$$\mathscr{H}^{\text{fermions}} \leftrightarrow \mathscr{H}^{\text{qubits}}$$

# How to do it?

## Step 2: Come up with an algorithm




- **Example: Real-time dynamics**

How does state $|\psi\rangle$ evolve over time?

 $= |\psi\rangle$

$$|\psi(t)\rangle = U(t)|\psi\rangle$$

final state

initial state

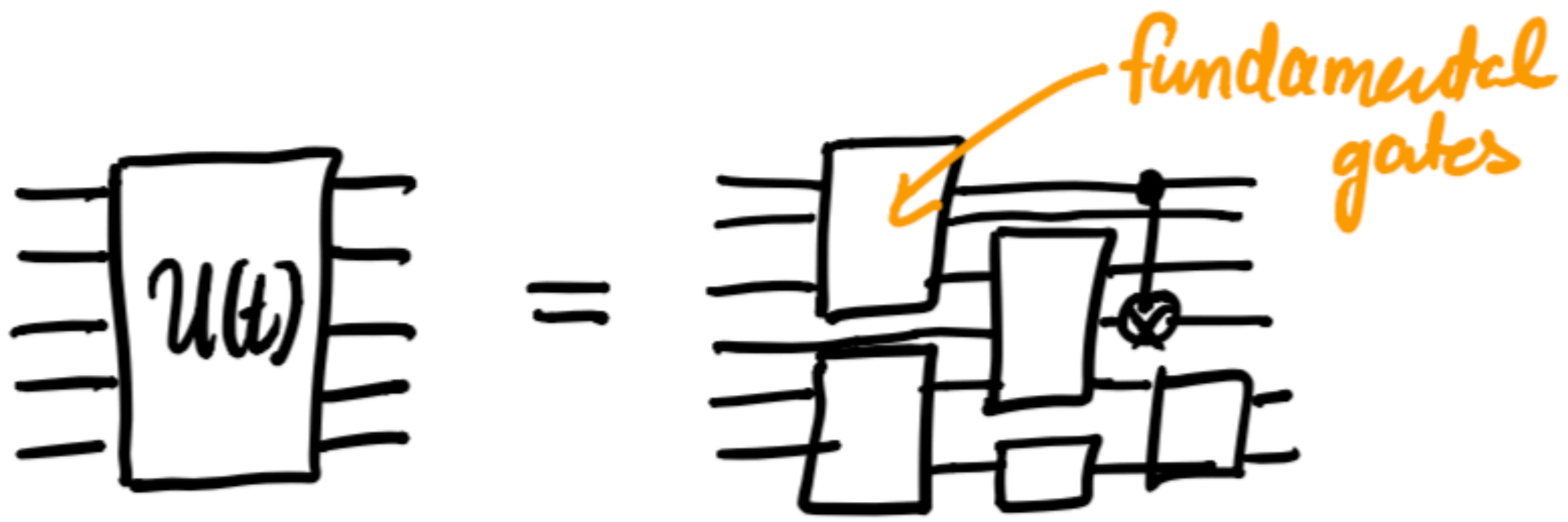
time evolution operator

$$U(t) = e^{-iHt}|\psi\rangle$$

# How to do it?

## Step 2: Come up with an algorithm

- **Decompose *U(t)* into circuit**



$$\text{“}\begin{pmatrix}0\\1\end{pmatrix} = \underbrace{\begin{pmatrix}0&1\\1&0\end{pmatrix}}_{\text{unitary}}\begin{pmatrix}1\\0\end{pmatrix}\text{”}$$

- **Figure out how to set up** $|\psi\rangle$

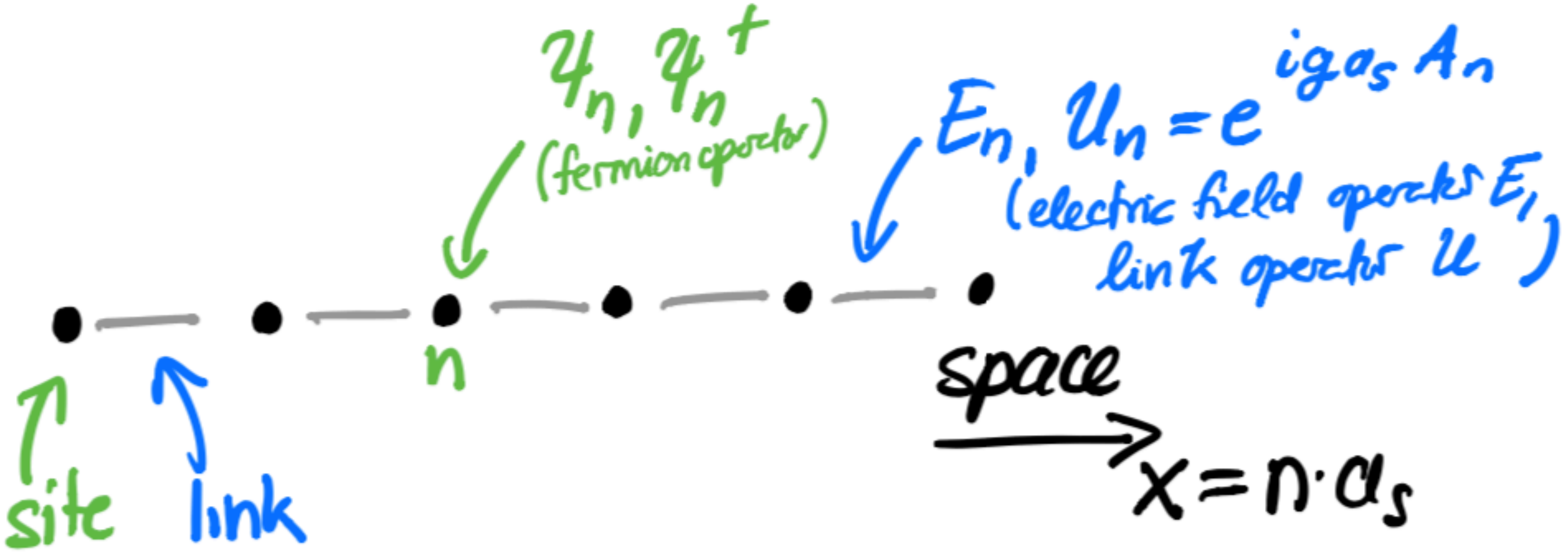
- **and how to extract information about** $|\psi(t)\rangle$ **through measurement**

# Operator formulation of Lattice Gauge Theory

*Let's dive a bit deeper. I will go a little faster now.*

- **QED$_{1+1}$: Schwinger-model** $$H = \int dx \left[\frac{E_x^2}{2} + \psi^\dagger \gamma^0 (i\gamma^1 D_x + m)\psi_x\right]$$

- **Lattice theory** $$H = a_s \sum_n \left[\frac{E_n^{\ 2}}{2} - \frac{i}{2a_s}(\psi_n^\dagger U_n \psi_{n+1} - h.c.) + m(-1)^n \psi_n^\dagger \psi_n\right]$$

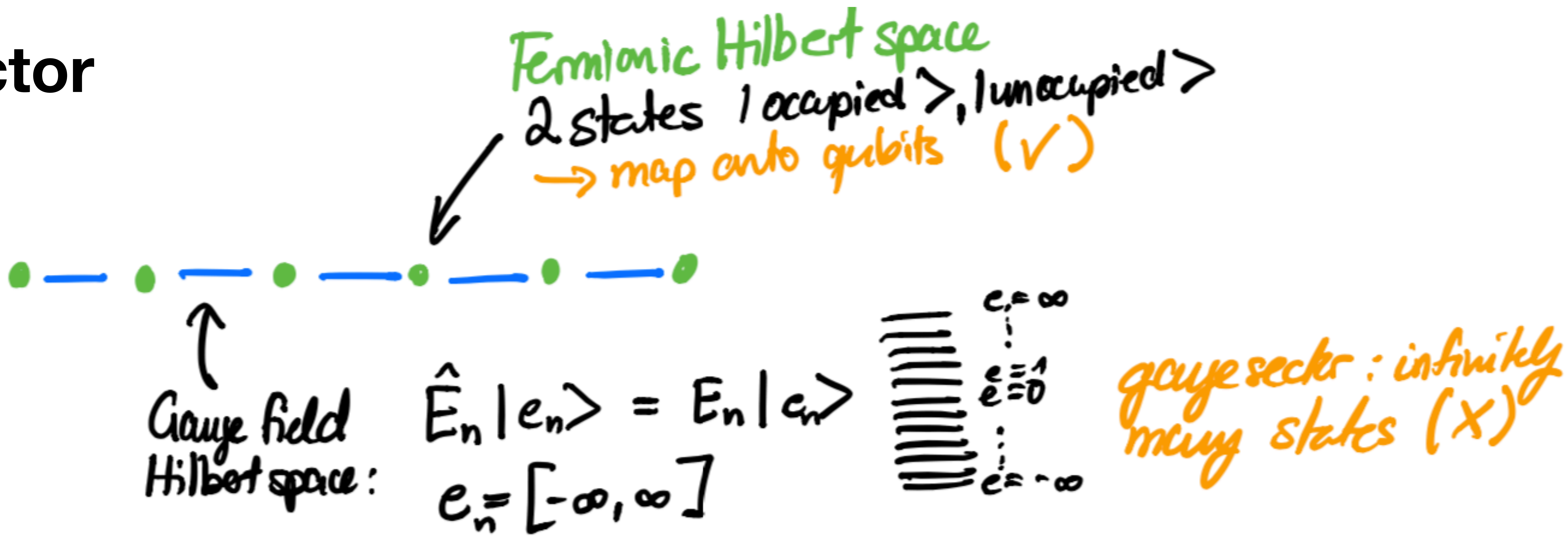


# Operator formulation of Lattice Gauge Theory

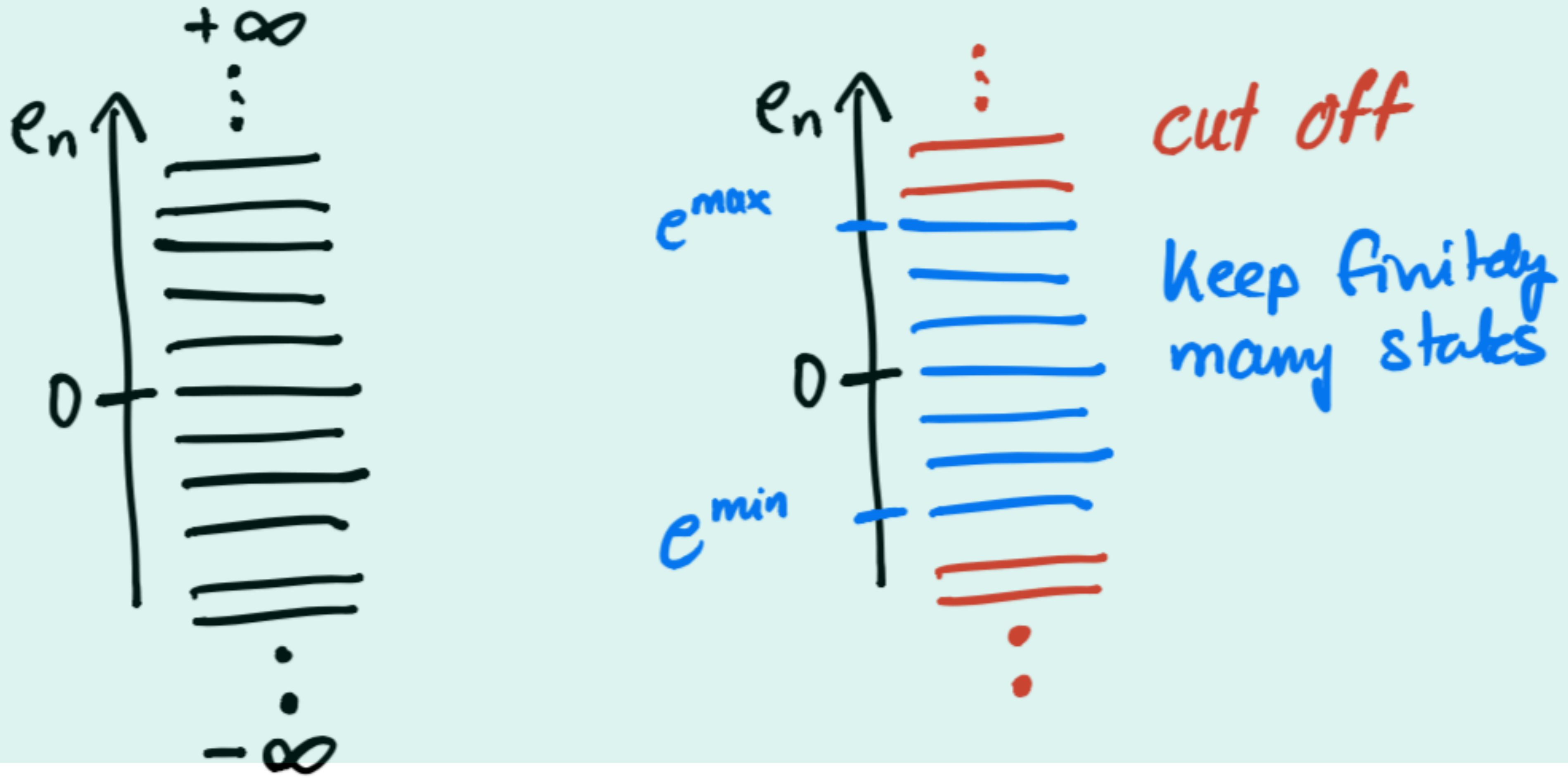
- **Hilbert space, gauge sector**

$$\hat{E}_n|e_n\rangle = E_n|e_n\rangle$$

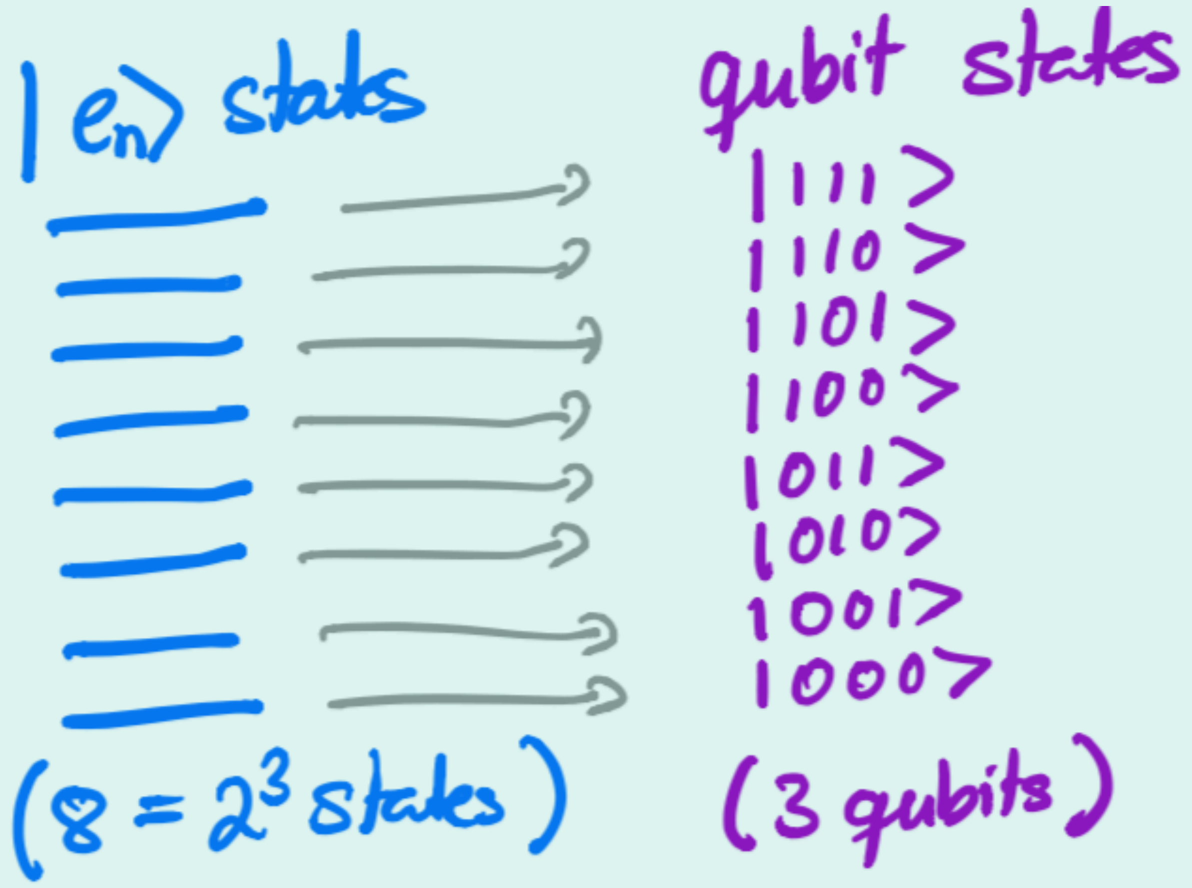
$$\hat{U}_n|e_n\rangle = |e_n + 1\rangle$$




- **Truncation / Digitization**

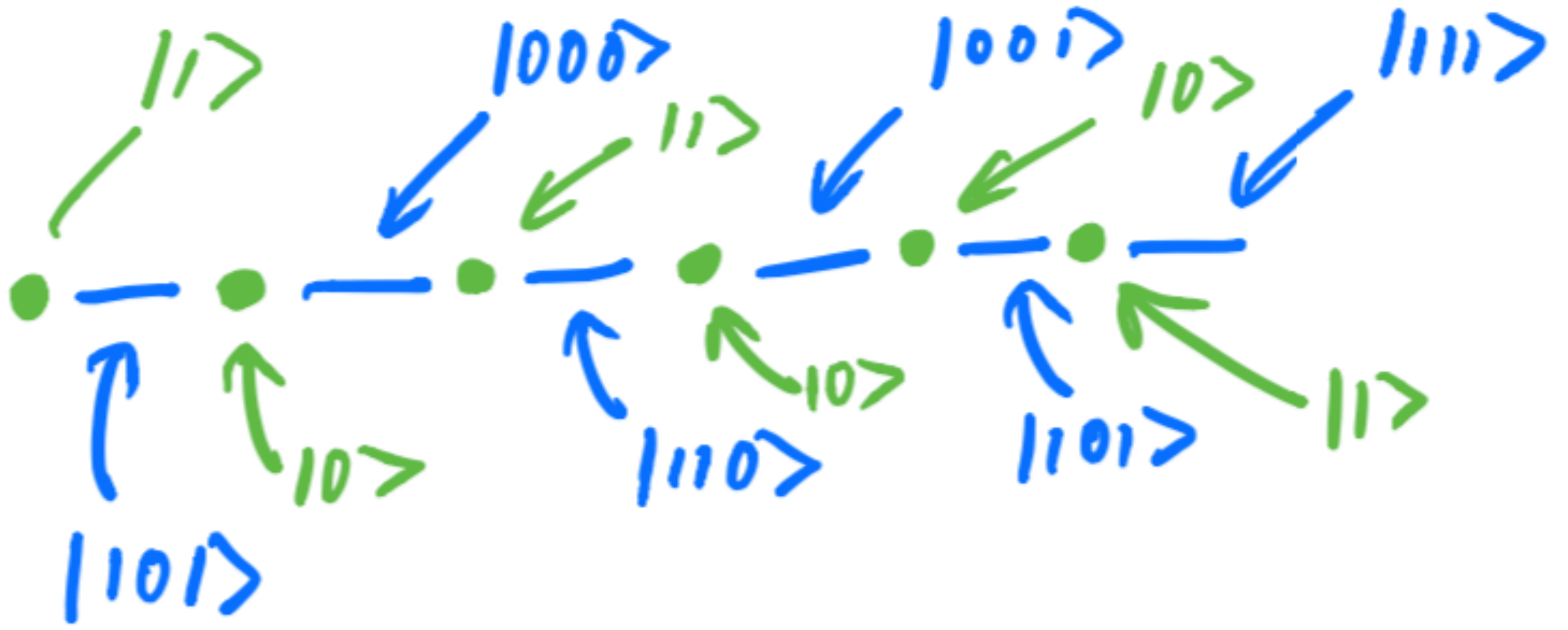



- **Map onto qubits**



# Operator formulation of Lattice Gauge Theory

- **A state of the full theory**




$|\psi\rangle = |110100001110000101011111\rangle$

(24 qubits)

- **Most of Hilbert space is unphysical, Gauss law** (*)

$$G_n = E_n - E_{n-1} - e\left[\psi_n^\dagger \psi_n + \frac{(-1)^n - 1}{2}\right]$$

(can see this because in 1+1d can integrate out Gauss law to remove gauge fields, physical Hilbert space can be represented with 6 qubits, instead of 24)

- **Hamiltonian commutes with Gauss law**

$[H, G_n] = 0$ If initial state is physical, it will stay physical

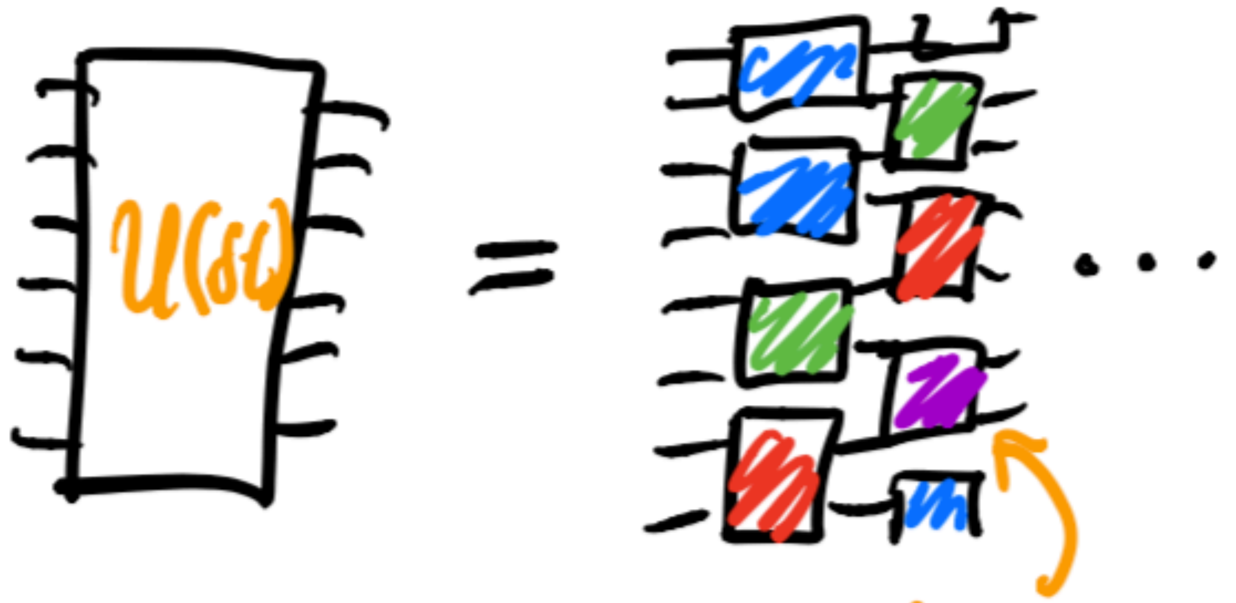
$$|\psi(t)\rangle = U(t)|\psi\rangle = e^{-iHt}|\psi\rangle$$

# Operator formulation of Lattice Gauge Theory

- $|\psi(t)\rangle = U(t)|\psi\rangle = e^{-iHt}|\psi\rangle$


- $U(t) = \prod_t U(\delta t)$

"Trotterization"


elementary gates

Trapped ions:

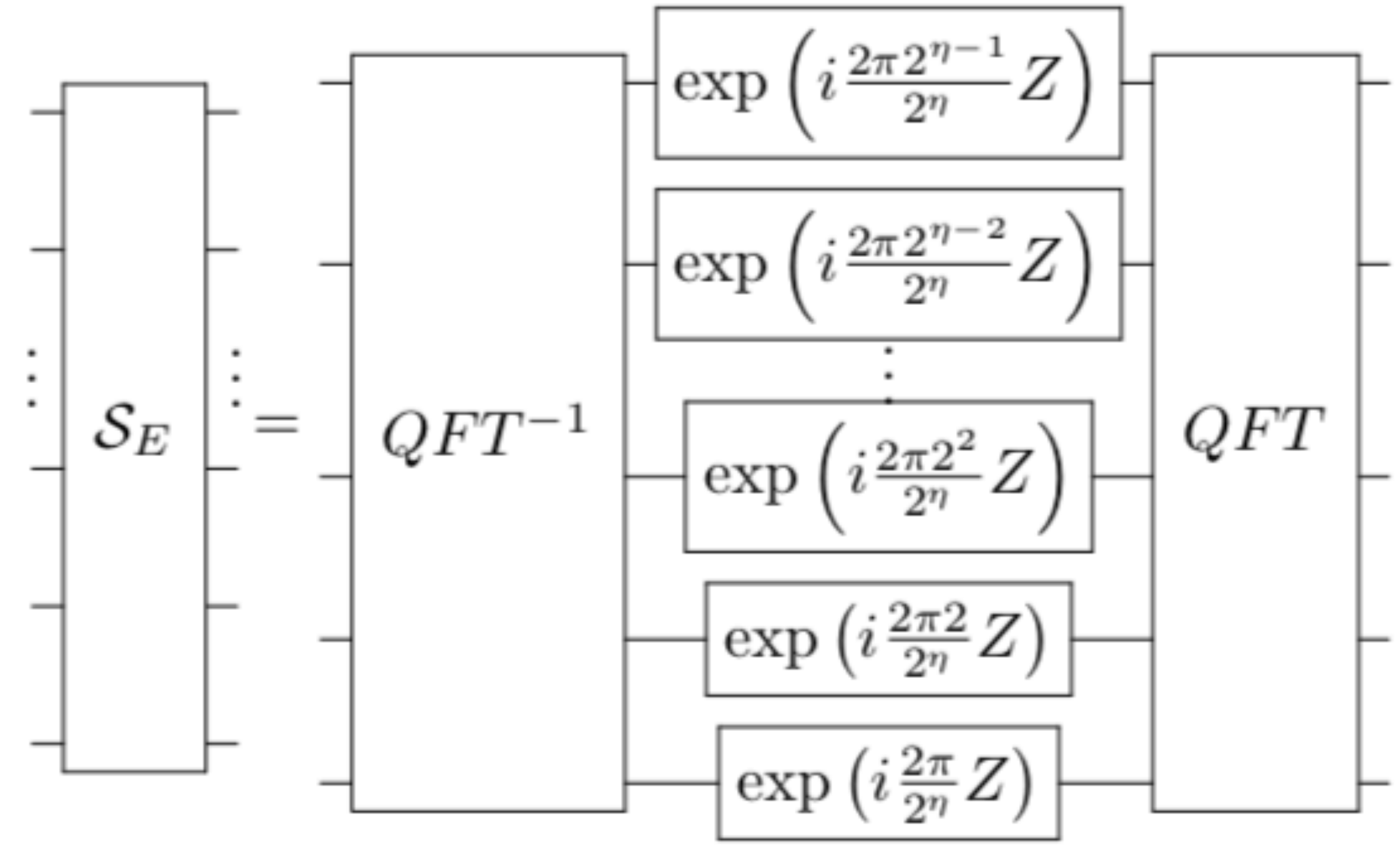
**Martinez et al, Nature 534 (2016) 516**

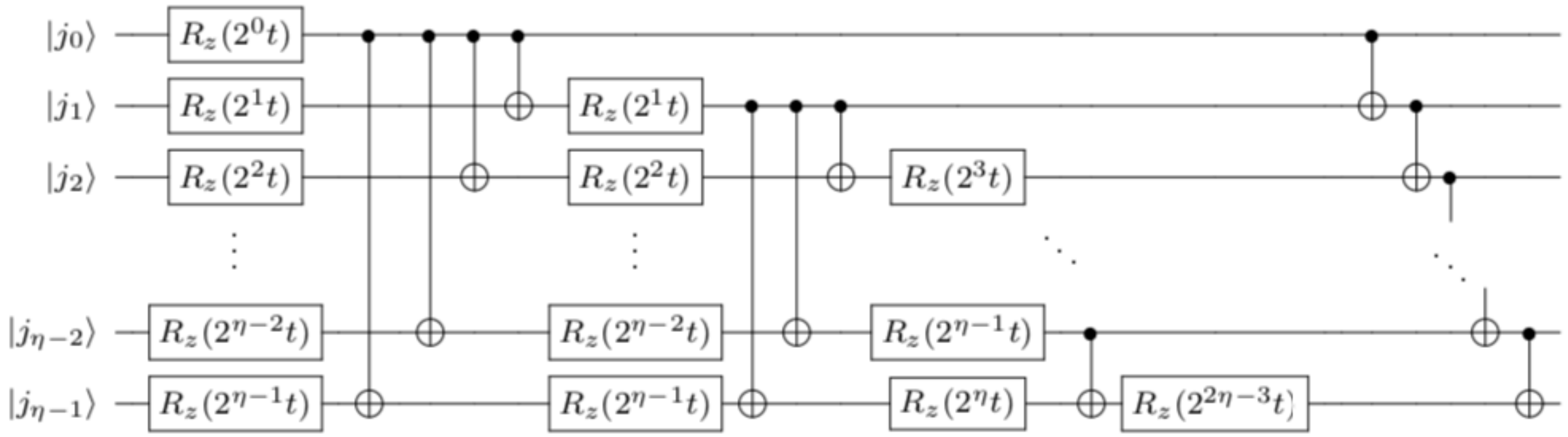
Physics world breakthrough of the year

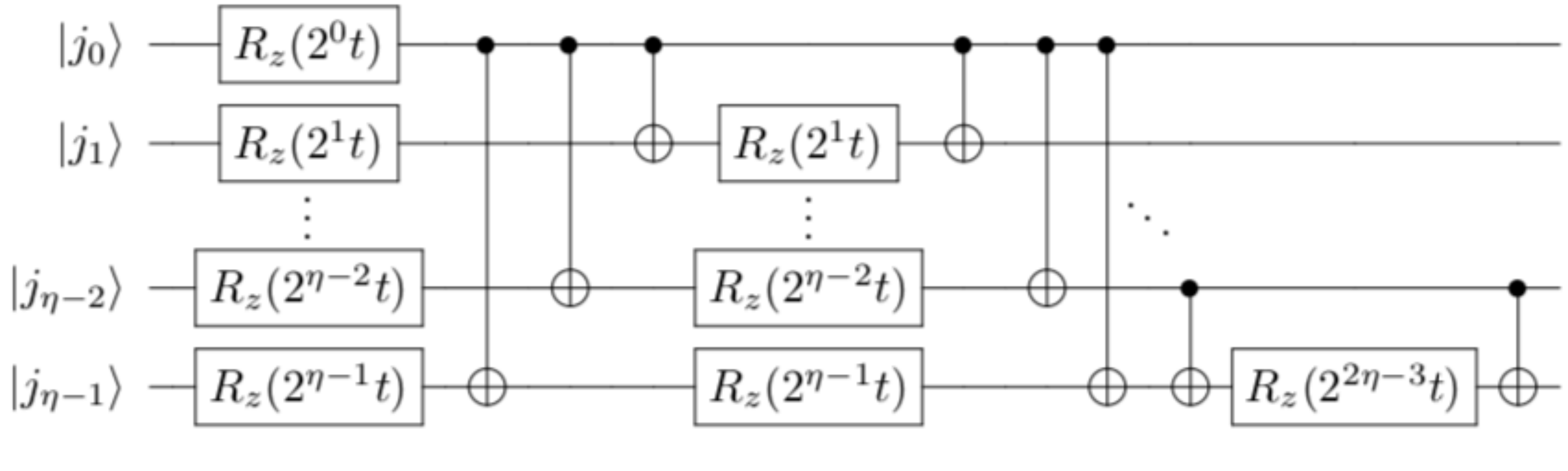
Martinez, Muschik, Schindler, Nigg, Erhard, Heyl, Hauke, Dalmonte, Monz, Zoller, Blatt, *Nature* 2016

- **Take a look at e.g. [https://arxiv.org/pdf/2002.11146.pdf](https://arxiv.org/pdf/2002.11146.pdf) to see examples of actual circuits !**

# Operator formulation of Lattice Gauge Theory




**circuits from https://arxiv.org/pdf/2002.11146.pdf**

# New Ideas

BROOKHAVEN NATIONAL LABORATORY

## Quantum Computation for the Electron Ion Collider

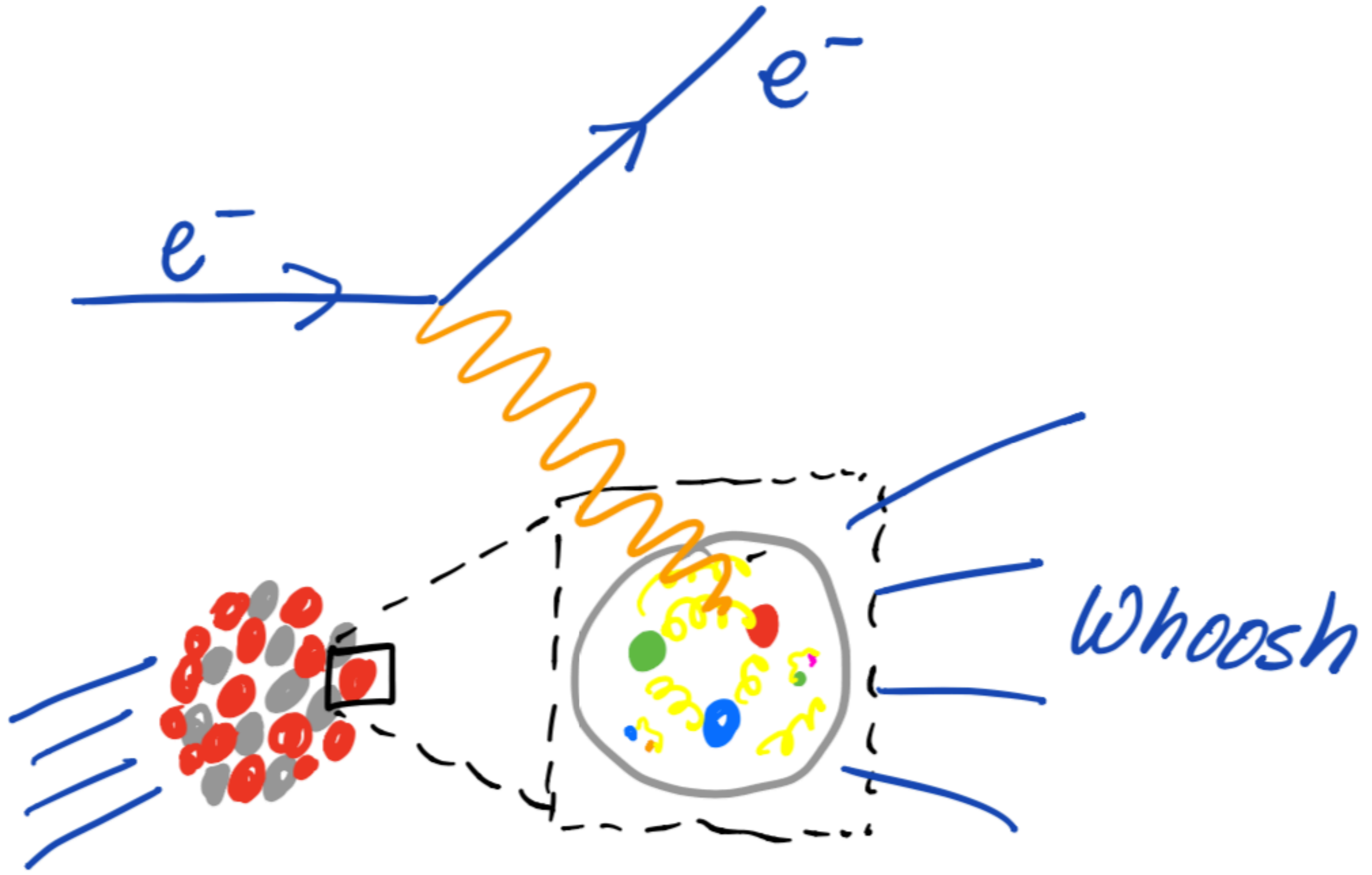
FYI SCIENCE POLICY NEWS FROM AIP Bulletin

Brookhaven Picked as Site for Electron-Ion Collider

SHARE THIS

**Publication date:** 17 January 2020 Number: 5

The Department of Energy has selected Brookhaven National Laboratory as the site for its proposed Electron-Ion Collider, a flagship nuclear science facility that is estimated to cost between $1.6 billion and $2.6 billion.

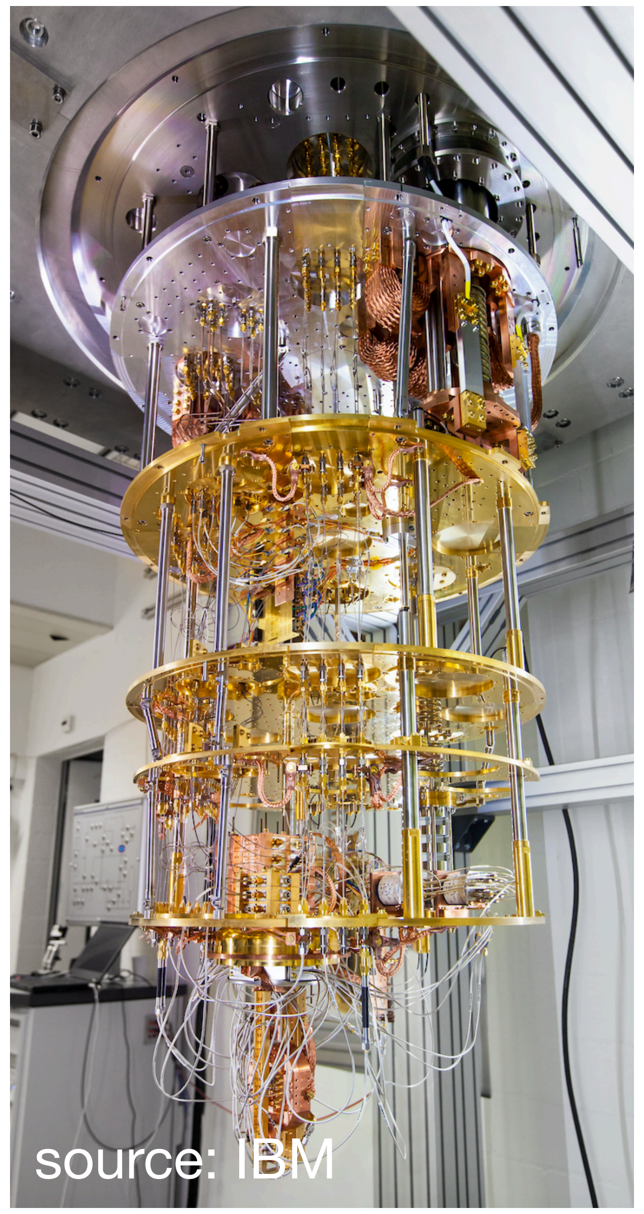


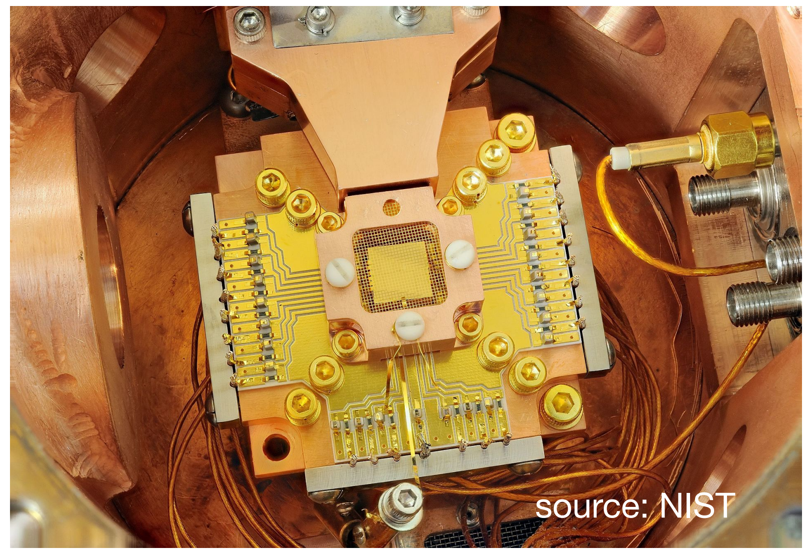

- **Measured are "real-time correlation functions"** $\langle P | J_\mu(x) J_\nu(0) | P \rangle$
- **What is the structure of the proton, what is** $|P\rangle$?

Quantum computers can go where classical computing fails!

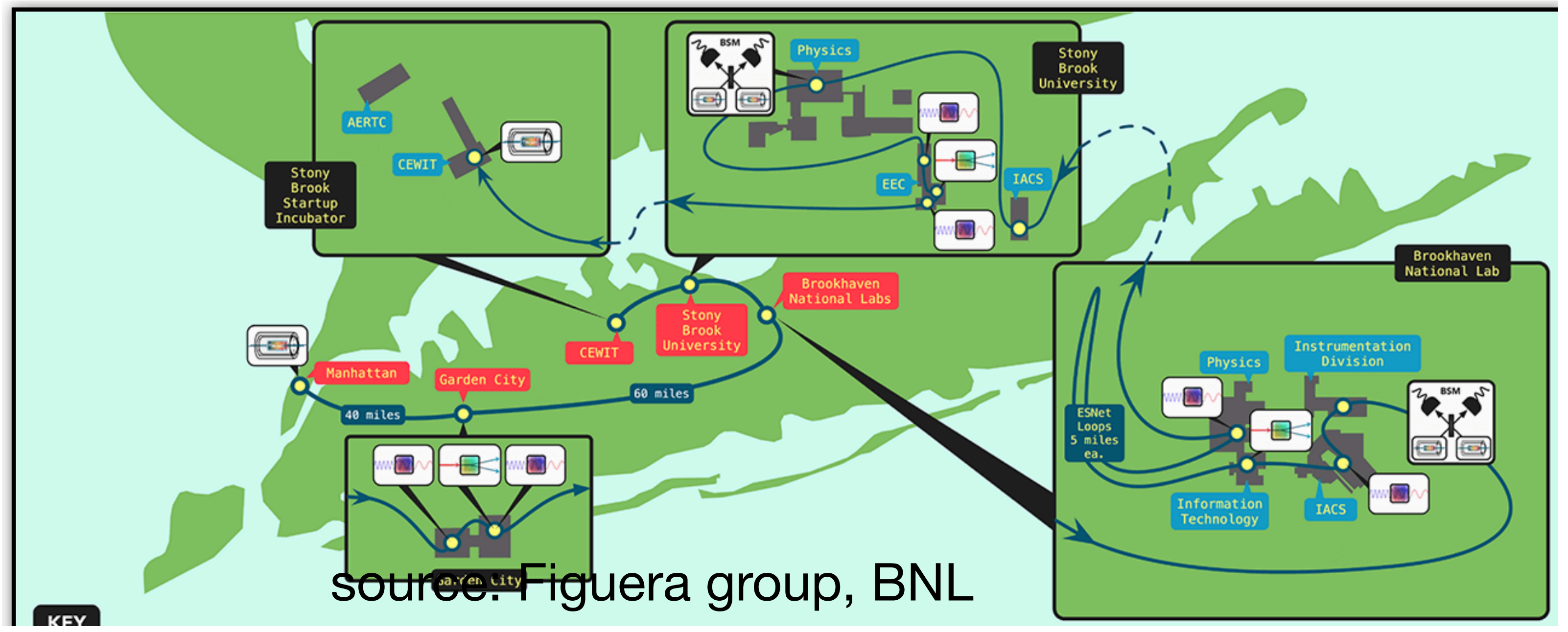
# Summary

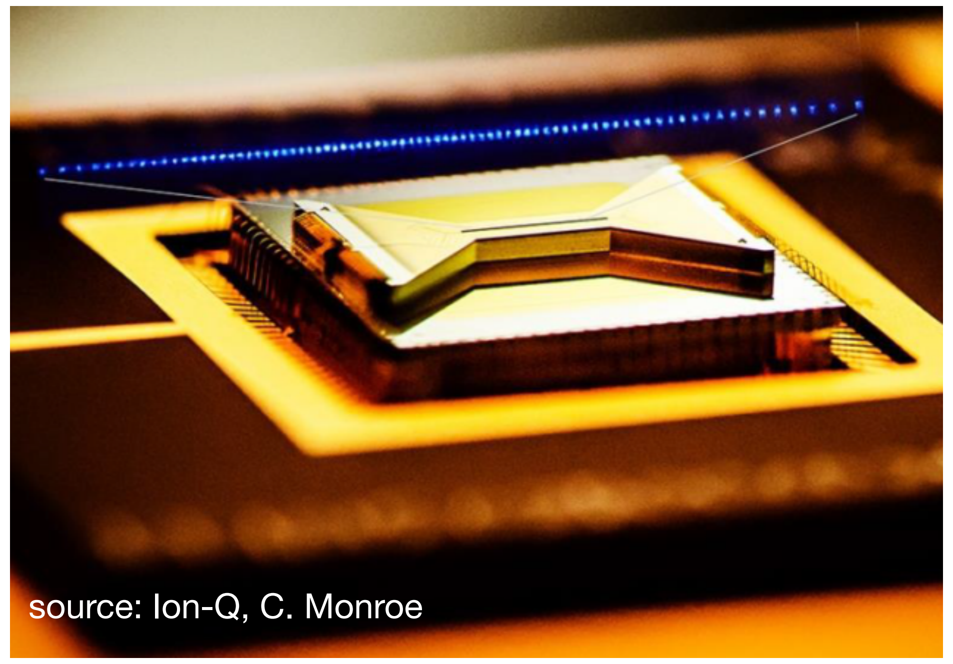
## Very exciting times ahead! - (Second) Quantum Revolution!

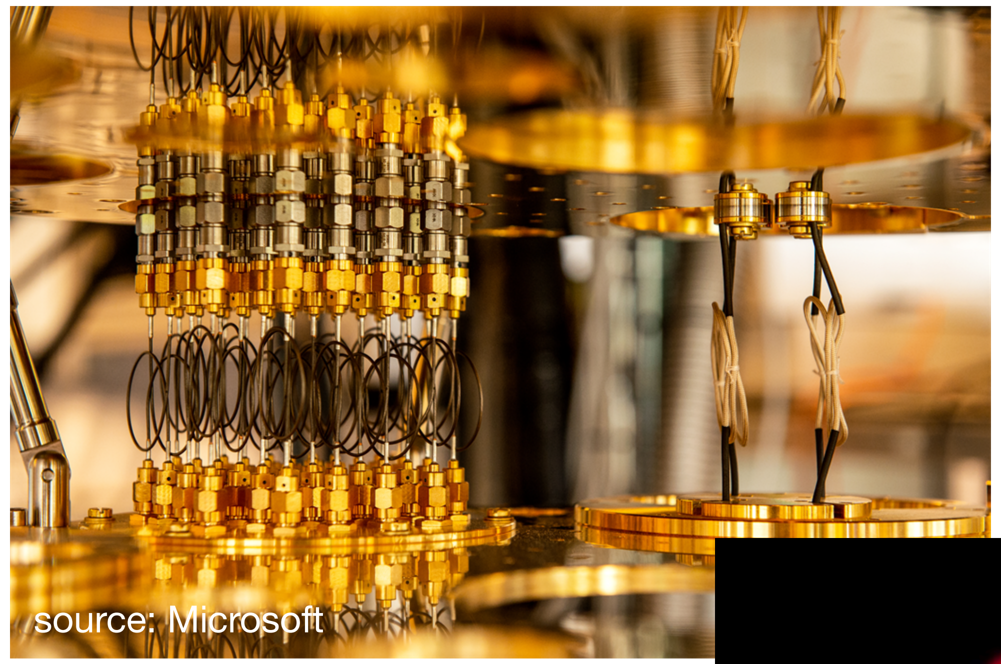

source: IBM


source: NIST


source: Google


source: Figuera group, BNL


source: Ion-Q, C. Monroe


source: Microsoft

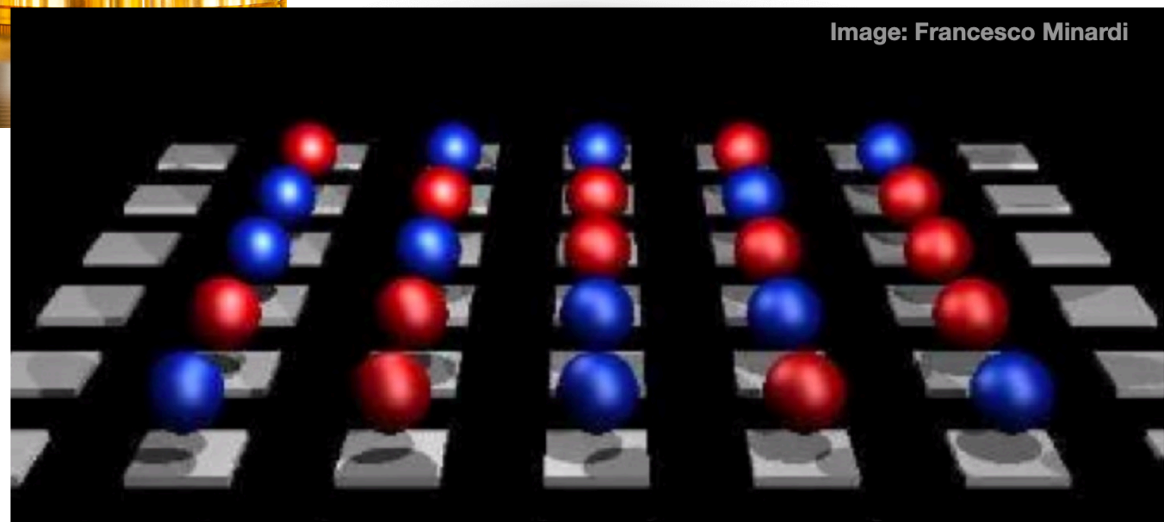
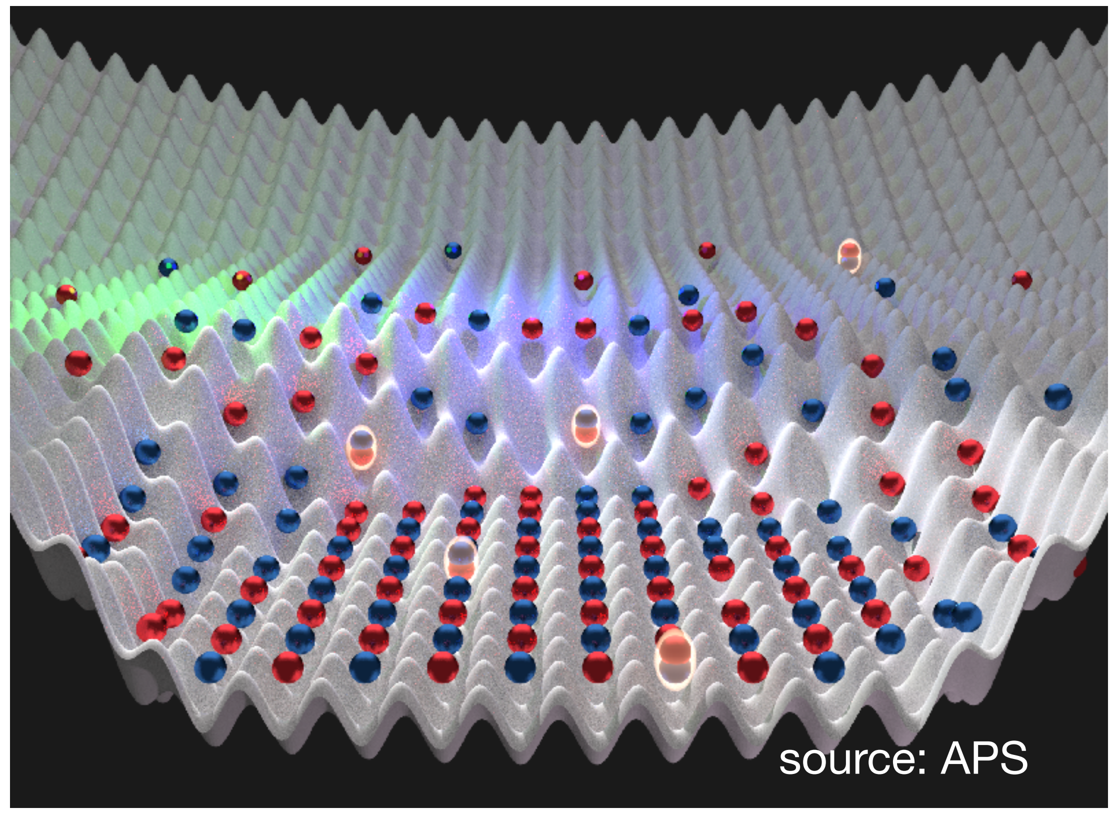


Image: Francesco Minardi


source: APS

## Enjoy thinking differently about problem? Go quantum!

# Your turn!

**Any questions?**

**I will hang around on Bluejeans after this lecture and we can discuss on <u>virtual</u> whiteboard**

(or email me: **nmueller@bnl.gov**)

# PS: Bye, bye BNL and thanks for all the fun!

(this was my last talk as a BNL'er here)

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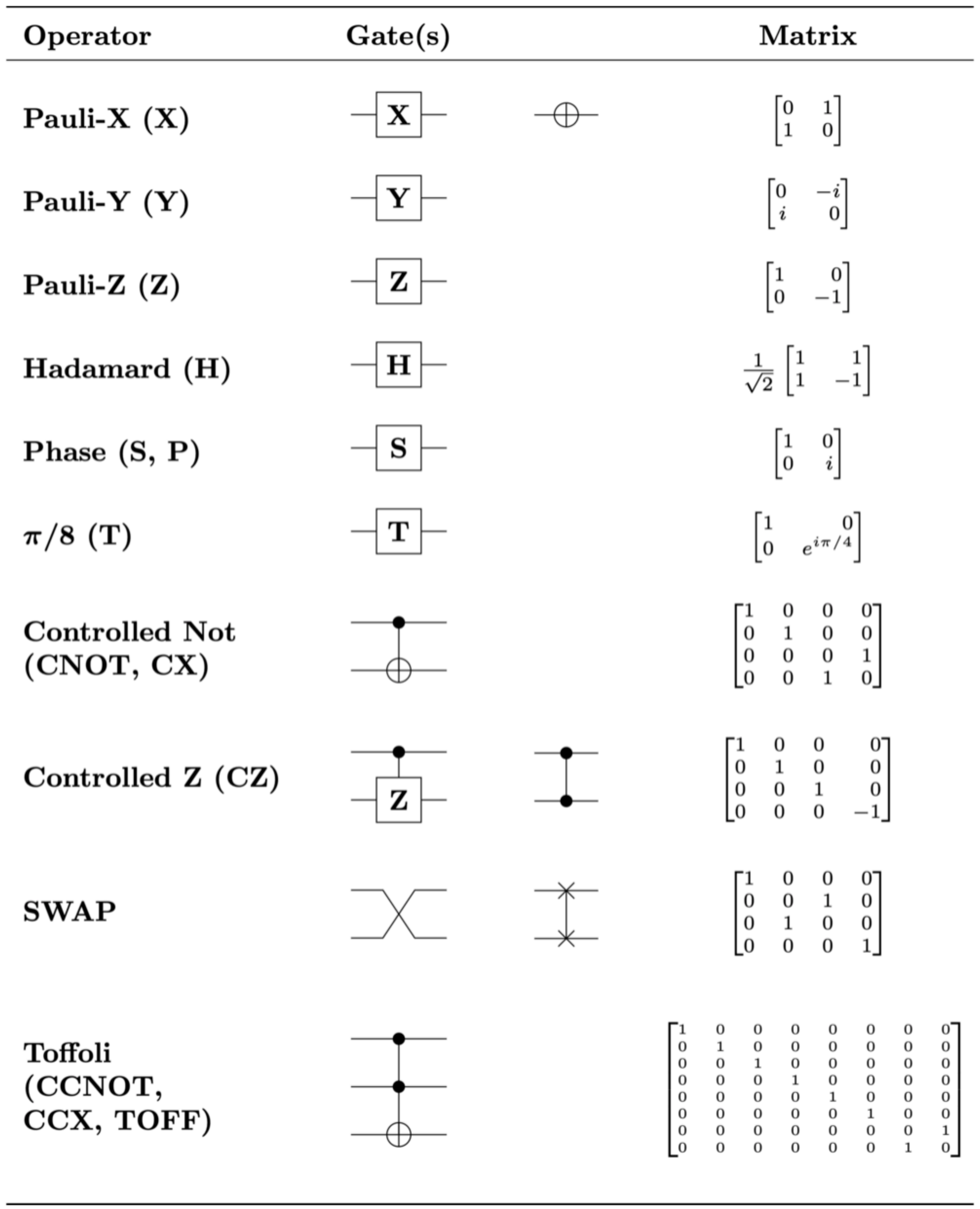
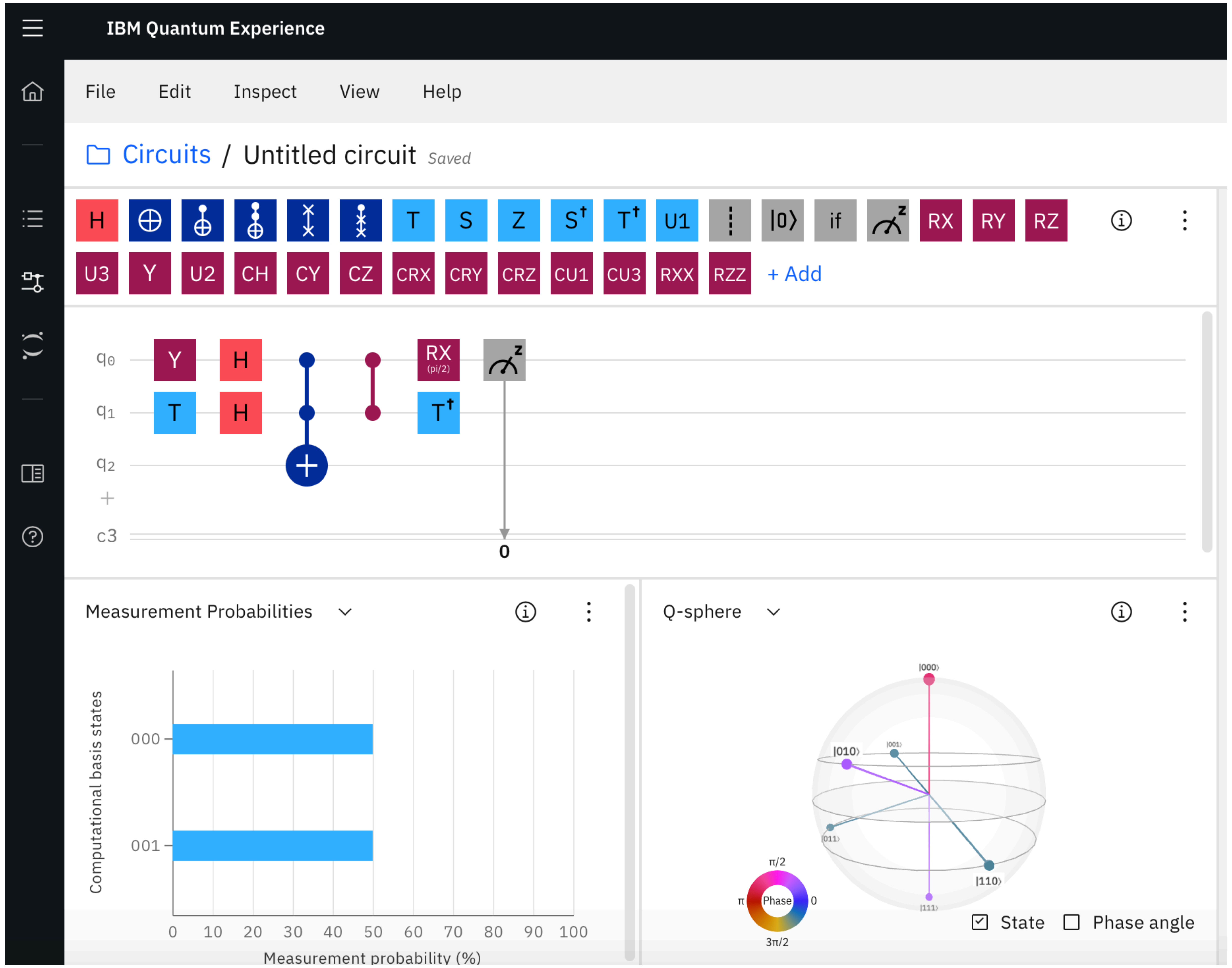
# Backup: Elementary Circuits / Gates



| Operator | Gate(s) | Matrix |
|---|---|---|
| Pauli-X (X) | X | $\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$ |
| Pauli-Y (Y) | Y | $\begin{bmatrix}0 & -i\\i & 0\end{bmatrix}$ |
| Pauli-Z (Z) | Z | $\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$ |
| Hadamard (H) | H | $\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}$ |
| Phase (S, P) | S | $\begin{bmatrix}1 & 0\\0 & i\end{bmatrix}$ |
| $\pi/8$ (T) | T | $\begin{bmatrix}1 & 0\\0 & e^{i\pi/4}\end{bmatrix}$ |
| Controlled Not (CNOT, CX) | | $\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{bmatrix}$ |
| Controlled Z (CZ) | Z | $\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&-1\end{bmatrix}$ |
| SWAP | | $\begin{bmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{bmatrix}$ |
| Toffoli (CCNOT, CCX, TOFF) | | $\begin{bmatrix}1&0&0&0&0&0&0&0\\0&1&0&0&0&0&0&0\\0&0&1&0&0&0&0&0\\0&0&0&1&0&0&0&0\\0&0&0&0&1&0&0&0\\0&0&0&0&0&1&0&0\\0&0&0&0&0&0&0&1\\0&0&0&0&0&0&1&0\end{bmatrix}$ |

source: wikipedia




source: IBM Q Experience

# Backup: What is a path integral?

- Path integral for single particle

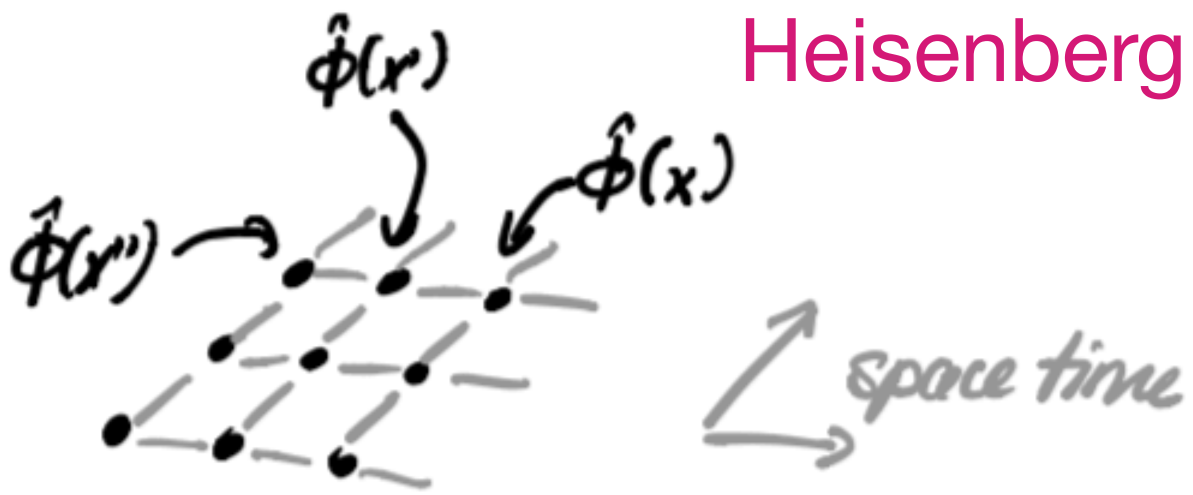
classically: $\vec{x}(t),\ \vec{p}(t)$

quantum mechanically $|x(t)\rangle\ \ |\vec{p}(t)\rangle$

one classical path

superposition of classical paths

- Path integral for many body theory: (Quantum) Field Theory




Heisenberg Field Operator

- with each $\hat\phi(x)$ comes a local Hilbert space

$$\hat\phi(x)\,|\Phi_x\rangle = \phi(x)\,|\Phi_x\rangle \qquad \mathcal{H} = \bigotimes_x \mathcal{H}_x$$

eigenvalue at $x$.

$$\hat\Pi(x)\,|\Pi_x\rangle = \Pi(x)\,|\Pi_x\rangle \qquad \mathcal{H}_x = \mathrm{span}\{|\Phi_x\rangle\} = \mathrm{span}\{|\Pi_x\rangle\}$$

- path integral: $\langle\Phi_B|\,e^{-i\mathcal{H}t}\,|\Phi_A\rangle$


Quantum mechanically superposition of a "paths".

# Backup: What is a path integral?

- Path Integral = Representation of quantum mechanical amplitude

$$\langle \Phi_B | e^{-iHt} |\Phi_A\rangle = \langle \Phi_B | e^{-iH\Delta} \int d\Pi |\Pi\rangle\langle\Pi| \int d\Phi |\Phi\rangle\langle\Phi| e^{-iH\Delta} \dots |\Phi_A\rangle$$

$$= \int \prod_t d\Pi_t \, d\Phi_t \langle \Phi_B | e^{-iH\Delta} |\Pi_0\rangle \underbrace{\langle \Pi_0 | \Phi_0 \rangle}_{e^{i\Pi_0\Phi_0}} \langle \Phi_0 | \cdots |\Phi_A\rangle$$

$$= \int D\Phi \, D\Pi \; e^{i\int dt (\dot\Phi \Pi - H)}$$

$$= \int D\Phi \, D\Pi \; e^{iS}$$

"weighted average over field operator eigenvalue"

not so crucial to understand now!

# Backup: Whiteboard space

# Backup: Whiteboard space

# Backup: Whiteboard space