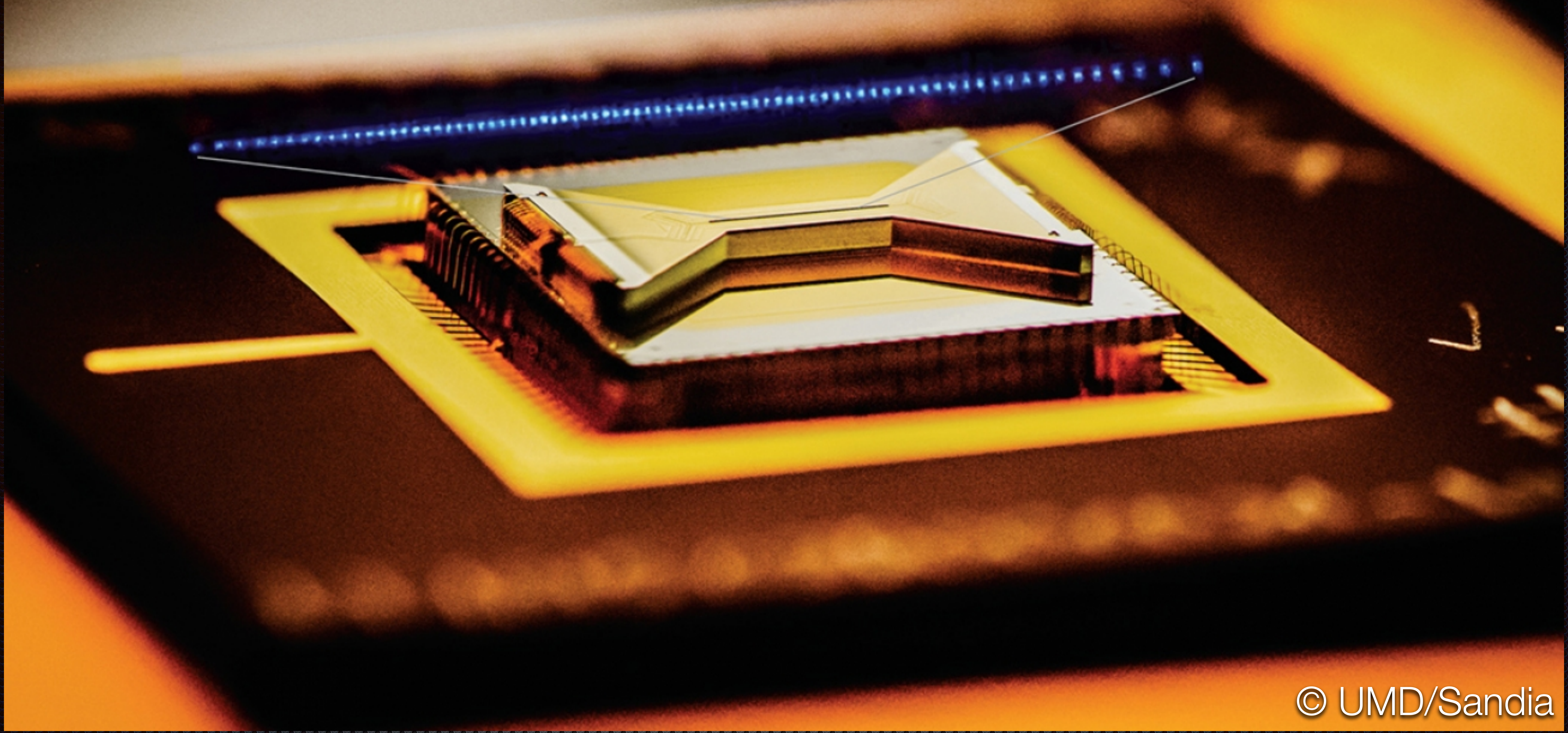


Quantum Computing for Nuclear Physics and Beyond

Niklas Mueller
University of Maryland

BNL Physics Department Summer Lectures
July 5, 2021

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."

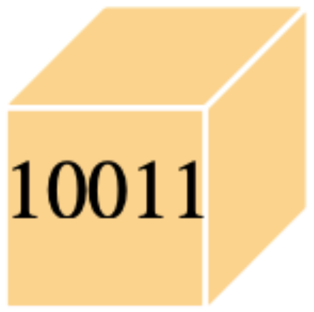
"…What I hoped to do was to design a computer
in which I knew how every part worked with everything
specified down to the atomic level. In other words I wanted
to write down a Hamiltonian for a system that could
make a calculation. "

What actually is quantum computation?

Question/Input

physical model
e.g the fundamental laws of chemistry,
or Quantum Chromodynamics
(“Quantum Many Body Systems”)

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



$\$ \sim \exp(V)$

Algorithm

?

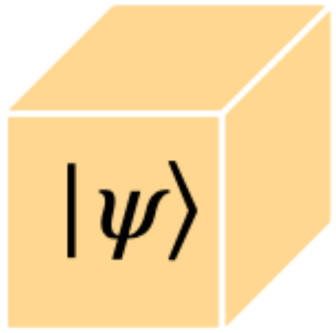
“practically computable” if resources required do not scale exponentially but polynomially with the complexity of the input

Today:
Nuclear Theory Perspective

Answer

understand how complex molecules, proteins etc. form from fundamental laws of nature;
understand how QCD thermalizes

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

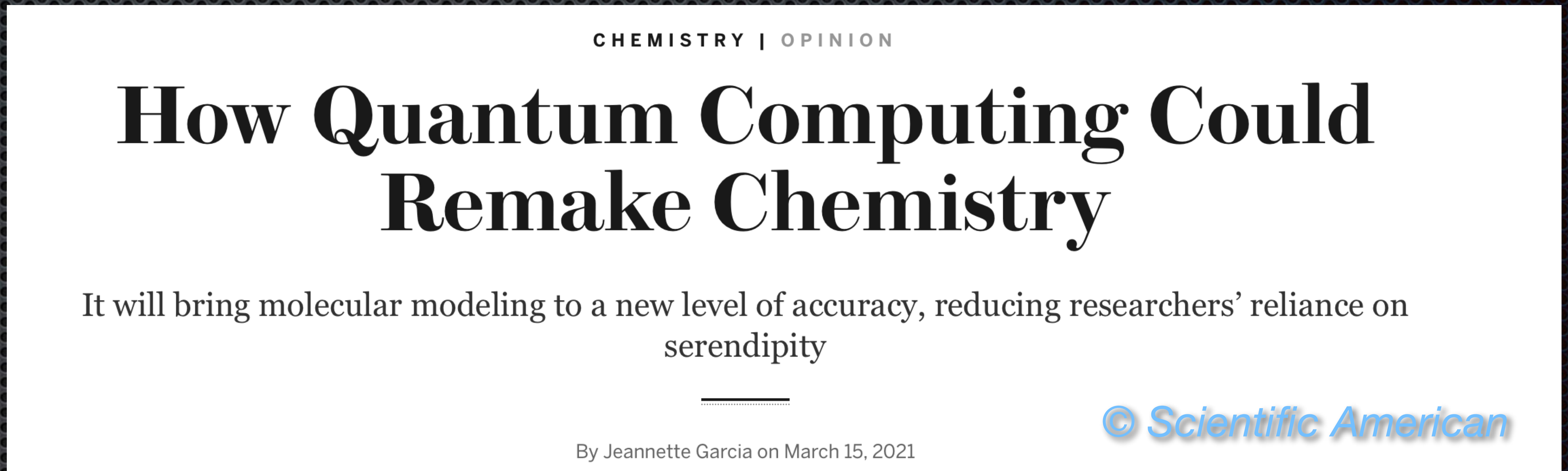


$\$ \sim V$

What actually is quantum computation?

Example: Carbon fixation

- find synthetic catalysts that transform CO_2 into chemicals of higher value
- Lengthy trial and error lab experiments, thousands of molecular combinations
- (classical) computer simulations: resources “exponentially” with the complexity of the problem



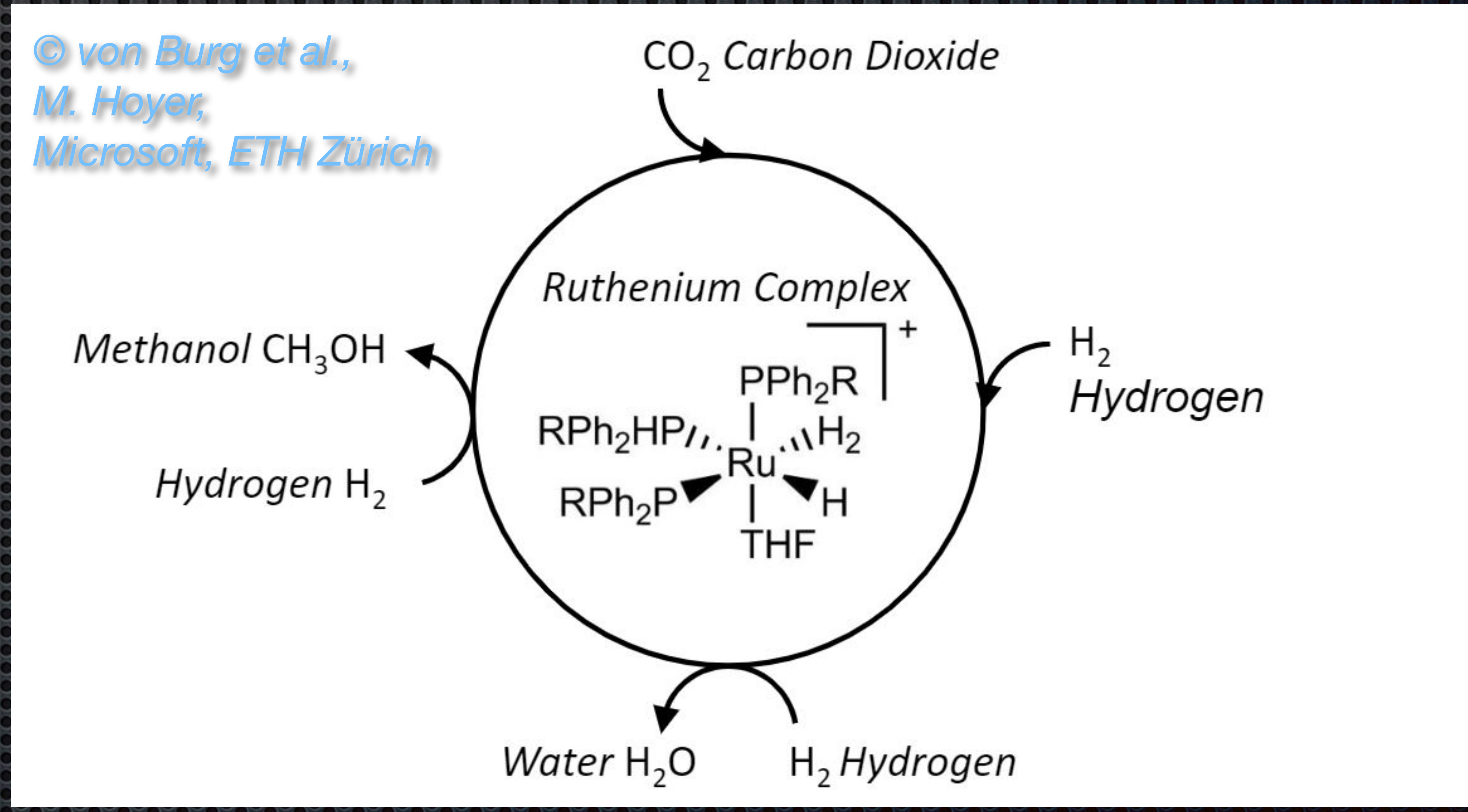
CHEMISTRY | OPINION

How Quantum Computing Could Remake Chemistry

It will bring molecular modeling to a new level of accuracy, reducing researchers’ reliance on serendipity

By Jeannette Garcia on March 15, 2021

© Scientific American



- Some problems are <u>quantum</u> computable (but not classical) because <u>their nature is essentially quantum mechanical</u> (such as chemistry)

disclaimer: I am not a chemist!

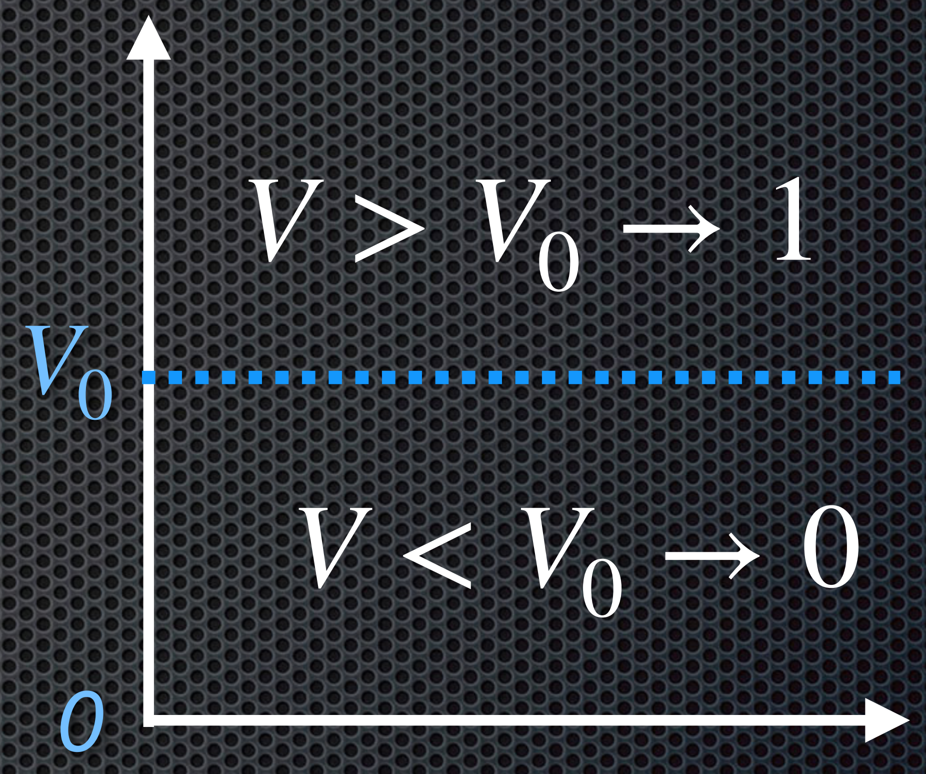
Basics: classical vs. quantum

Classical

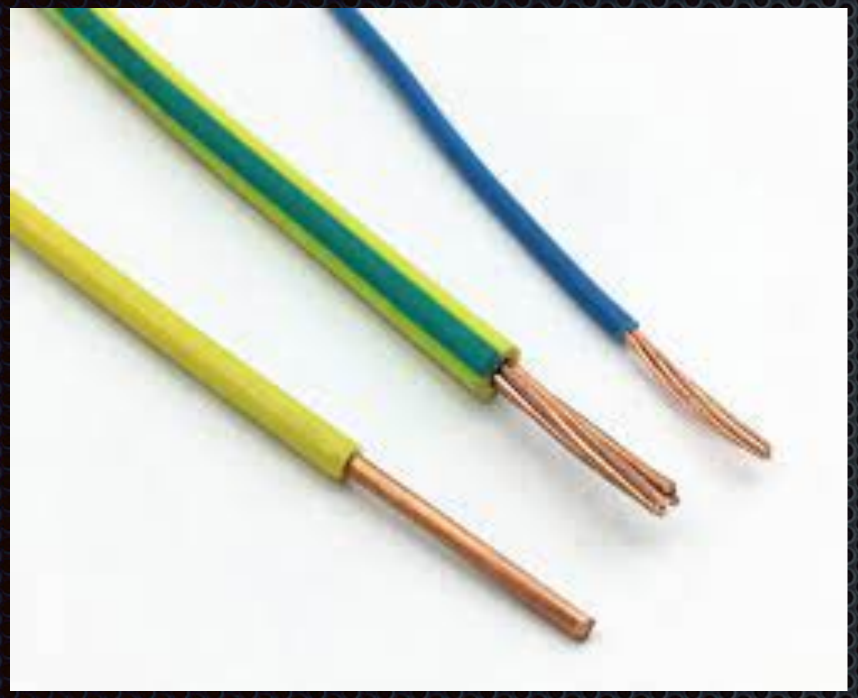
1	0	1	1

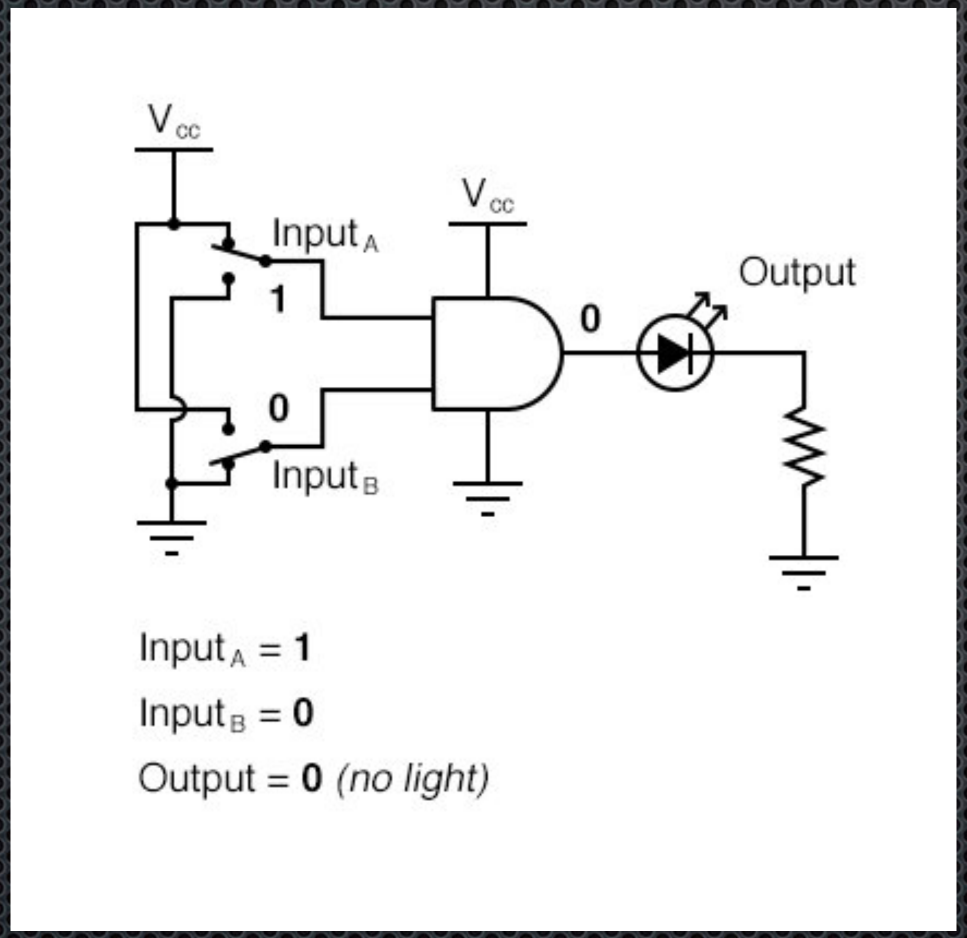
"bits" can be either 1 or 0

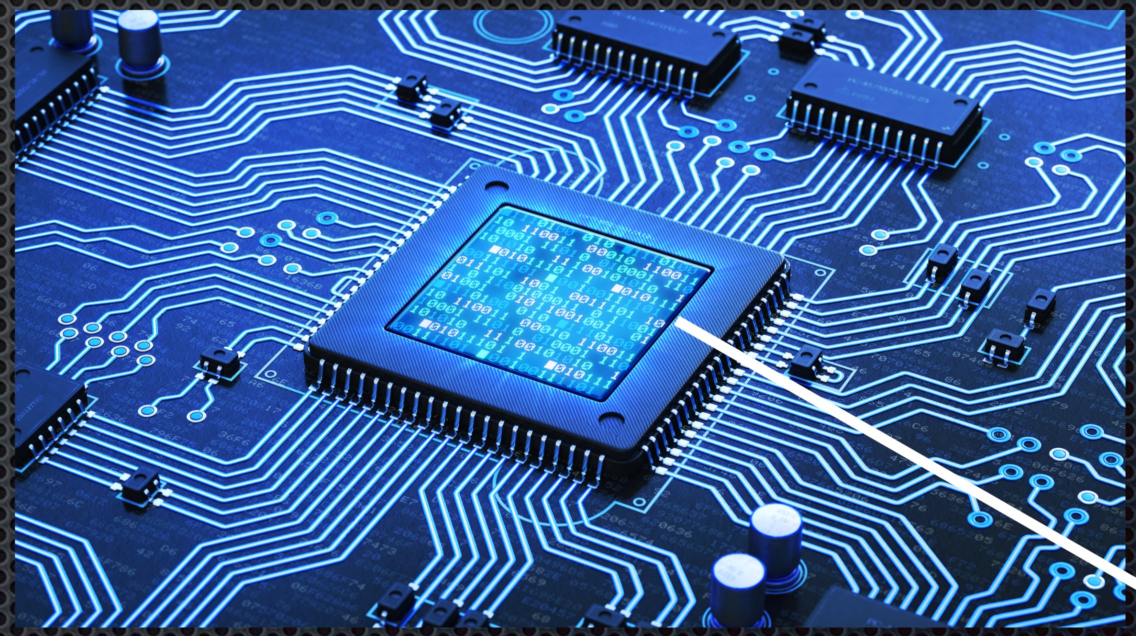
$2^0 + 2^1 + 2^3 = 11$



- what this actually means in a computer: electric current in "wires" and circuits







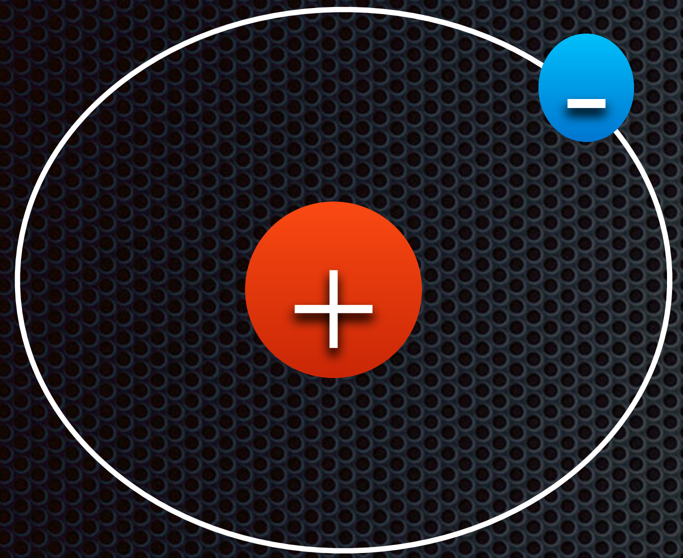
10^9 from 0 to 1 per sec

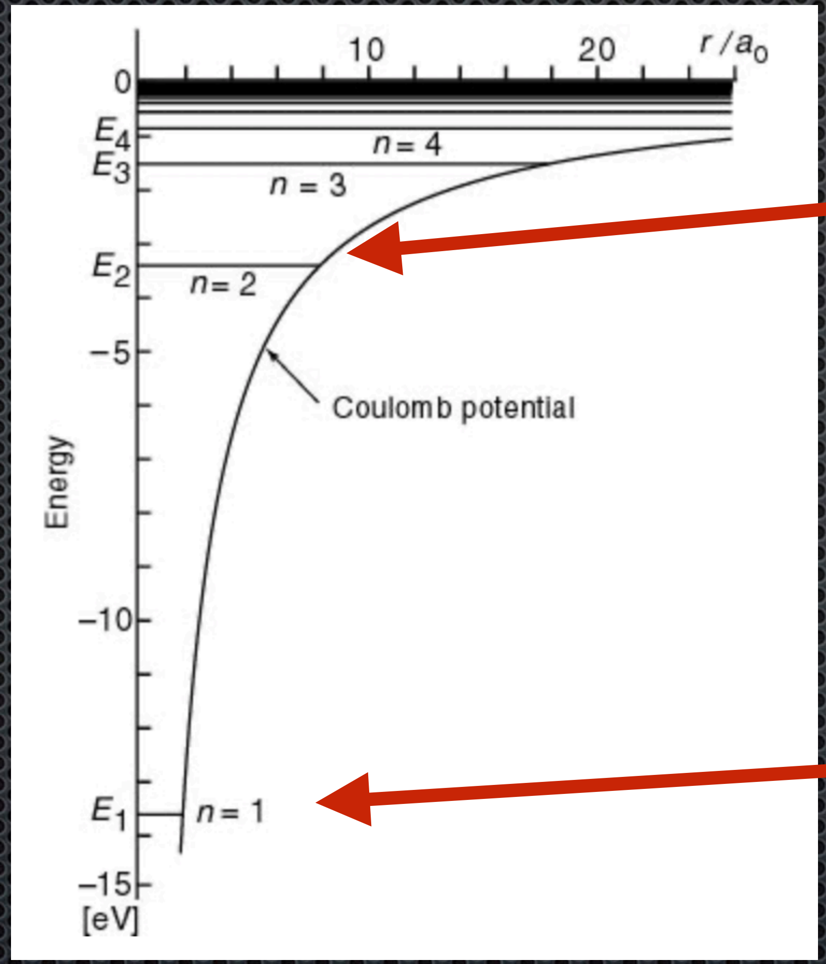
60 billion transistors

~5nm $(=5 \cdot 10^{-9}\text{m})$

Basics: classical vs. quantum

- What happens at $5 \cdot 10^{-11}$ m ("Bohr radius" ~ size of atoms) ?
- At this scale, the laws of quantum mechanics become important
- Atoms also have discrete "states", just like bits!





1 $|1\rangle$

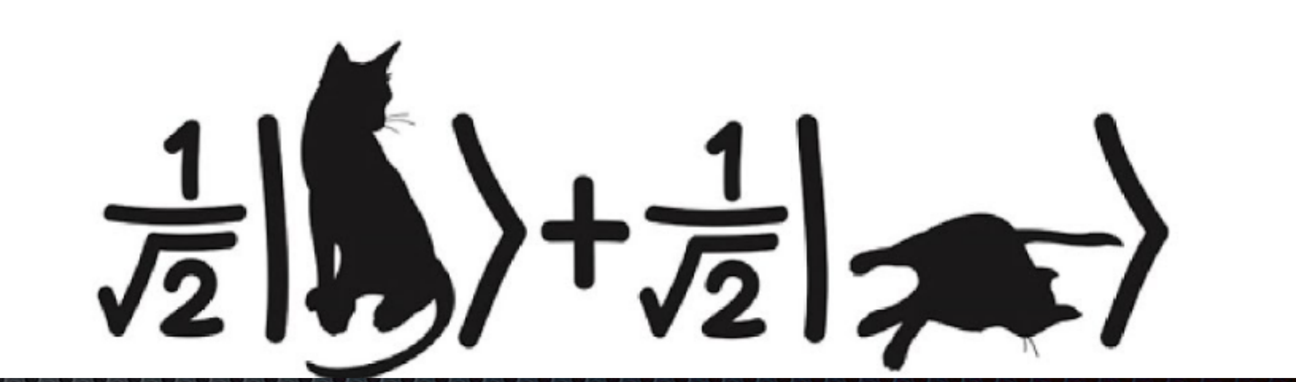
"qubits"

0 $|0\rangle$

Richard Feynman 1981
*"**Nature isn't classical**, dammit, and if you want to make a simulation of **nature**, you'd better make it quantum mechanical…"*

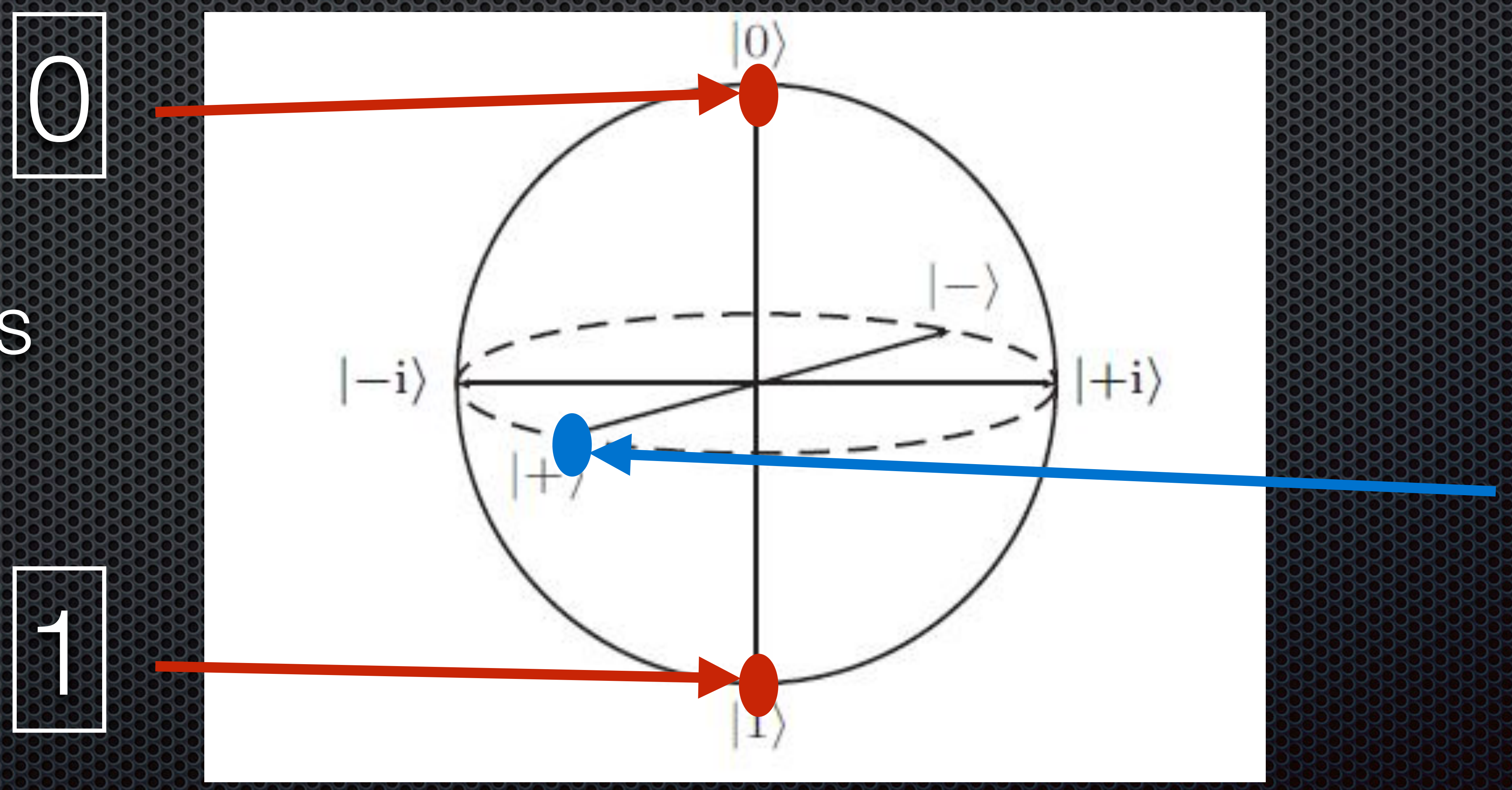
- What if we could harness the laws of quantum mechanics to make a computation?

Basics: classical vs. quantum



- What is so different about quantum bits (qubits)?
- Of course … you all waited for it … Schroedinger's cat! (*) 😻
- Quantum mechical superposition: can be in multiple states simultaneously

classically, the north and south pole are allowed states ("either 0 or 1", no super-position)



quantum mechanically, any point on the sphere is allowed, e.g. here

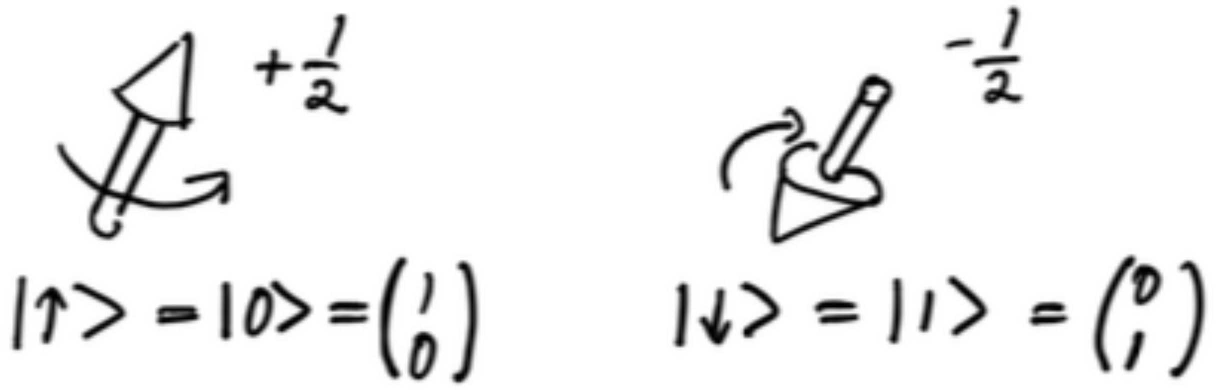
$$\frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|0\rangle$$

("any superposition of 1 and 0")

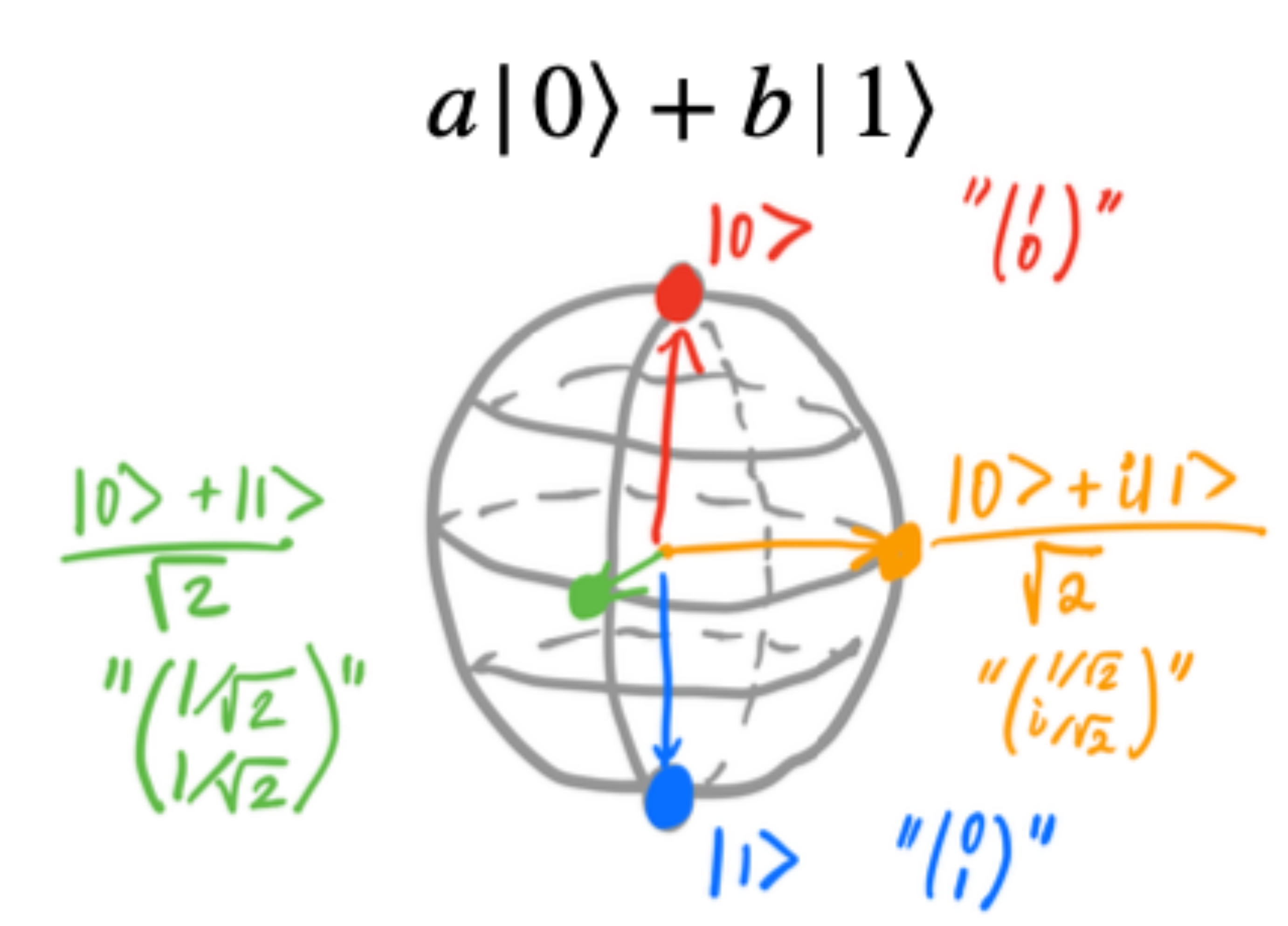
(*) no cats were harmed during the making of this presentation

Basics: Quantum 101

- **Qubit = spin 1/2**



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



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

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

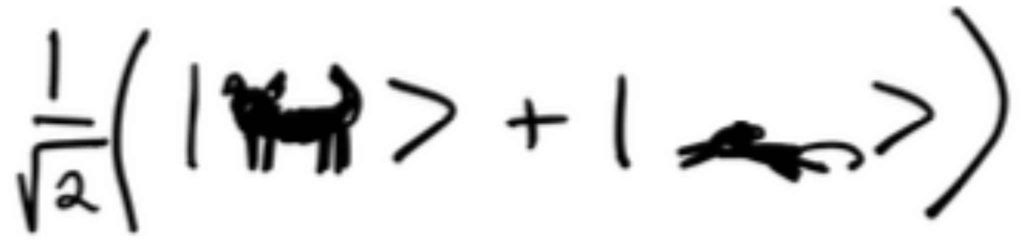
$$\begin{pmatrix} a_0 \\ b_0 \end{pmatrix} \otimes \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} a_0a_1 \\ a_0b_1 \\ b_0a_1 \\ b_1a_1 \end{pmatrix}$$

Size of Hilbertspace grows exponentially ~2^N with quantum mechanical degrees of freedom N!

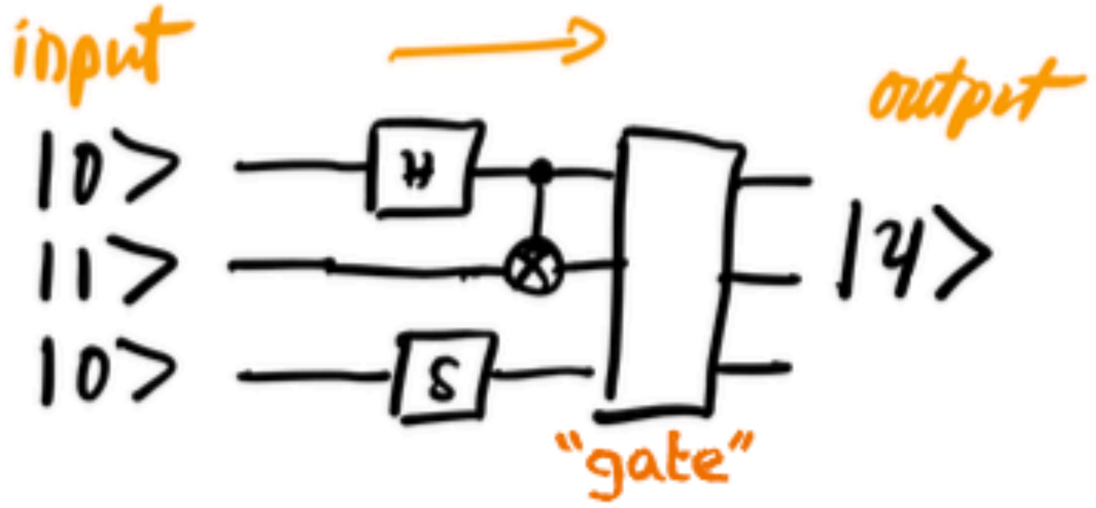
Basics: Quantum 101

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

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

Basics: Quantum 101

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

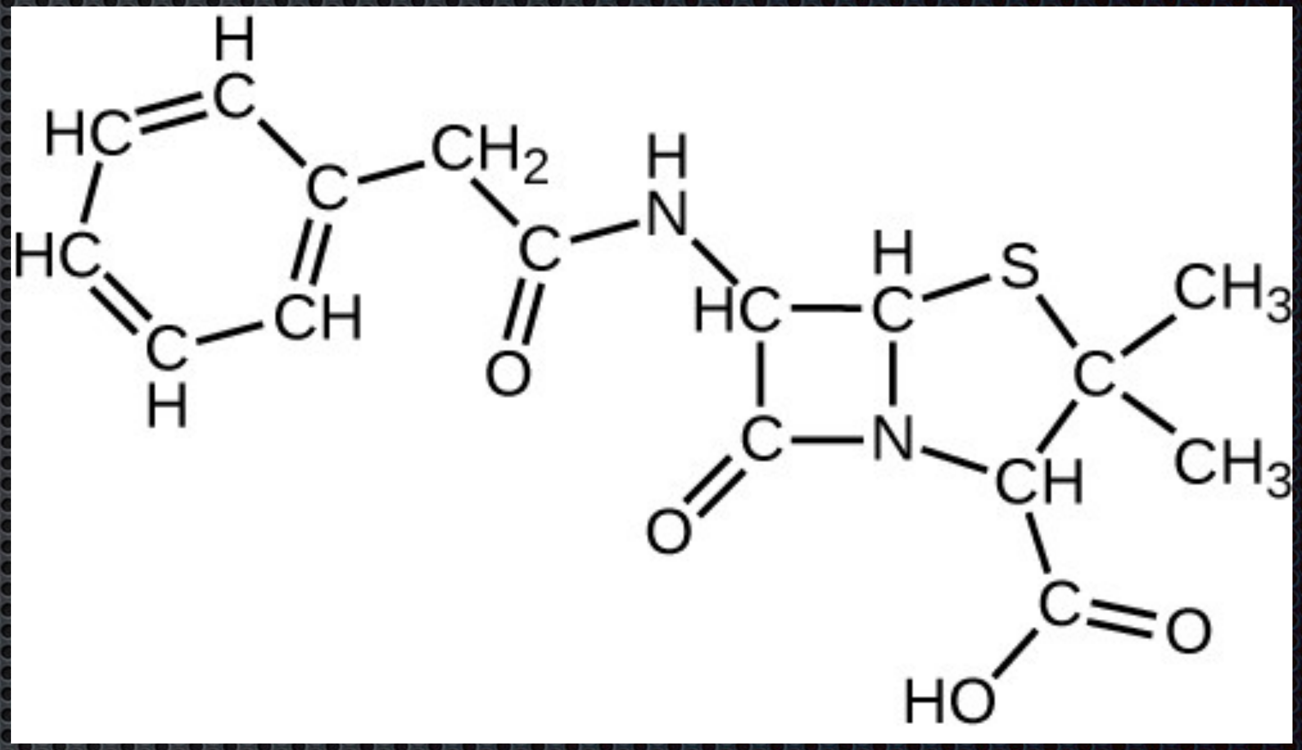
- **Extracting answer from Quantum Computer: subtile issue**

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

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

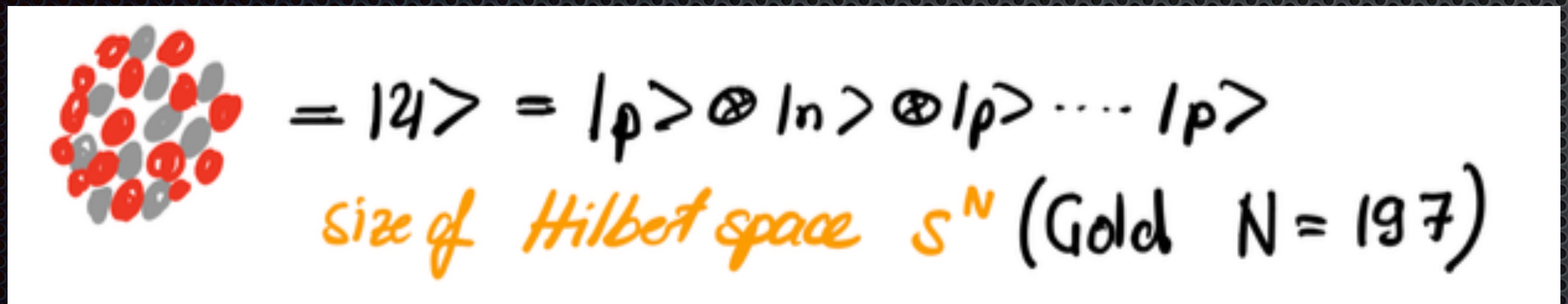
Basics: classical vs. quantum

- Classical computers have a hard time computing something that is quantum mechanical
- How many states can the atoms, making up this molecule, be in?
- simplification: assume 2 states per atom
- What about the states of a **gold ion?**



200 “2 state”atoms = $2^{200} \sim 10^{60}$ coefficients, earth consists of $\sim 10^{50}$ atoms. Not enough atoms to build (classical) RAM memory

Yet if you could use 200 qubits, you could do the computation



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

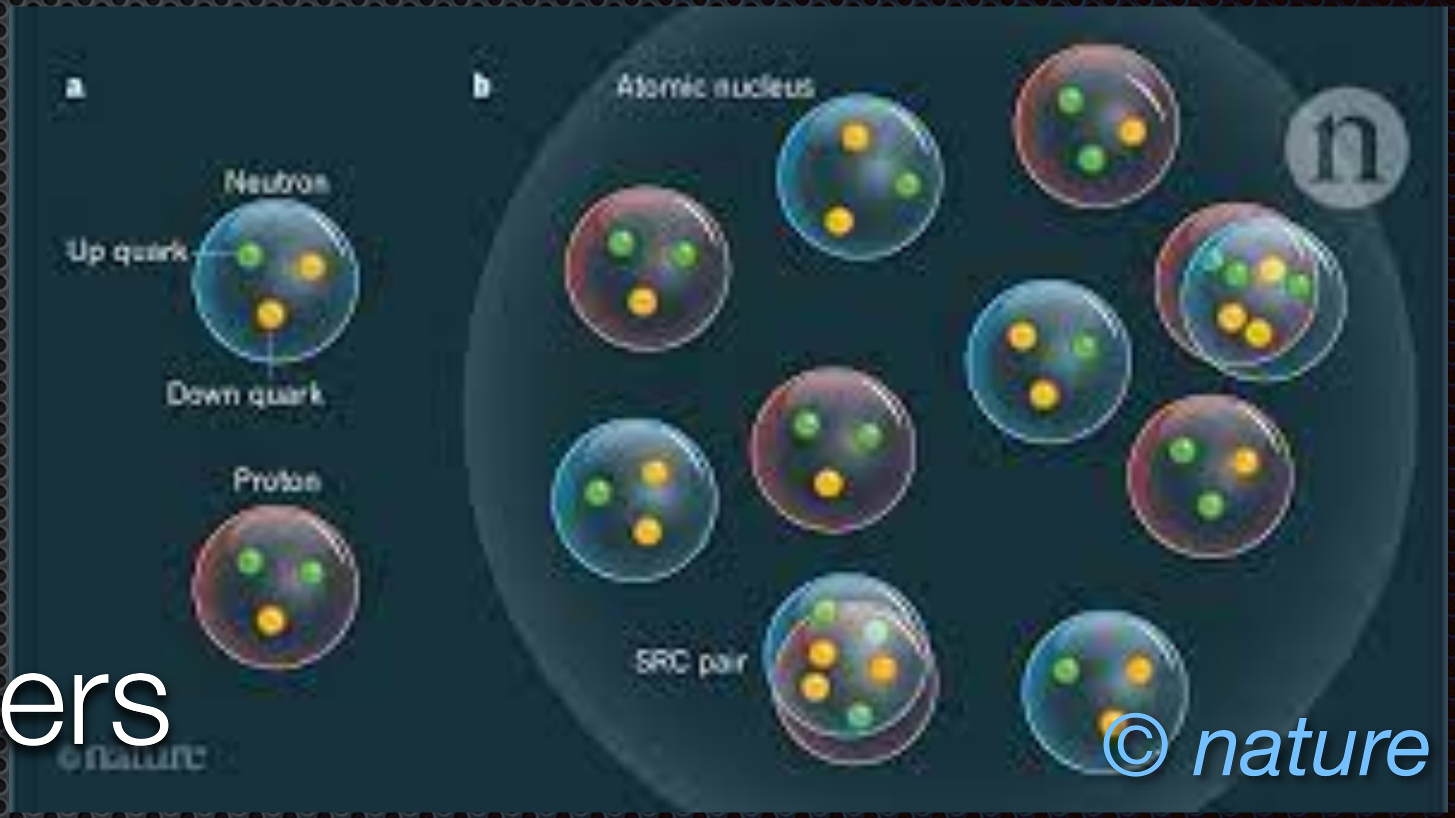
(Hamiltonian operator)

Matrix equation of size

$$2^{197} \sim 10^{59}$$

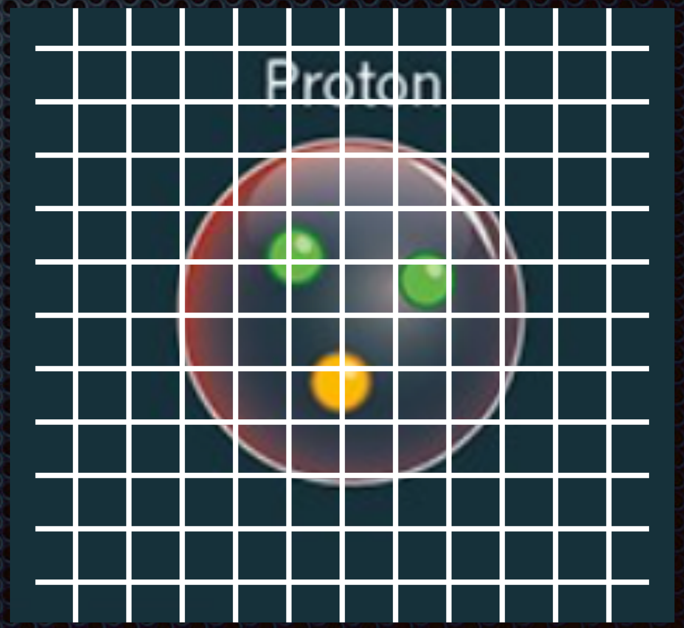
Quantum Computation for Physics

- What can we learn about the fundamental forces of nature, such as the theory of the strong interactions that binds together protons, neutrons and nuclei?

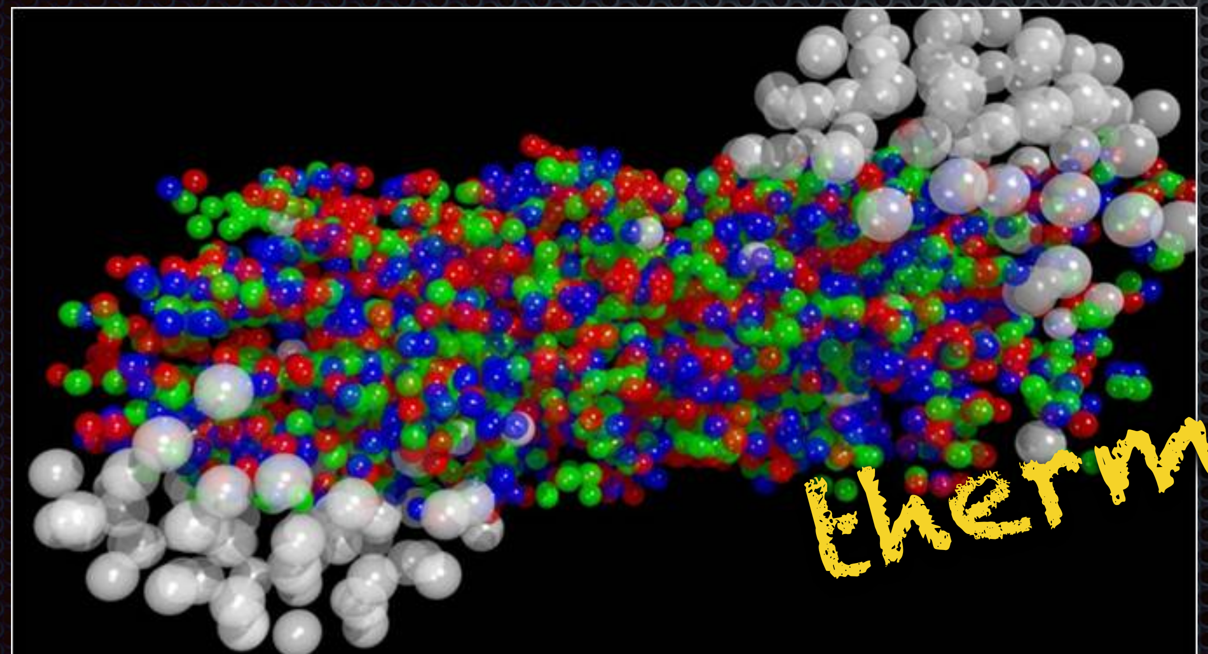


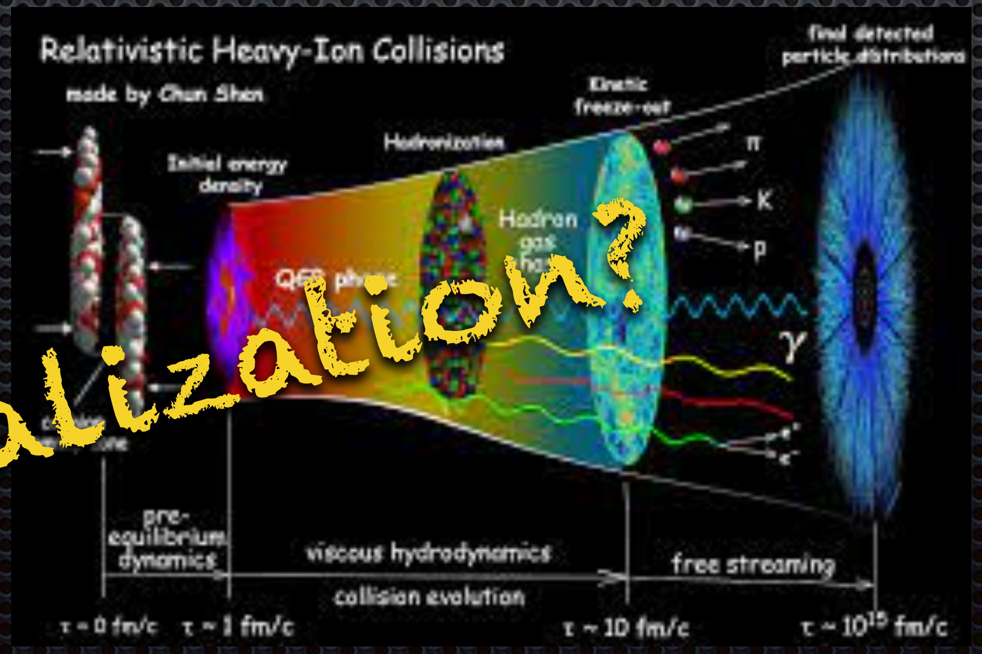
- Very few problems can be solved on classical computers

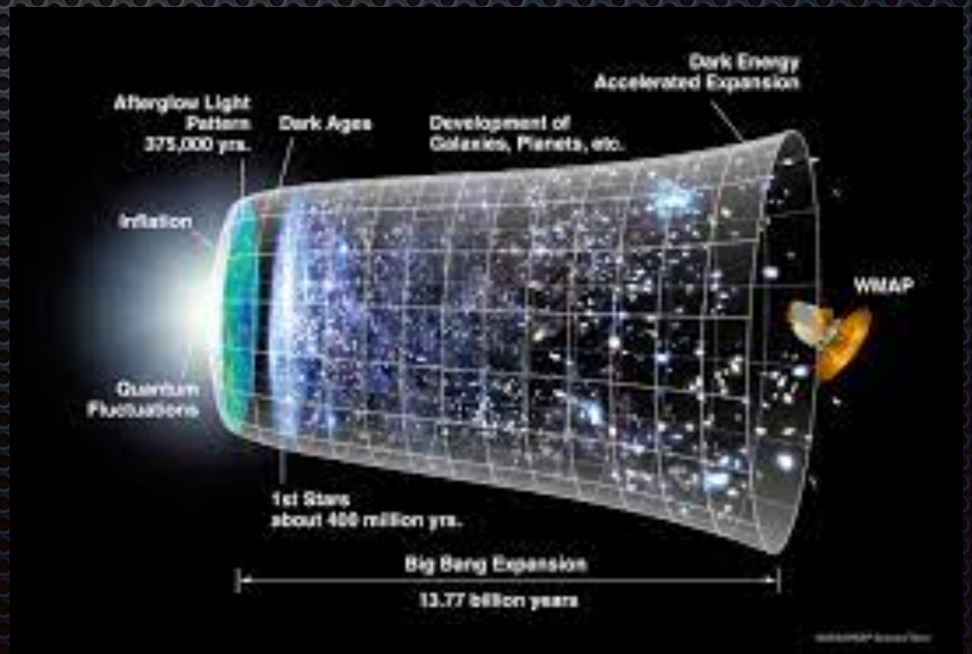
mass of the proton ✅
(after ~45 years of development only cost us a lot of $$)



- The interesting problems can't!







"Lattice Gauge Theory"

Quantum Computation for Physics

- Quantum Many-Body Theory → Quantum Field Theory

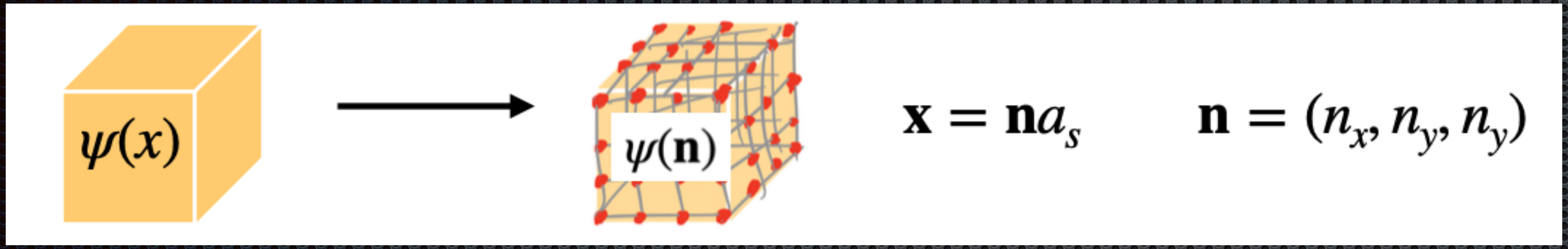
- Example: (Quantum) Electrodynamics

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

- Every x lables on quantum mechanical degree of freedom

Quantum Computation for Physics

- Quantum Field Theory → **Lattice** Quantum Field Theory



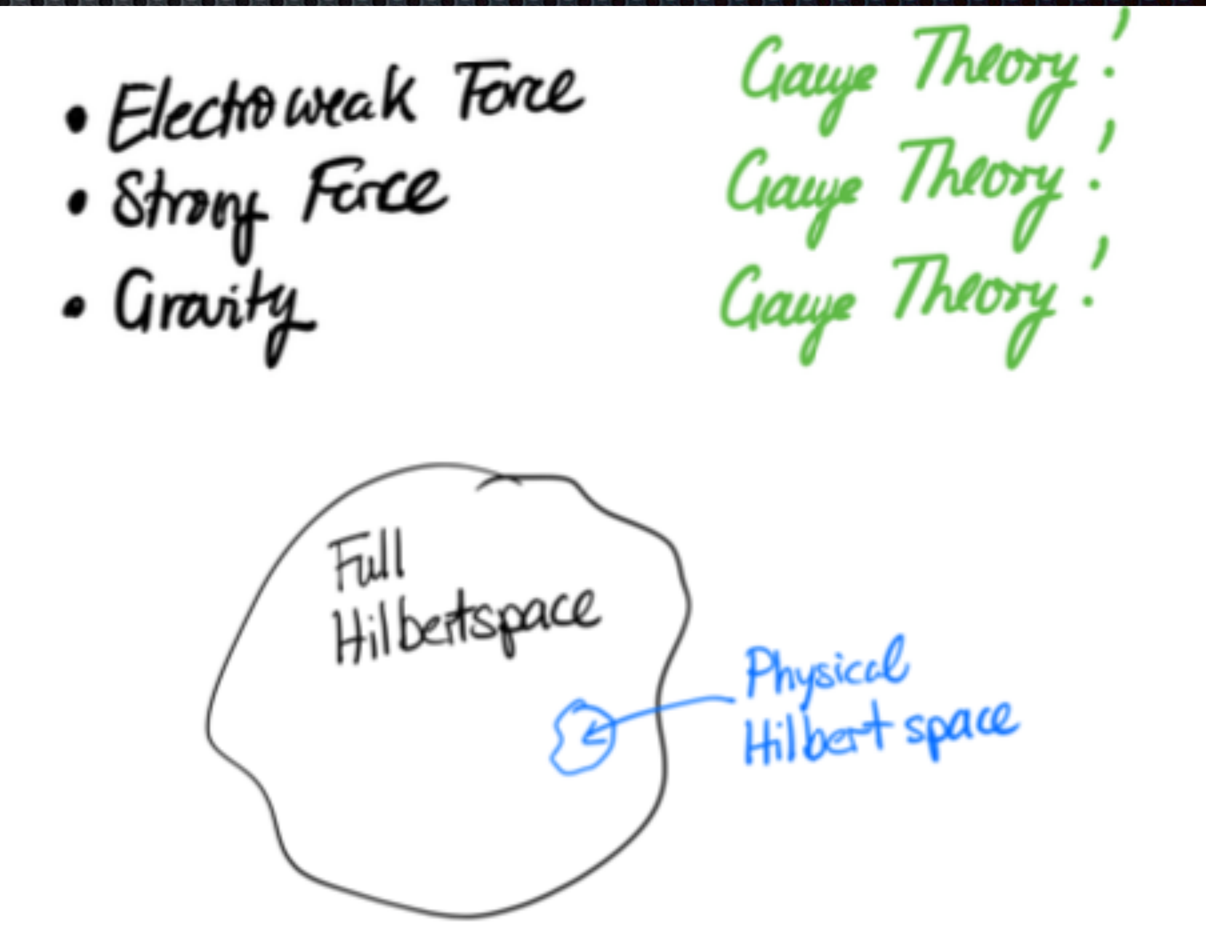
- Lattice Quantum Field Theory ~ Quantum Many Body Theory

Quantum Computation for Physics

Challenges

- Gauge Theories (e.g. Quantum Electrodynamics, QED)

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

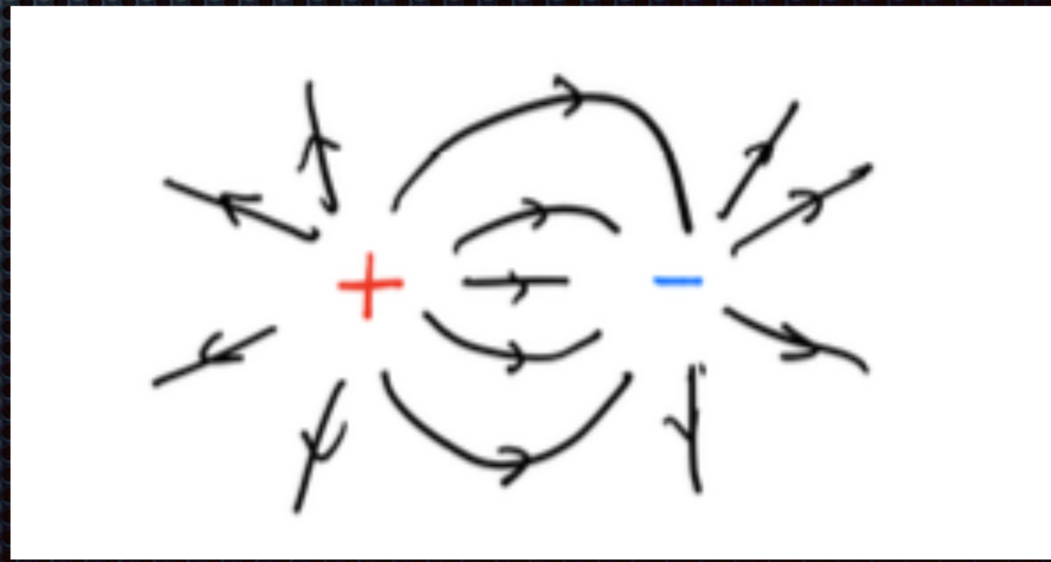


- Redundancy, not all dofs are physical

- Gauss law (operator) defines physical sector

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

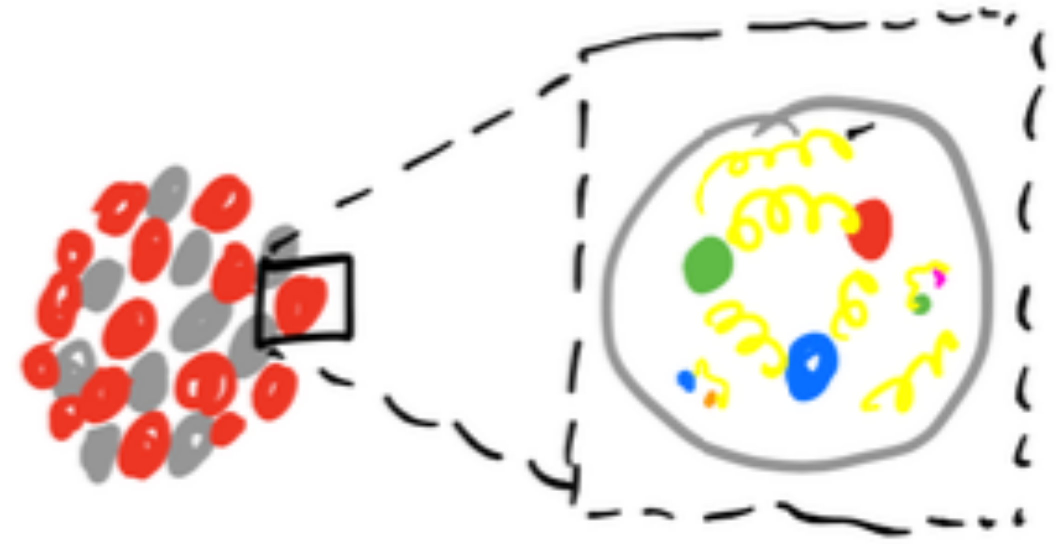
$$G(\mathbf{x}) = \nabla_{\mathbf{x}} E(\mathbf{x}) - J(\mathbf{x})$$



Quantum Computation for **Nuclear** Physics

Lattice QCD Simulations

Quantum Chromodynamics (QCD)



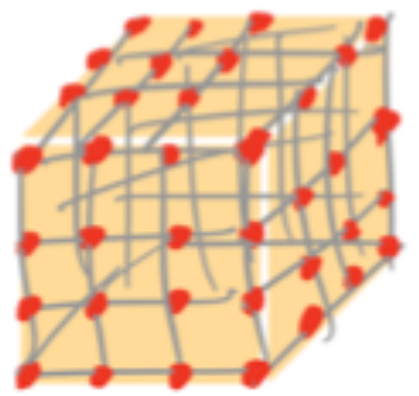
- From Hamiltonian to Lagrangian

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

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

- … to path integral

$$Z = \int dA\, e^{iS_{\mathrm{QCD}}[A]}$$



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

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

- in Euclidean Spacetime: statistical mechanics problem

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

Lattice Monte-Carlo simulations work in many dimensions!

Quantum Computation for **Nuclear** Physics

Lattice QCD Simulations

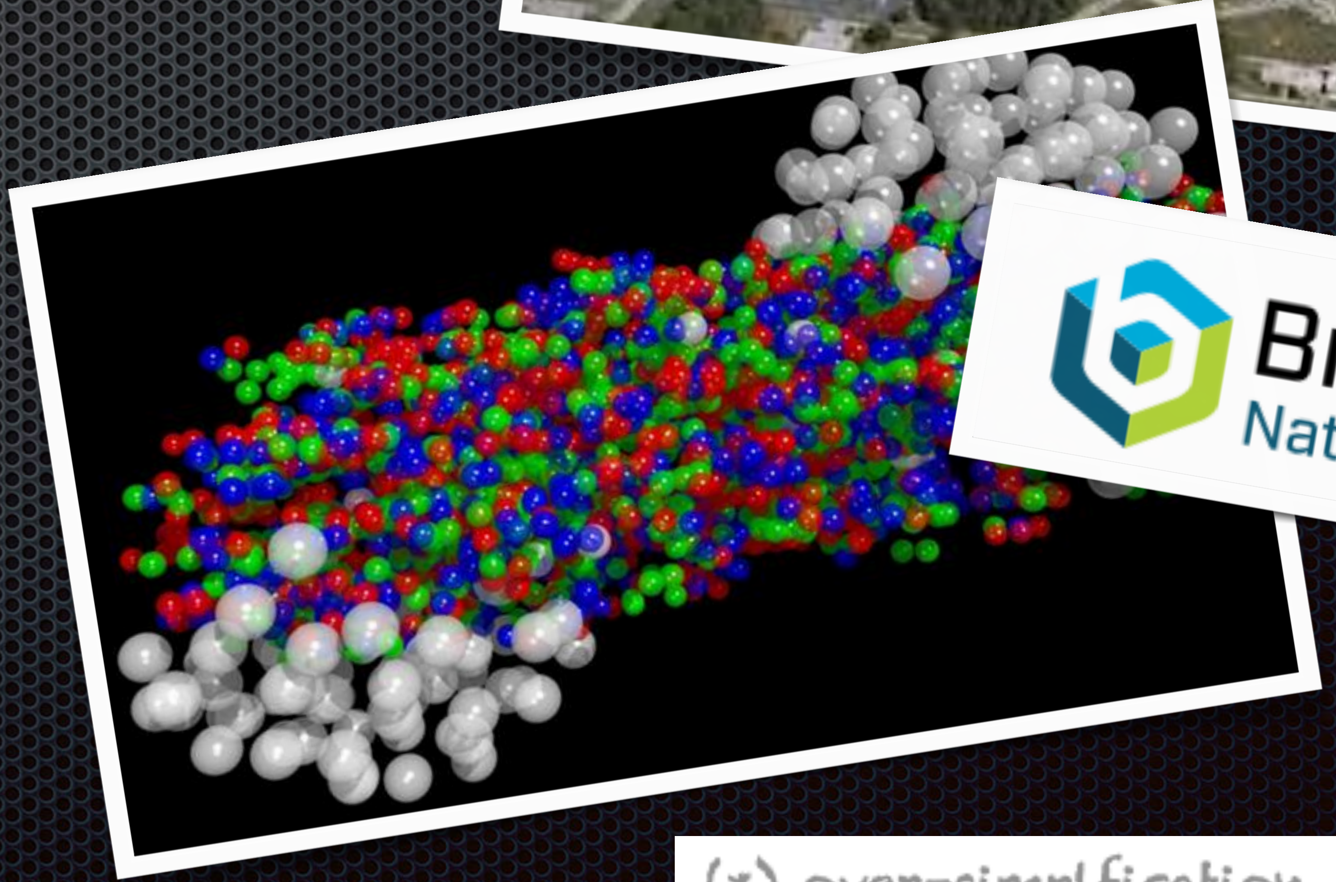
- very expensive
- do not work for various interesting problems (*)

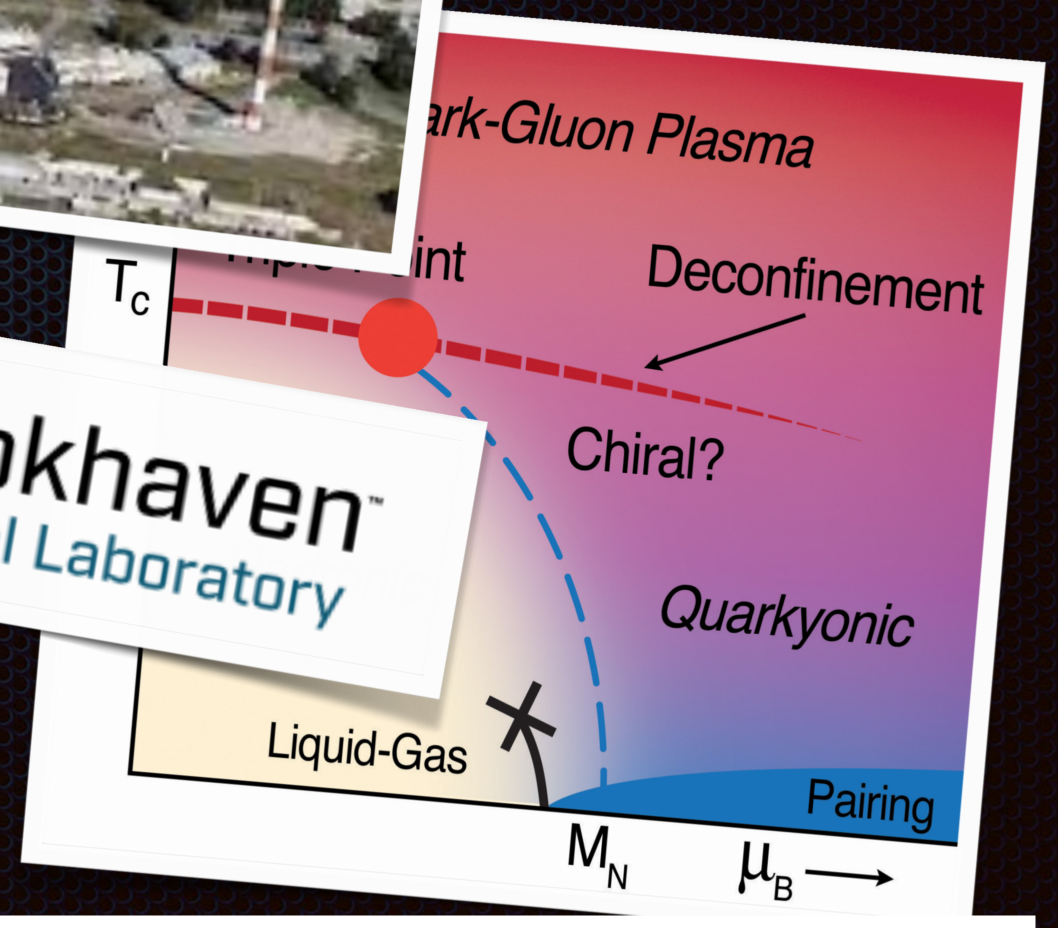
- ~~Real-time physics, systems out of Equilibrium~~ Nope, euclidean space time remember?

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

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

imaginary!

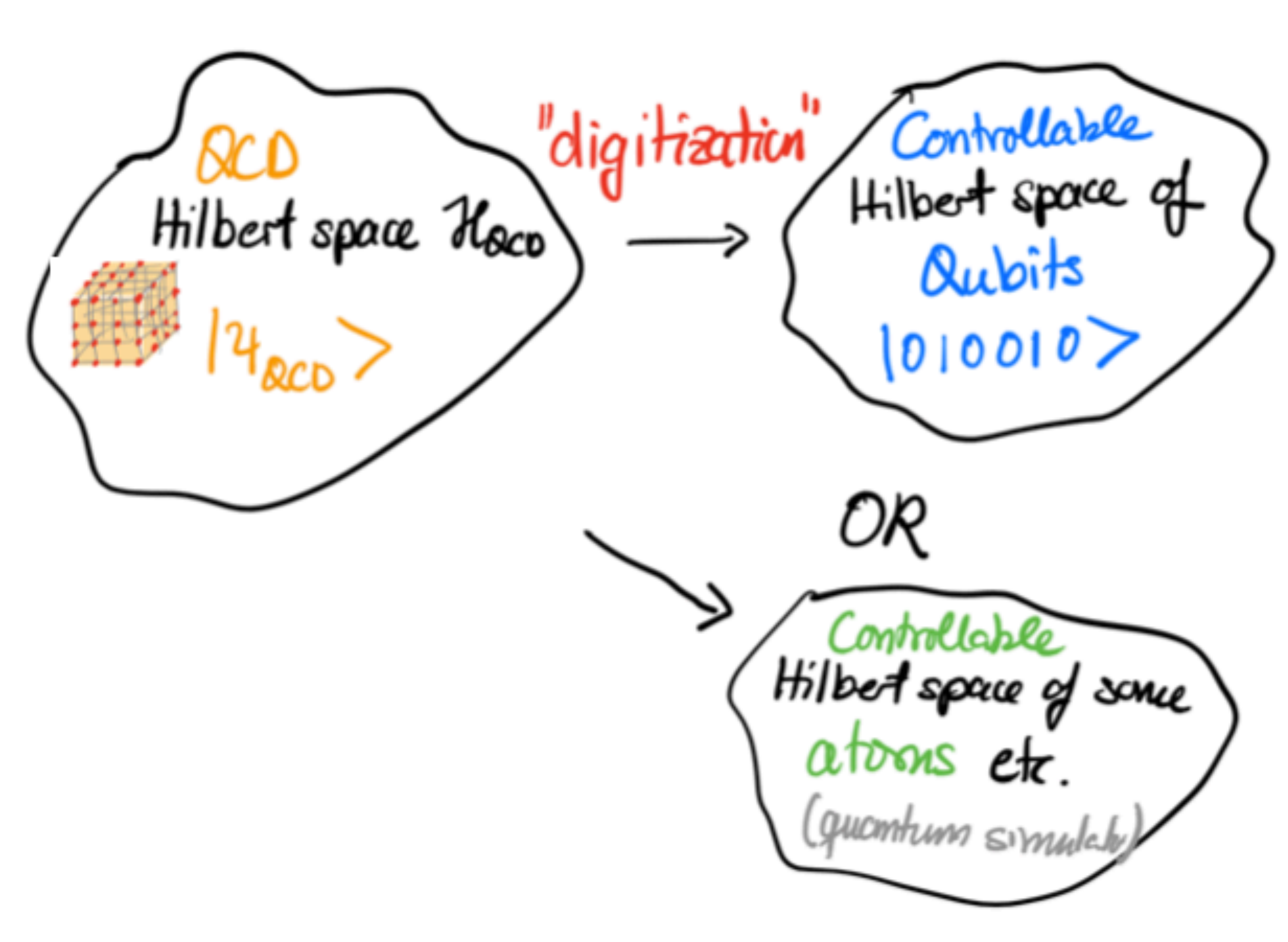




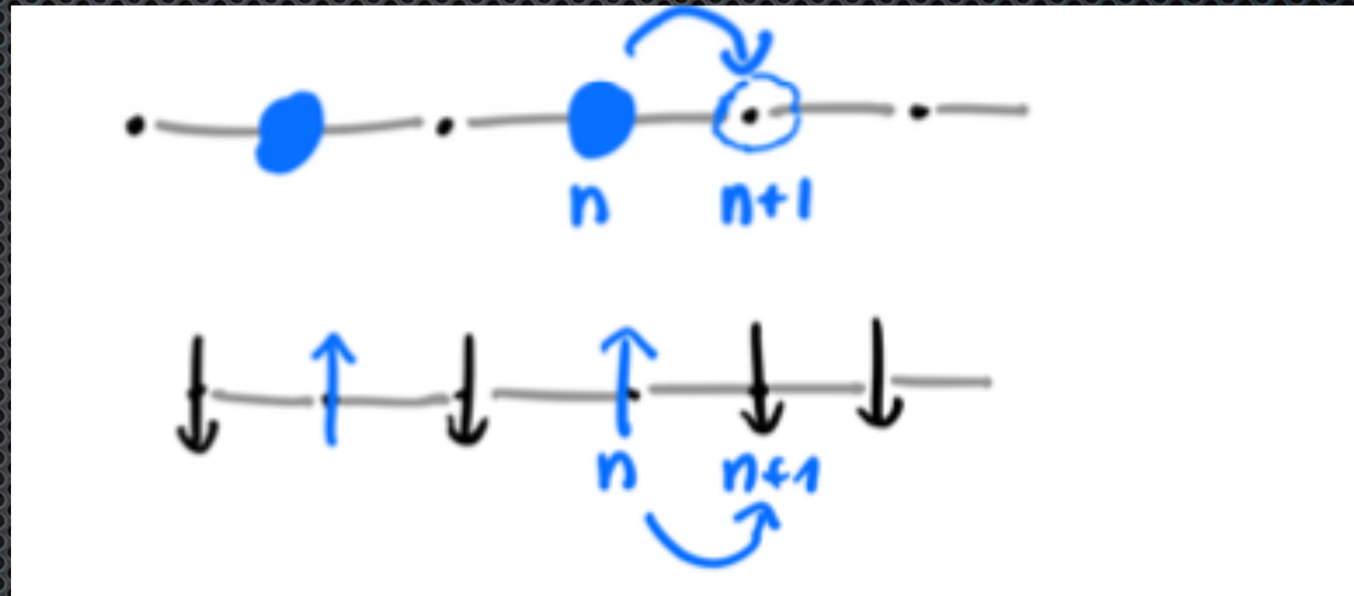
(*) over-simplfication. Please dont be mad, lattice practitioners

Quantum Computation: How to do it?

step 1: Digitization



- example fermions in 1d



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

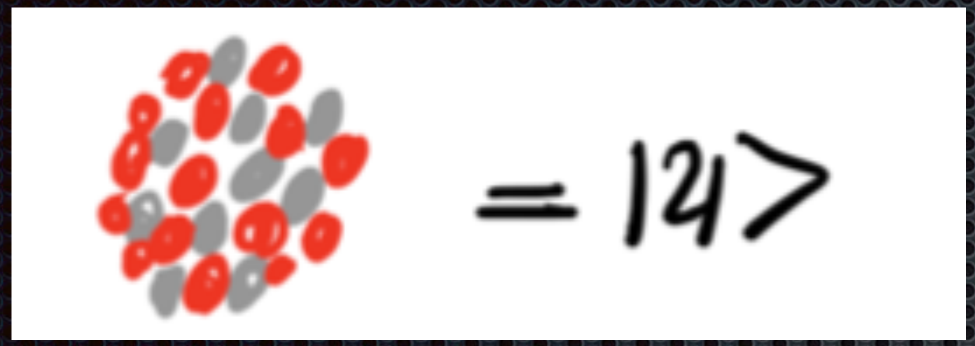
- Local Hilbert space $\mathscr{H} = \bigotimes_n \mathscr{H}_n$

- Fermion = 2 states (occupied/unoccupied)
- qubit = 2 states $(|1\rangle, |0\rangle)$

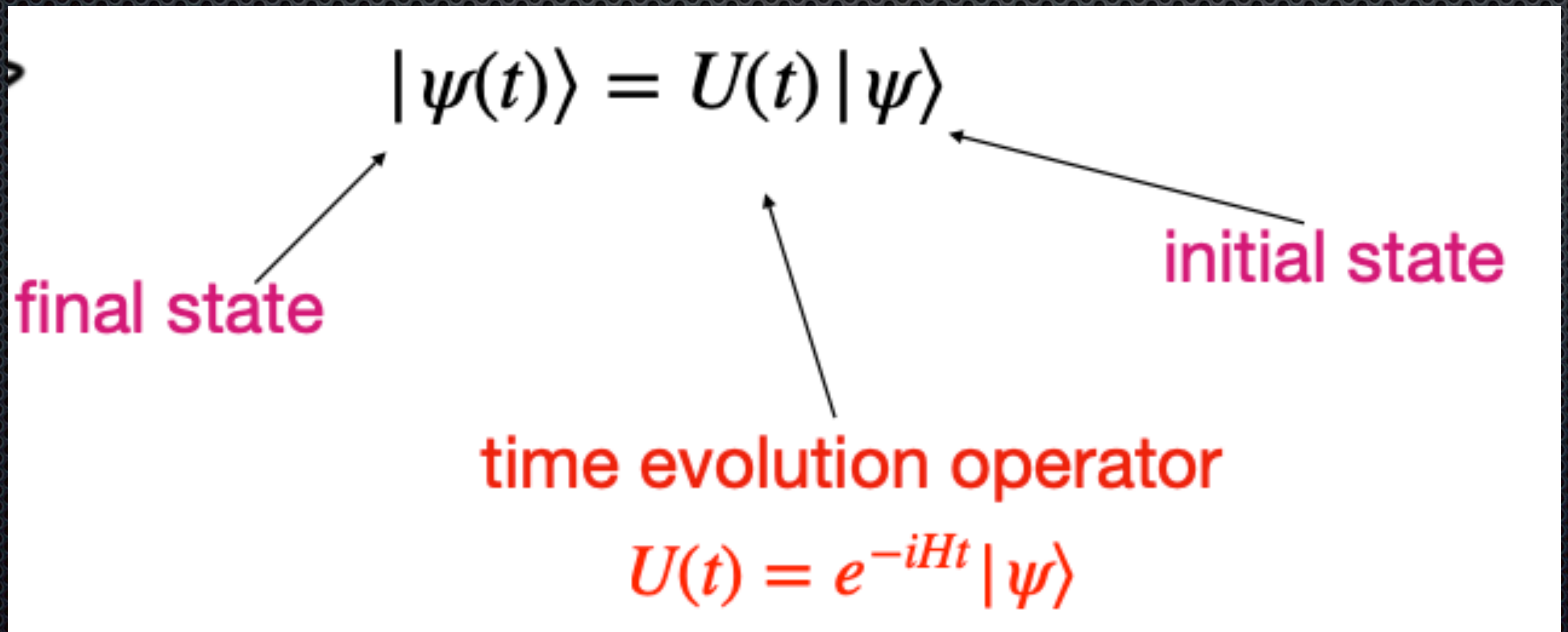
Quantum Computation: How to do it?

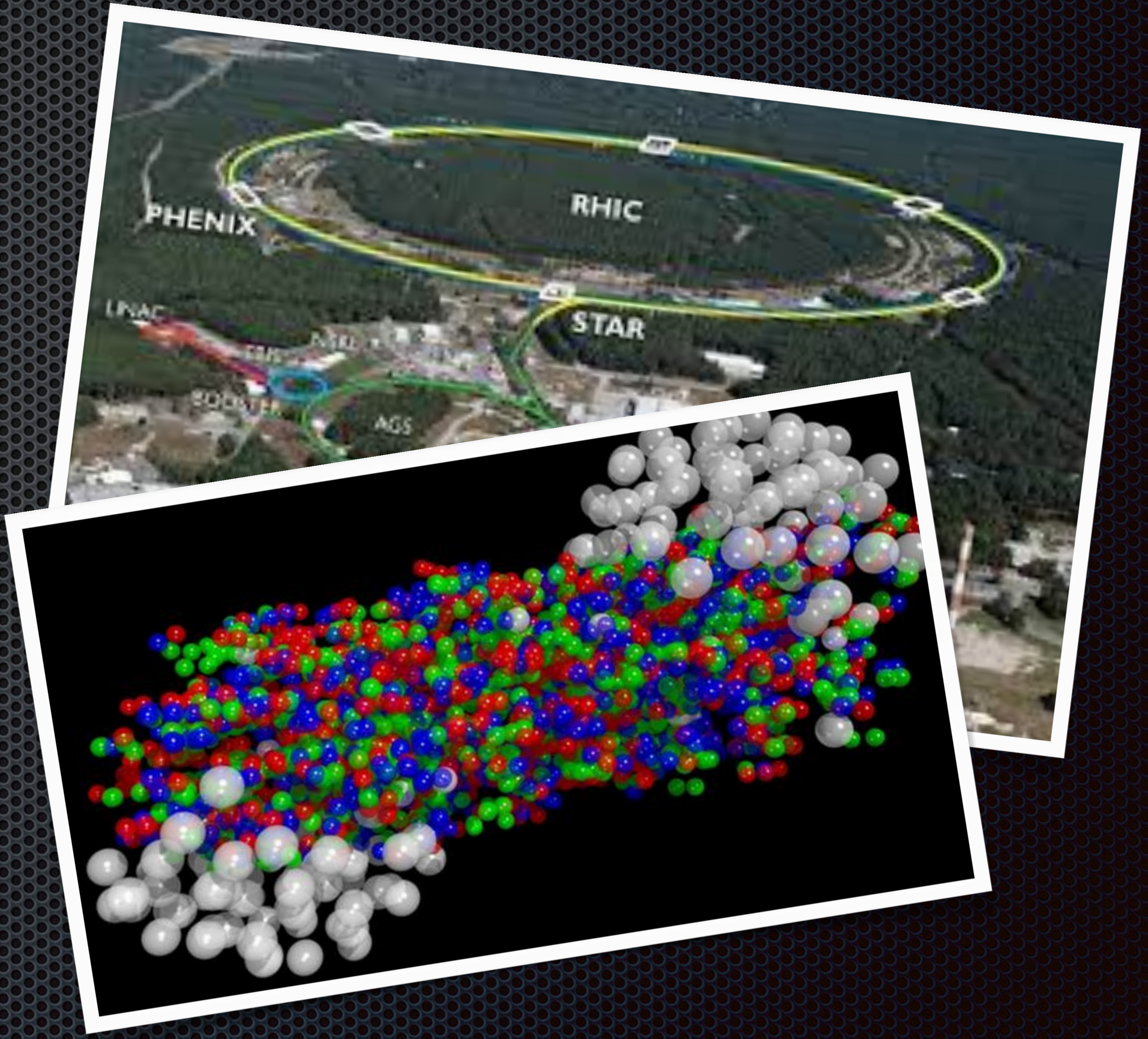
step 2: come up with an algorithm

- example: real-time dynamics



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

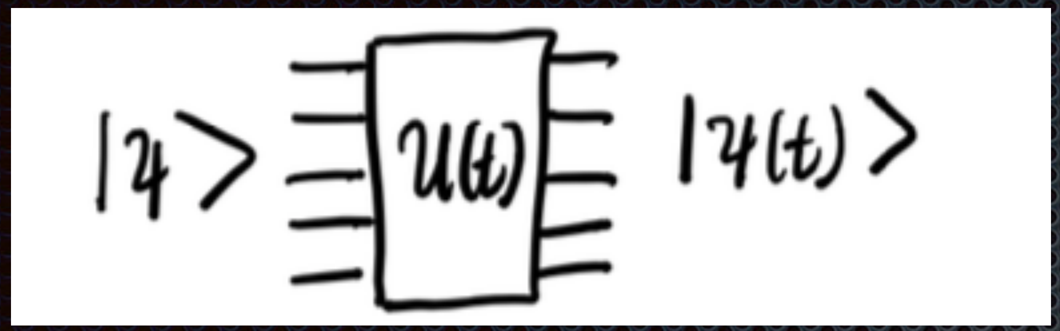


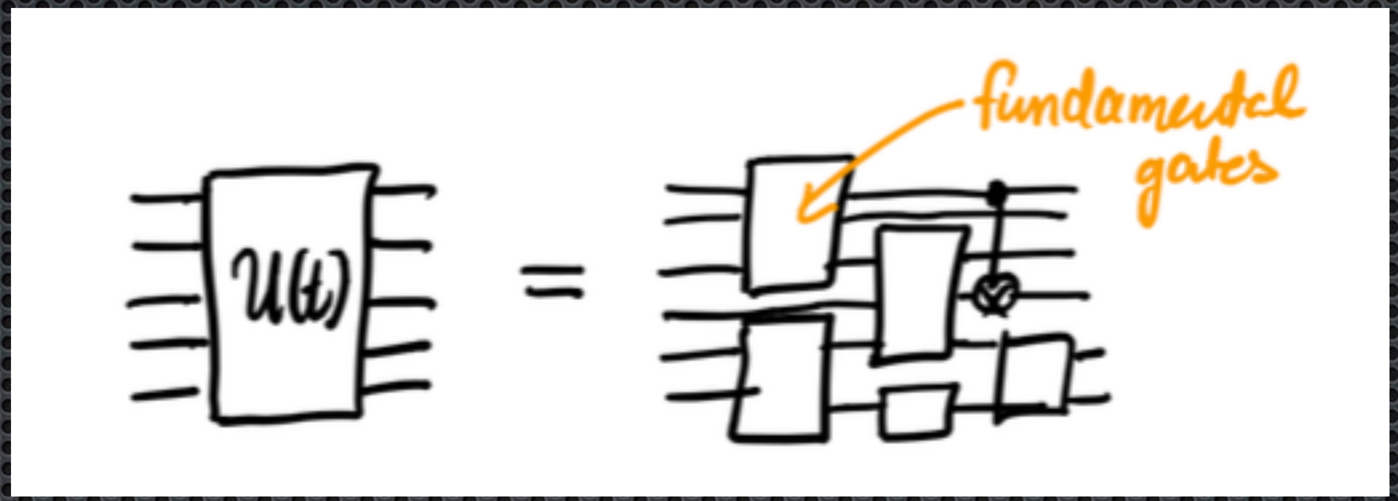


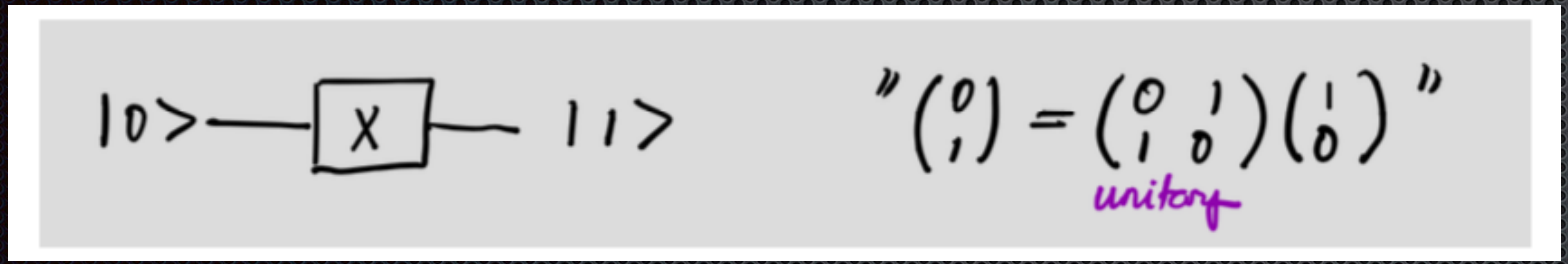
Quantum Computation: How to do it?

step 2: come up with an algorithm

- Decompose time evolution operator $U(t)$ into a circuit







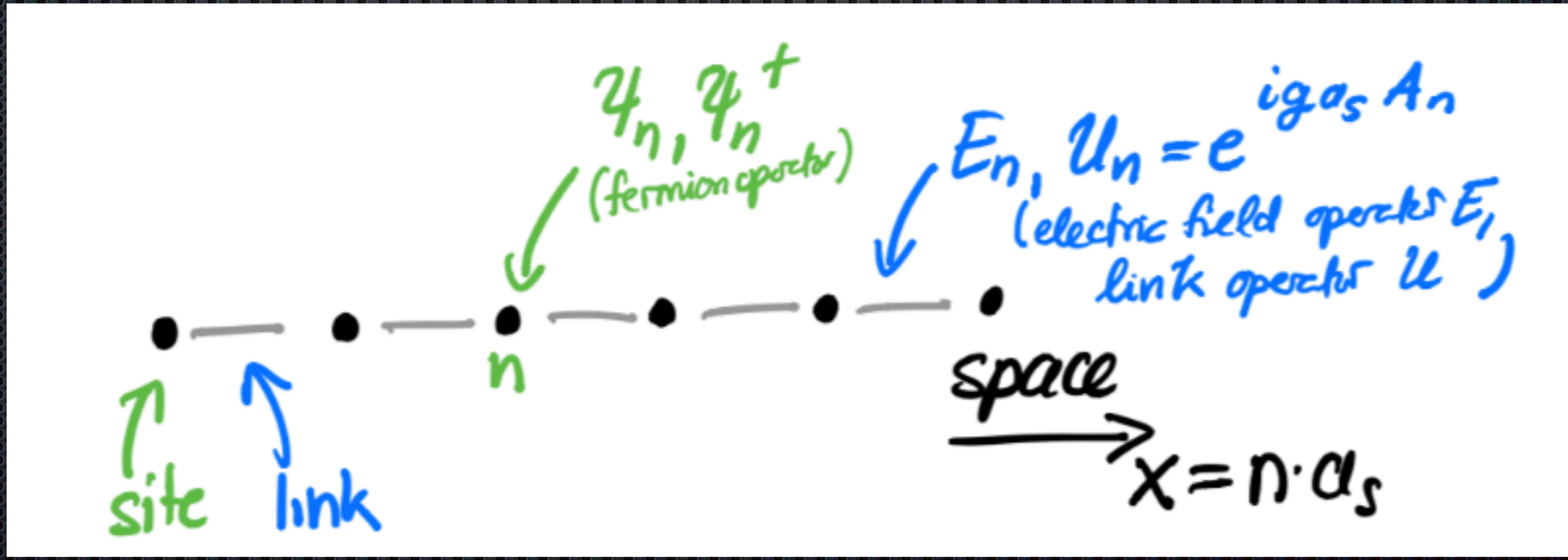
- Details beyond this lecture.

  However, for one fermion/spin with Hamiltonian
  $H = -\sigma^z$, can you figure out a circuit?
  Hint: use the gates in "Quantum Computation and Quantum Information"
  Nielsen & Chuang

Quantum Computation: How to do it?

Diving deeper. I will go a little faster now. Sit back and relax.

- QED_{1+1} Schwinger model: $$H = \int dx [\frac{E_x^2}{2} + \psi^\dagger \gamma^0 (i\gamma^1 D_x + m)\psi_x]$$
- Lattice Theory $$H = a_s \sum_n [\frac{E_n^2}{2} - \frac{i}{2a_s}(\psi_n^\dagger U_n \psi_{n+1} - h.c.) + m(-1)^n \psi_n^\dagger \psi_n]$$

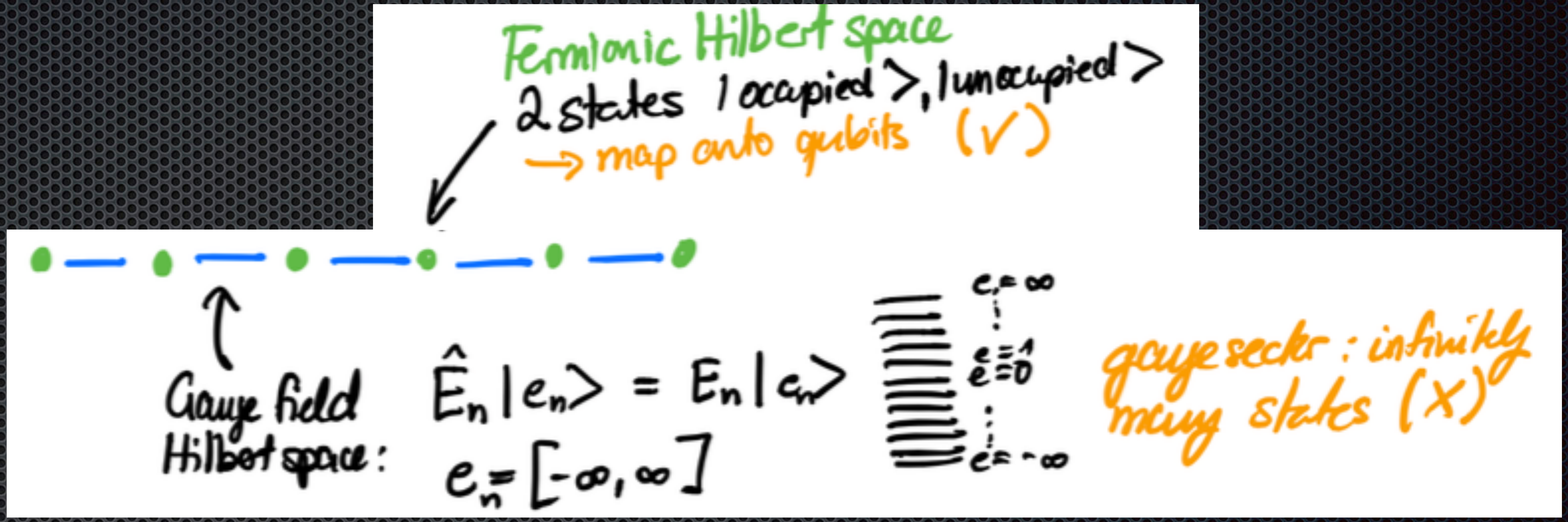


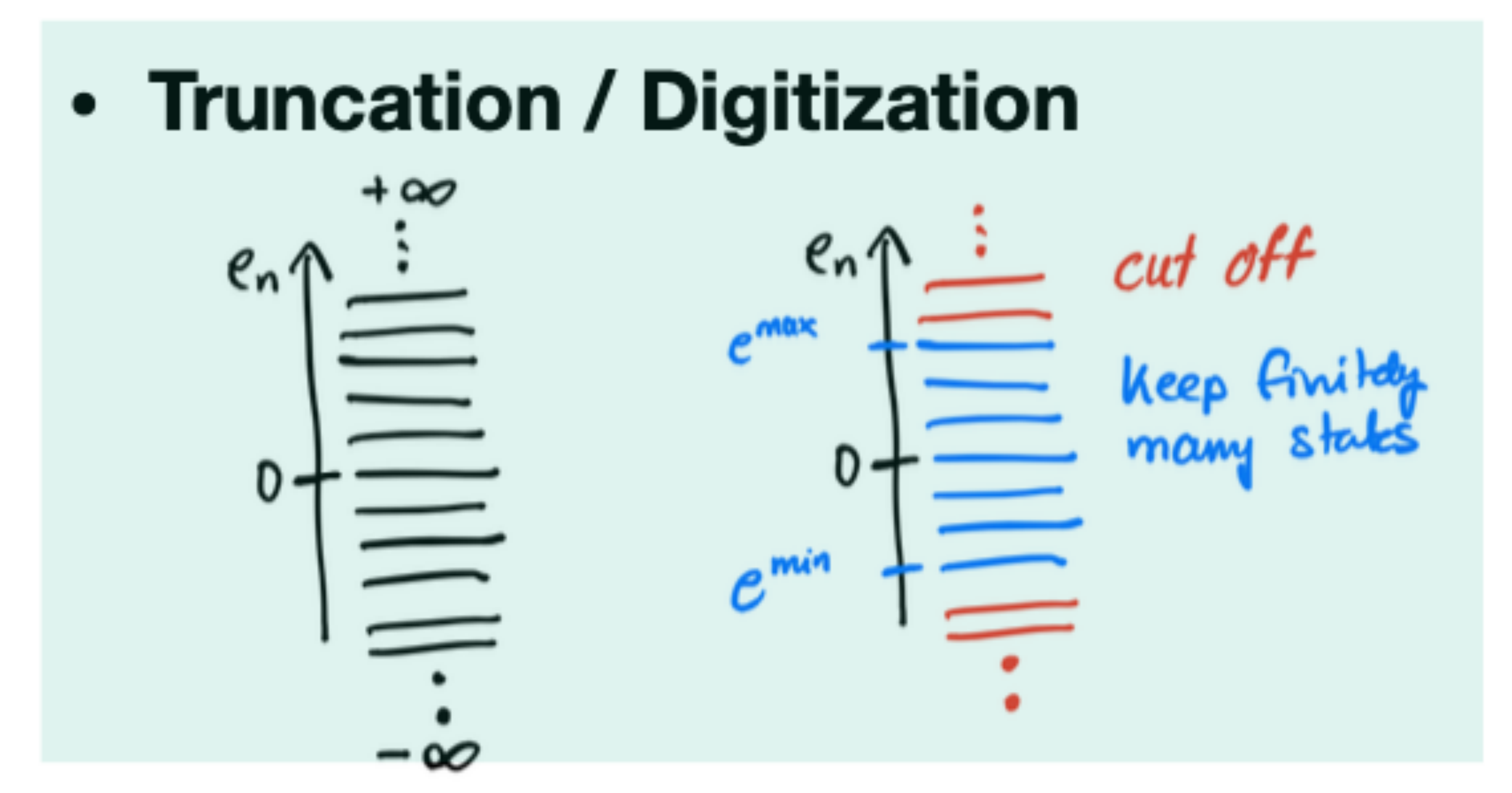
Operator Formulation of Lattice Gauge Theory

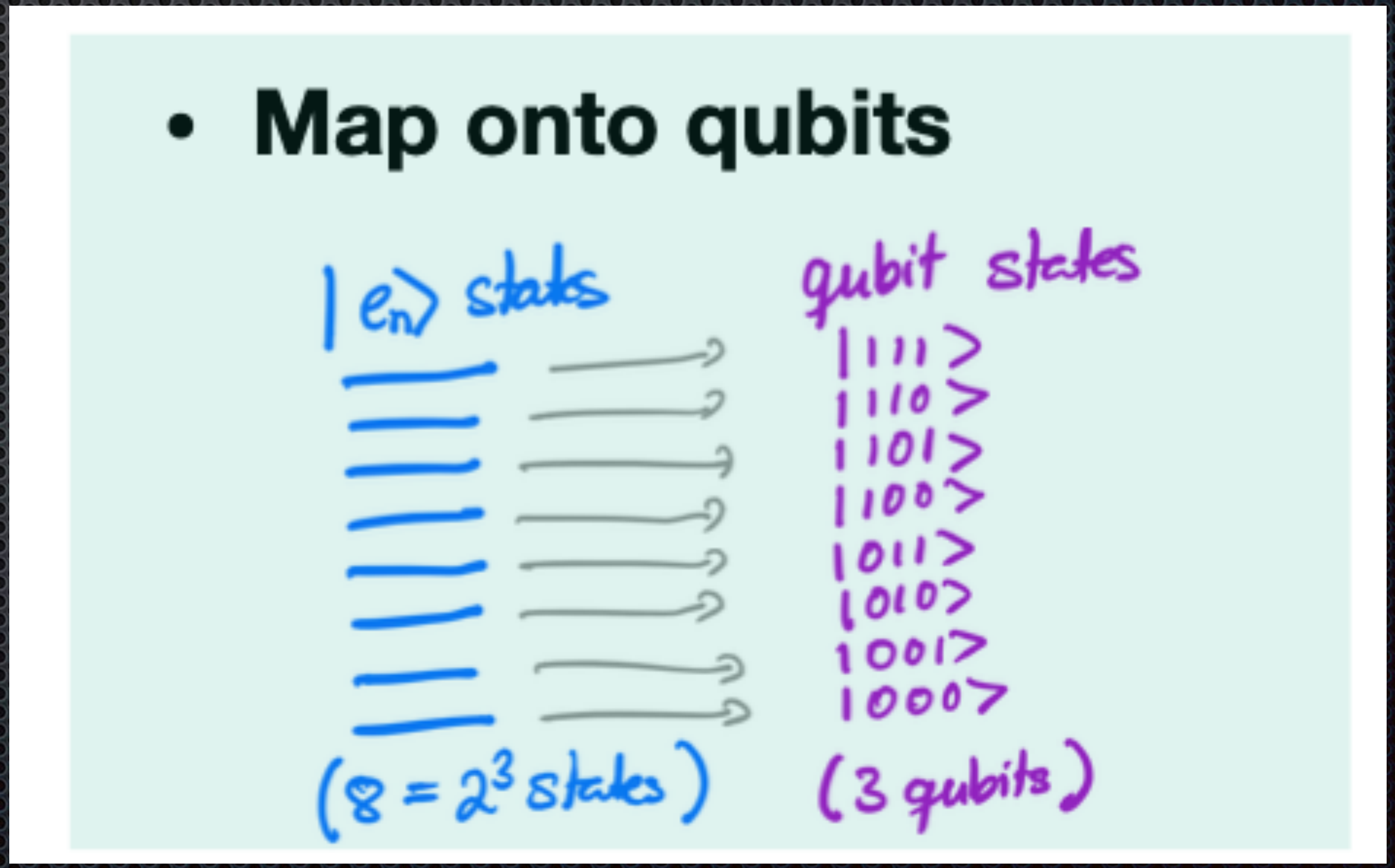
- Hilbert space, gauge sector

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

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

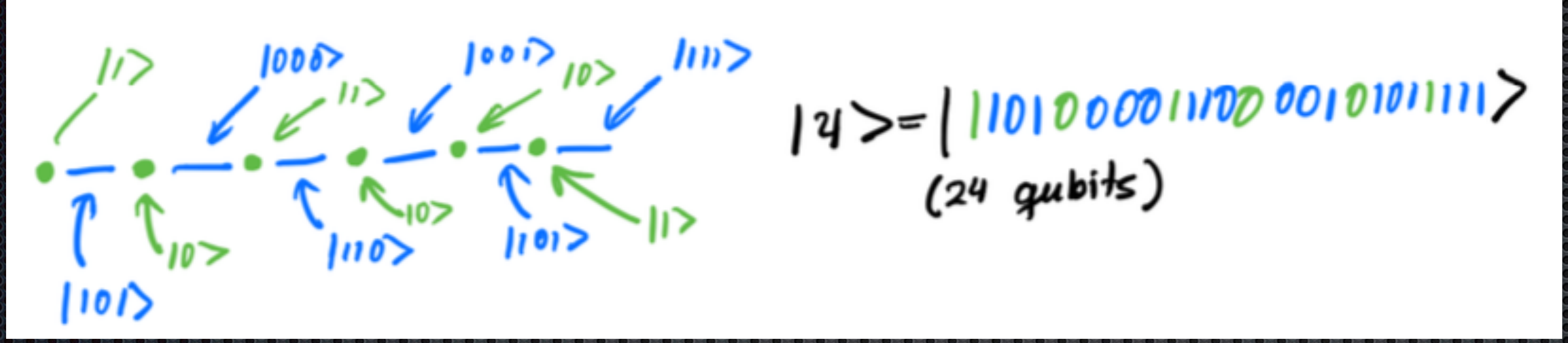






Operator Formulation of Lattice Gauge Theory

- A state of the full theory



- Most of Hilbert space 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 physical, it will stay physical

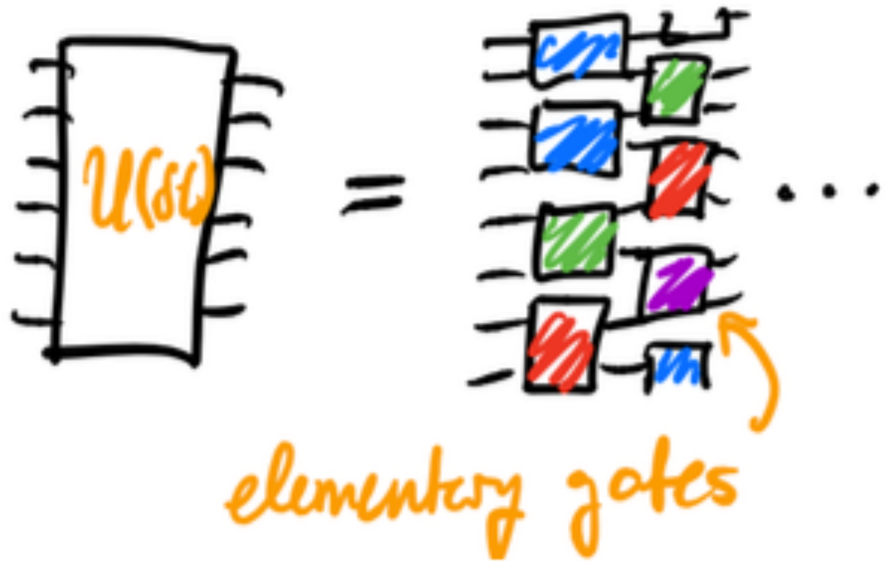
$$|\psi(t)\rangle = U(t)\,|\psi\rangle = e^{-iHt}\,|\psi\rangle$$

Operator Formulation of Lattice Gauge Theory

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

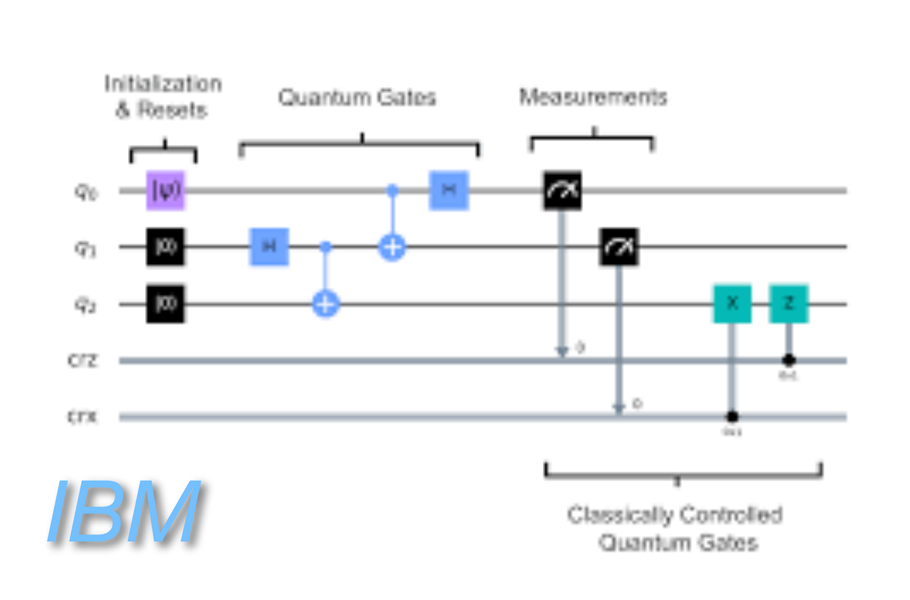
- $U(t) = \prod_t U(\delta t)$

"Trotterization"



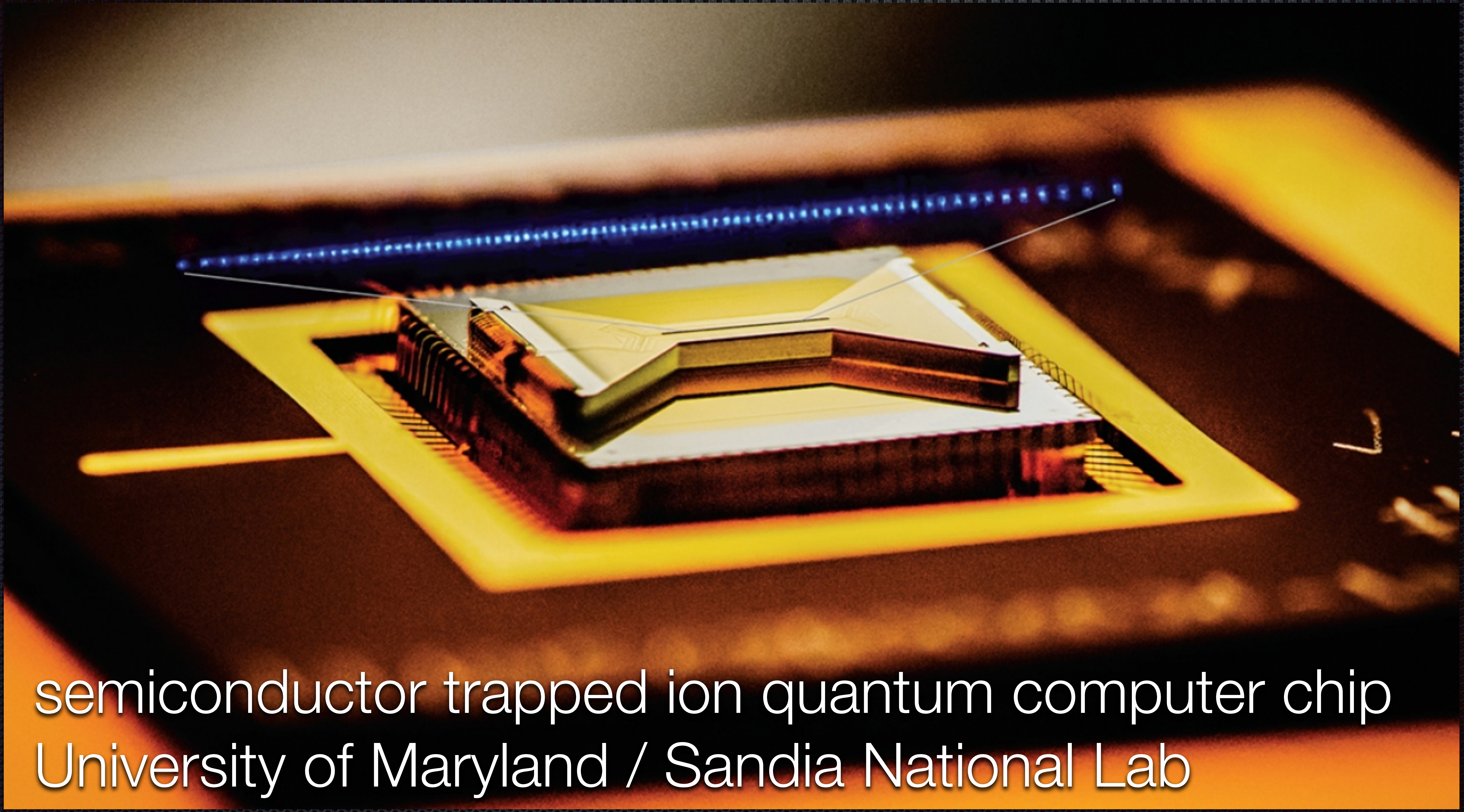
Trapped ions:
Martinez et al, Nature 534 (2016) 516

Physics world breakthrough of the year
Martinez, Muschik, Schindler, Nigg, Erhard, Heyl, Hauke, Dalmonte, Monz, Zoller, Blatt, *Nature* 2016



- Take a look at https://quantum-journal.org/papers/q-2020-08-10-306/ to see actual circuits!

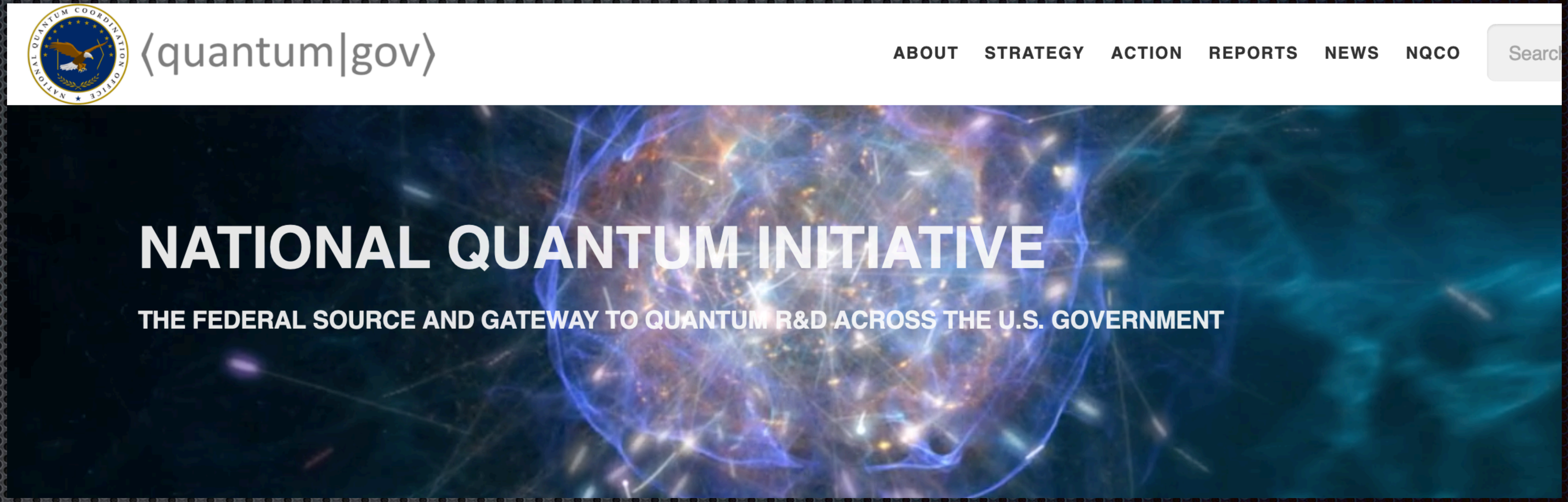
Science Fiction?



semiconductor trapped ion quantum computer chip
University of Maryland / Sandia National Lab

Quantum is picking up speed!

National Quantum Initiative
quantum.gov



U.S. DEPARTMENT OF ENERGY | Office of Science

NSF

Brookhaven National Laboratory

At Brookhaven:

https://www.bnl.gov/quantumcenter/

https://science.osti.gov/Initiatives/QIS/QIS-Centers

C^2QA Co-design Center for Quantum Advantage

more shameless advertisement

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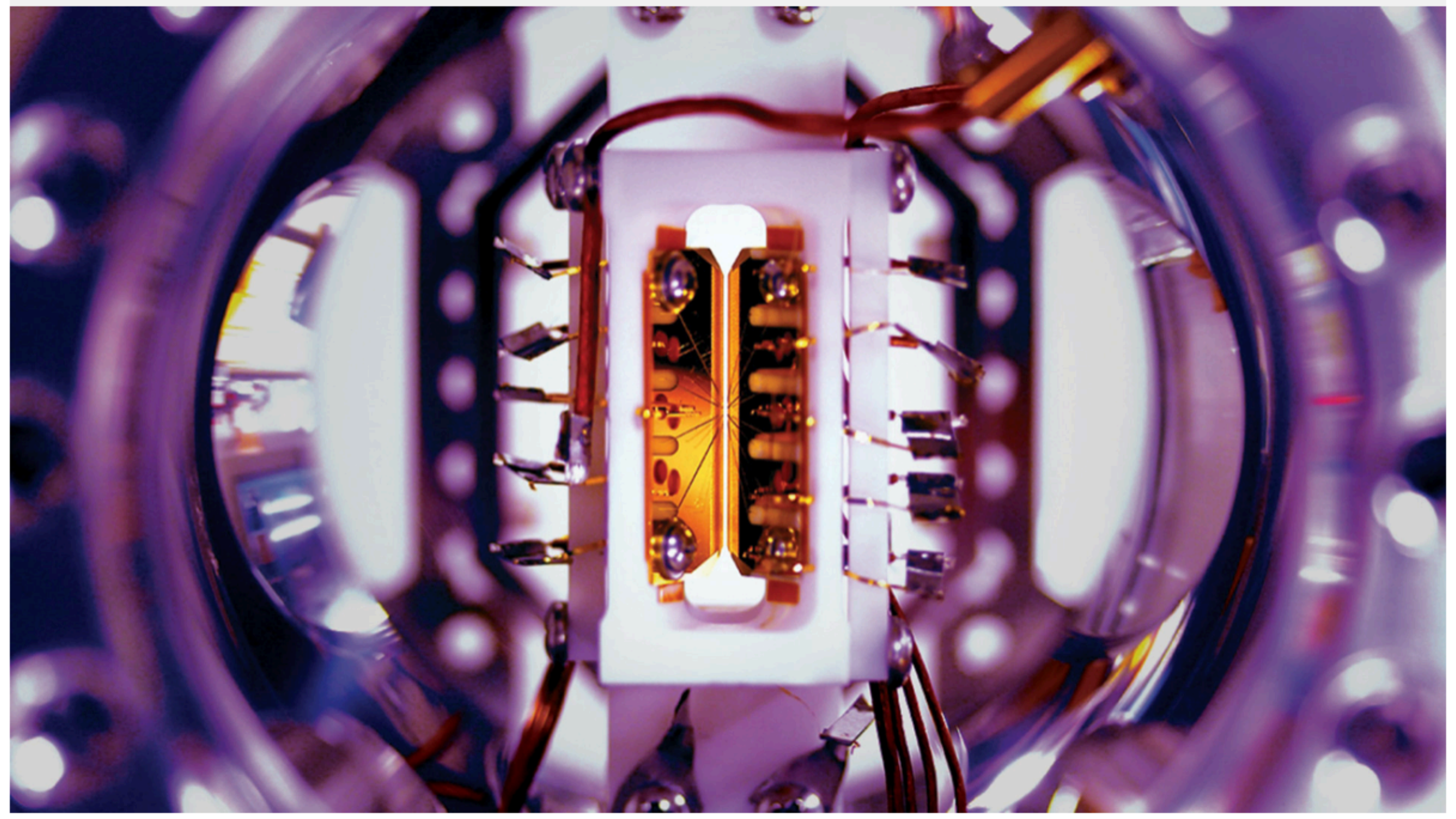
Produced by the Office of Strategic Communications

THURSDAY, APRIL 22, 2021



CAMPUS & COMMUNITY

From Innovation to Inauguration

Pines Announces New Quantum Business Incubator, Presents Invention and Entrepreneurship Awards

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DEPARTMENT OF PHYSICS ← where you find me! ("nuclear theory")

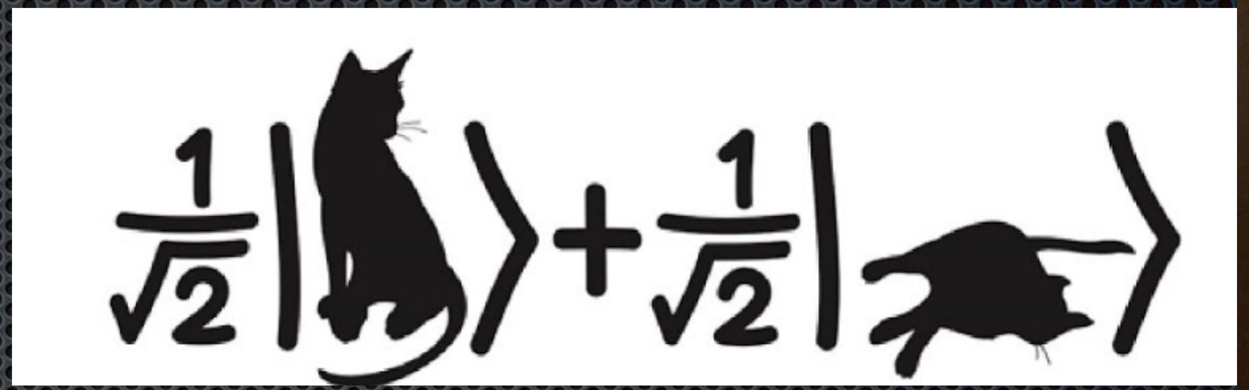
DEPARTMENT OF COMPUTER SCIENCE

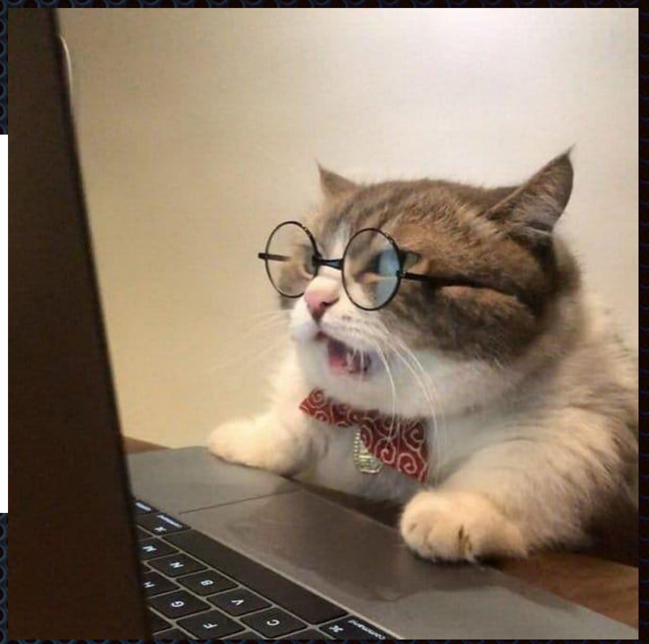
Quantum is picking up speed!

5 minutes of googling found all this

Where are we now?

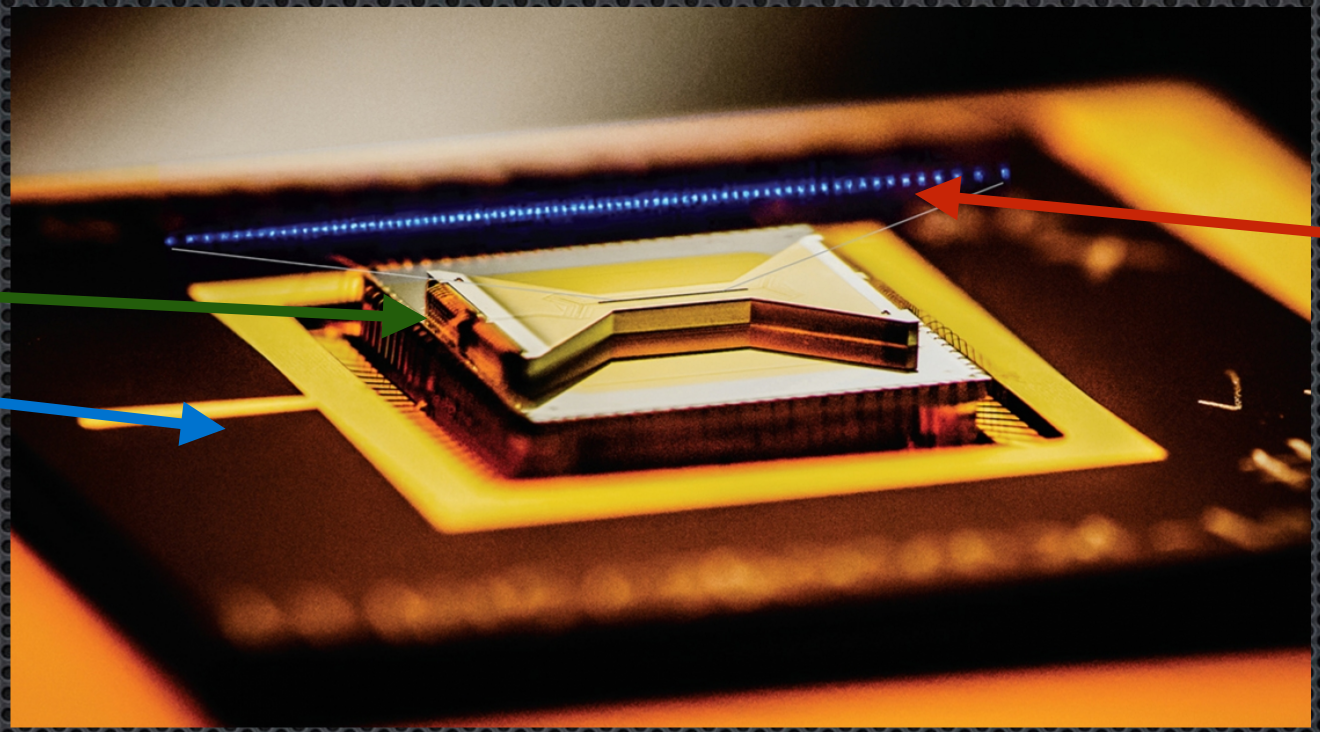
- Cats do not make good quantum computers



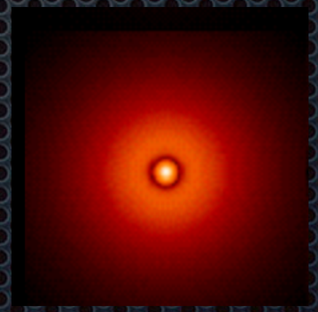


- Single atoms / qubits are never alone. They are surrounded by billions of other atoms

other stuff: walls,
air molecules,
also made of atoms
also like to talk to our "isolated" quantum mechanical system



atom (actually an ion) we would like to control as "isolated quantum mechanical system"



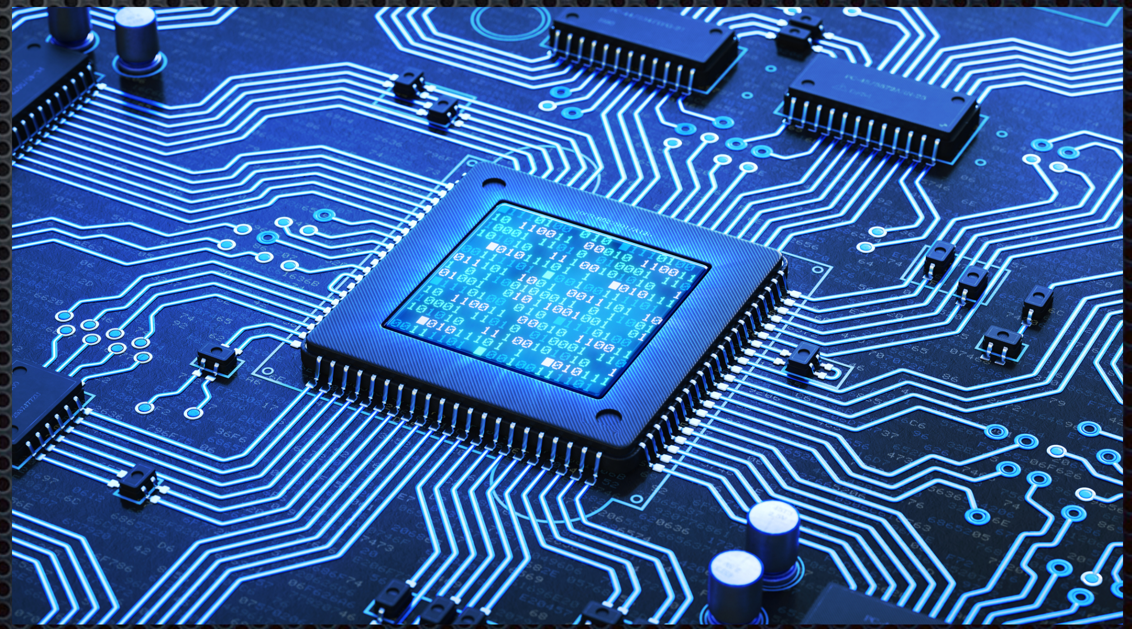
- Achieving "Quantum coherence" is hard.

- Challenge today: separating and controlling qubits from noisy environment + "quantum error correction"

Where are we now?

- Today: multitude of different architectures. We don't know yet which is the best.

- 1-50 qubits, very noisy, tens to hundreds of operations before thing breaks down (after ~10 years of serious development)
  - compare to classical computers (after 80+ years of development)



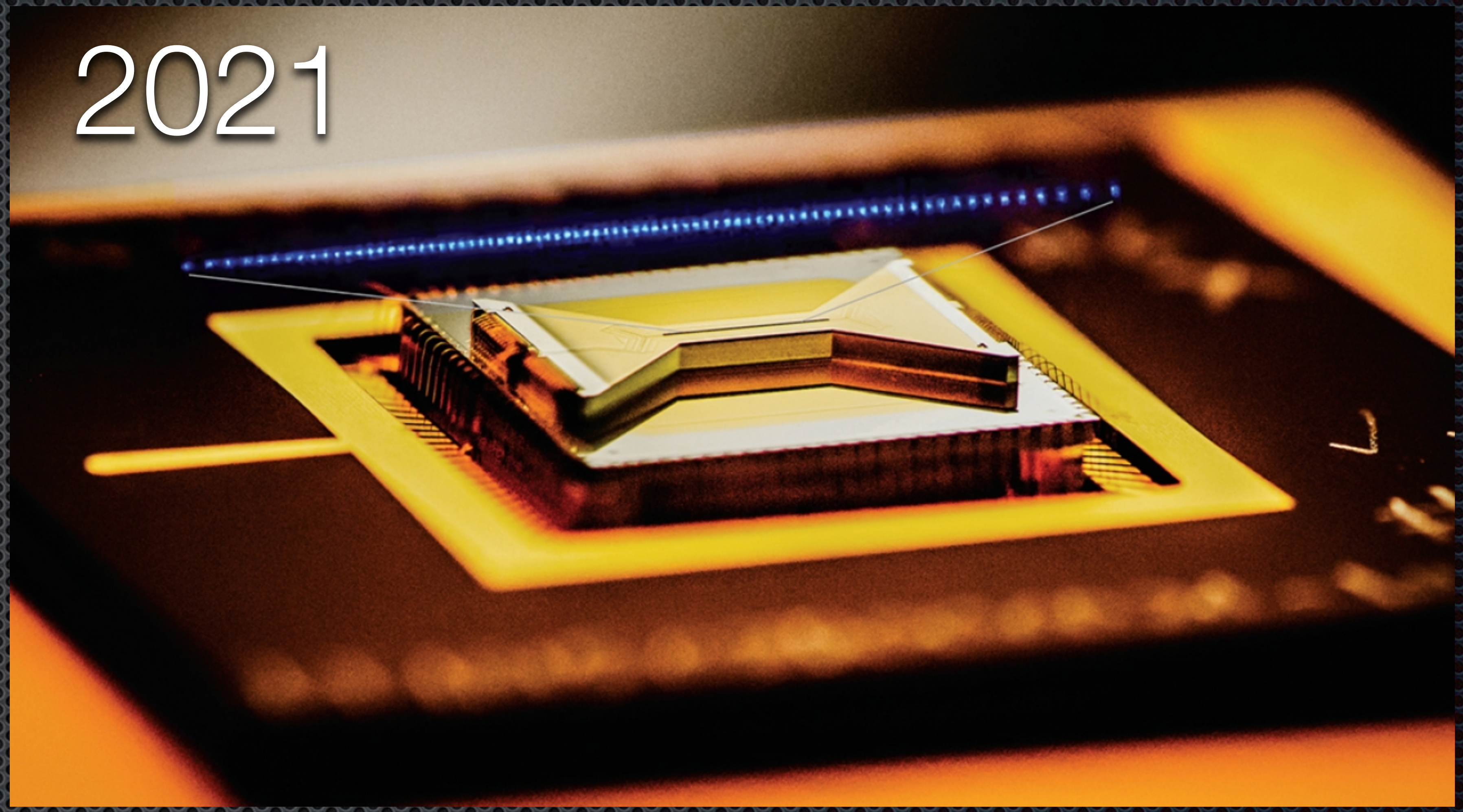
10^9 operations per sec

60 billion transistors

- break even point 50-100 "good qubits"

Where are we now?

> >



This will change very soon.

The myriad possibilities of quantum

- So basic idea then: use quantum mechanics to compute something else …in quantum mechanics …

- … or elsewhere: RSA encryption of emails

```
RSA-240 = 124620366781718784065835044608106590434820374651678805754818788883289666801
          188210855036039570272508747509864768438458621054865537970253930571891217684
          318286362846948405301614416430468066875699415246993185704183030512549594371372
          159029236099
```

```
RSA-240 = 509435952285839914555051023580843714132648382024111473186660296521821206469746700620316443478873837606252372049619334517
        × 244624208838318150567813139024002896653802092578931401452041221336558477095178155258218897735030590669041302045908071447
```

900 core years on a 2.1 GHz Intel Xenon Gold 6130 CPU

quantum computer:
piece of cake (Shor's algorithm)

- but also: quantum cryptography

- many more applications in science and industry

"big data" "quantum communication" "quantum sensors" "quantum optimziation"