DFG 2020
BECAUSE RESEARCH MATTERS

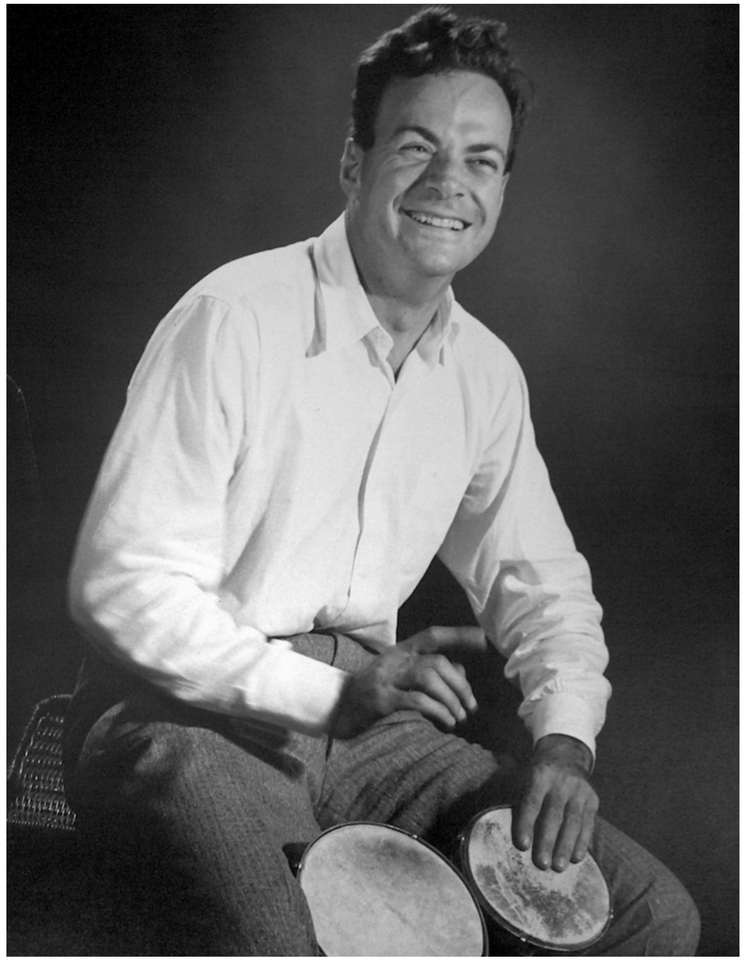
BROOKHAVEN NATIONAL LABORATORY

Quantum Computation for Nuclear Physics

Niklas Mueller
Nuclear Theory Group
Brookhaven National Laboratory

BNL Physics Department Summer Lectures 2020

What is quantum computation?



Richard Feynman (1981)
"Simulating Physics with Computers"

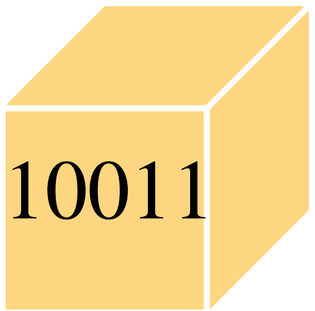
"Nature isn't classical
... and if you want to make a simulation of Nature,
you'd better make it quantum mechanical,
and by golly it's a wonderful problem,
because it doesn't look so easy."

"…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. "

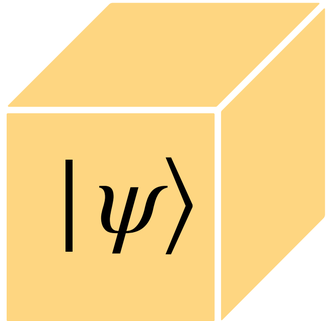
What is quantum computation?

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

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



$\$ \sim \exp(V)$

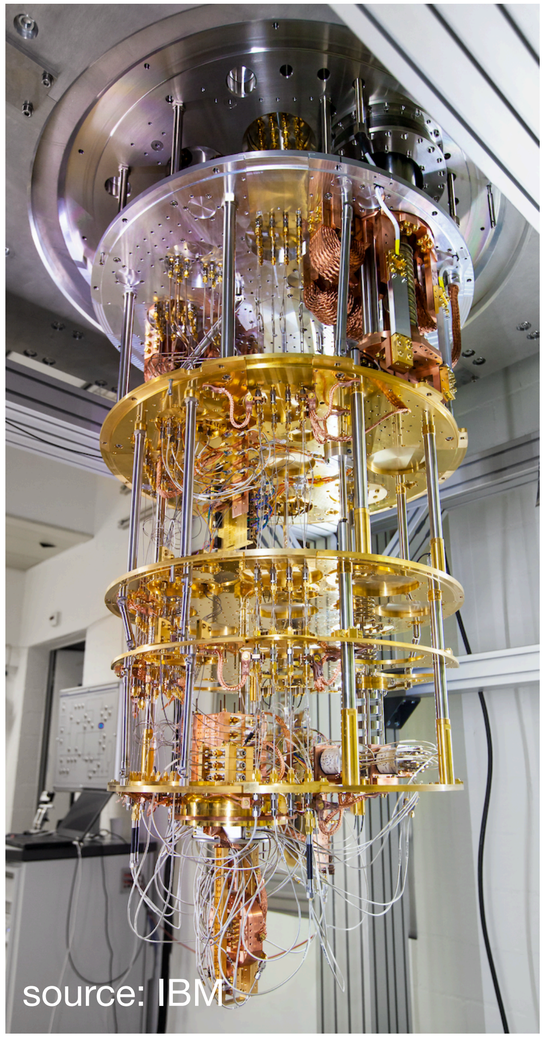


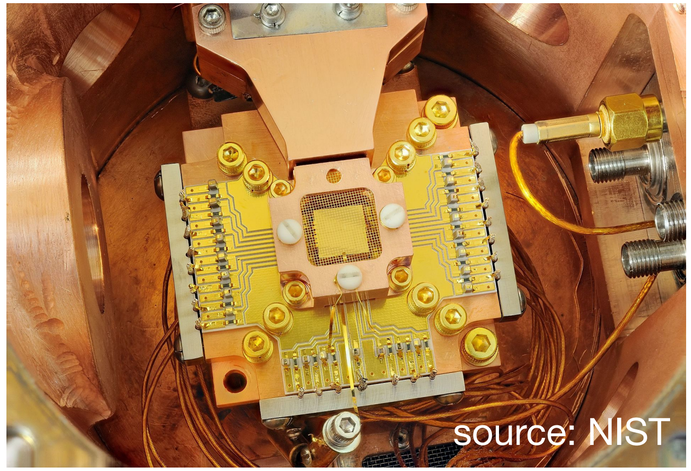
$\$ \sim V$

Today: A (nuclear) theorists perspective

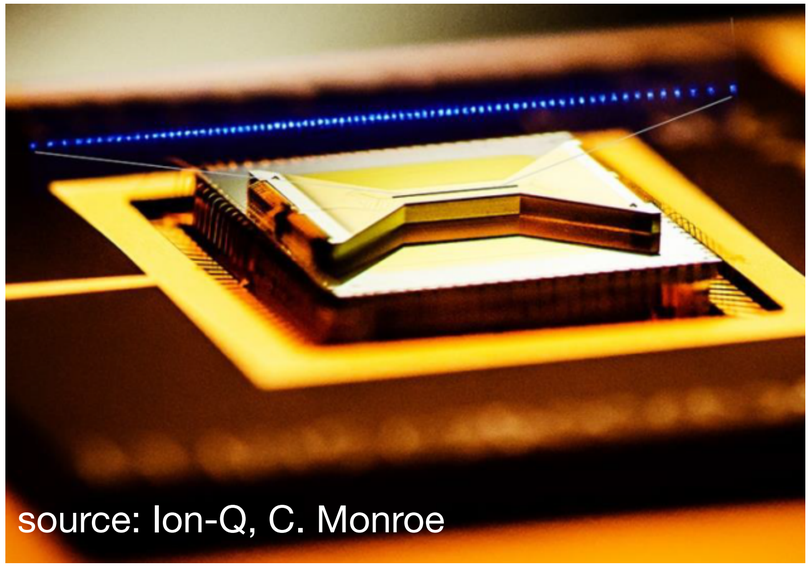
What is quantum computation?

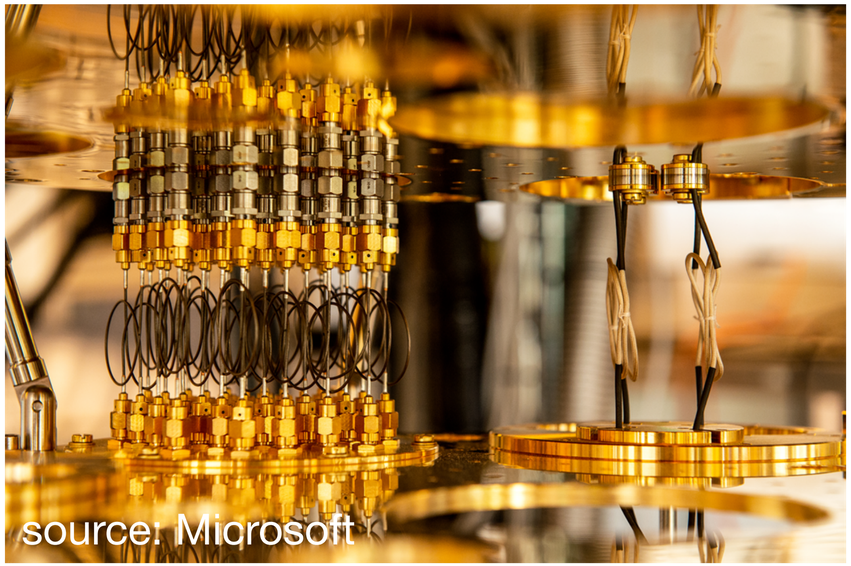
Digital (universal) Quantum Computers


source: IBM


source: NIST

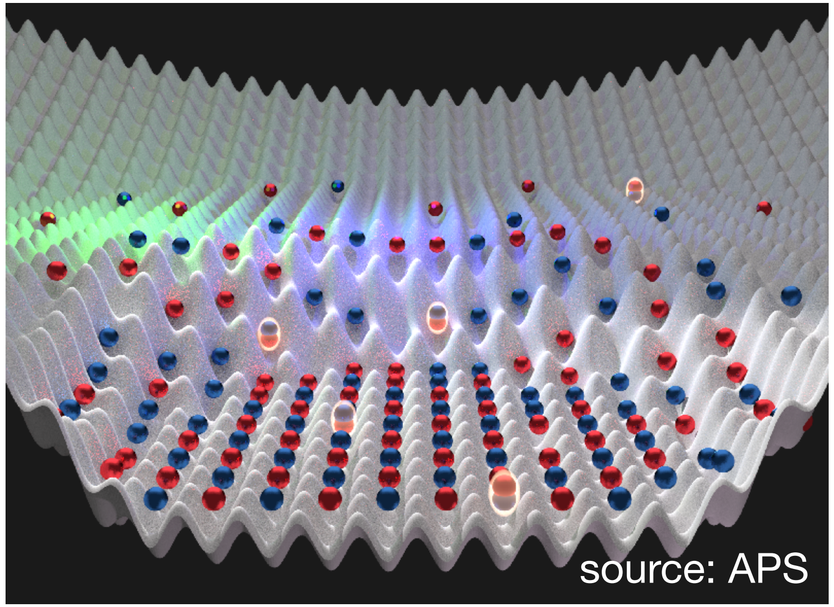

source: Google

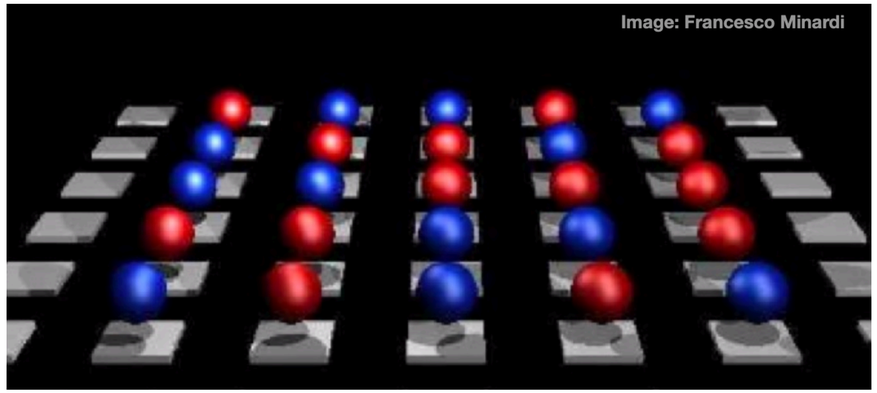

source: Ion-Q, C. Monroe


source: Microsoft

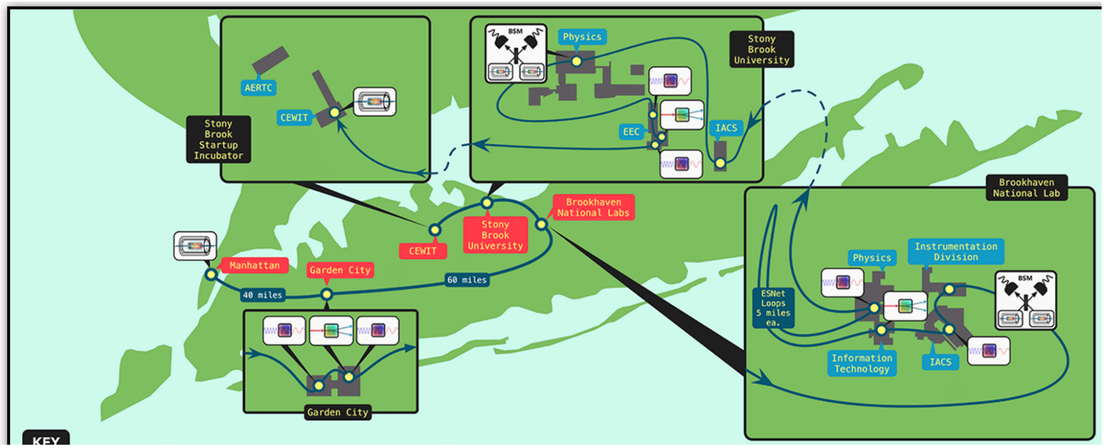
What is quantum computation?

Analog (non-universal) Quantum Simulators



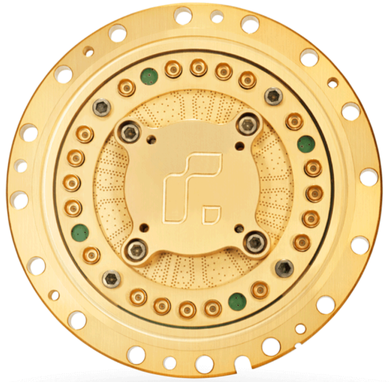


Quantum Communication and Cryptography



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

- 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**

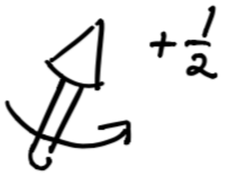
Outline of this lecture

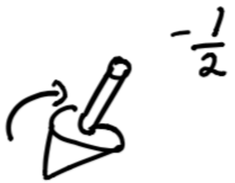
1. Basics - Quantum 101
2. Quantum Computing (Nuclear) Physics
3. How to do it?
4. New Ideas

Basics - Quantum 101

Basics - Quantum 101

- **Qubit = spin 1/2**





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

Basics - Quantum 101

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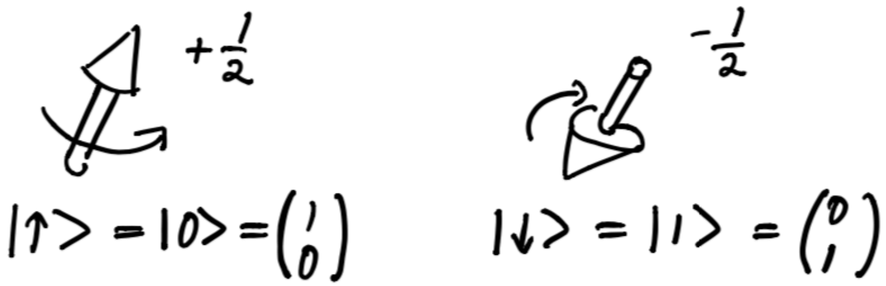
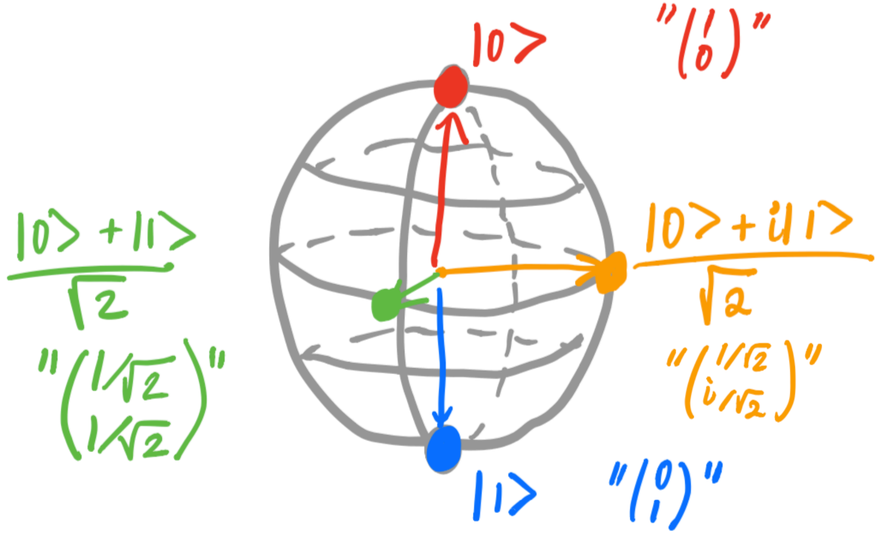


- **Hilbert space** $\mathscr{H} = \text{span}(|0\rangle, |1\rangle)$

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



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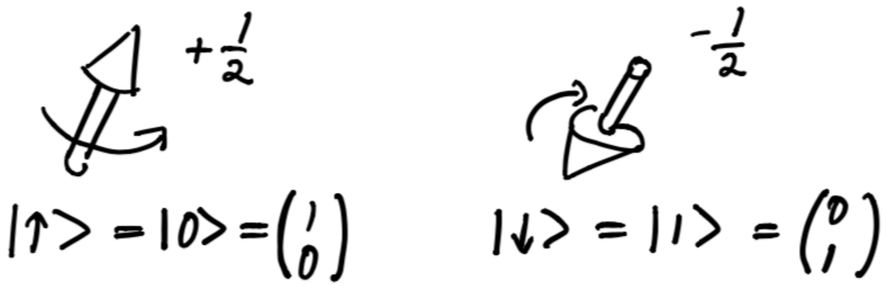

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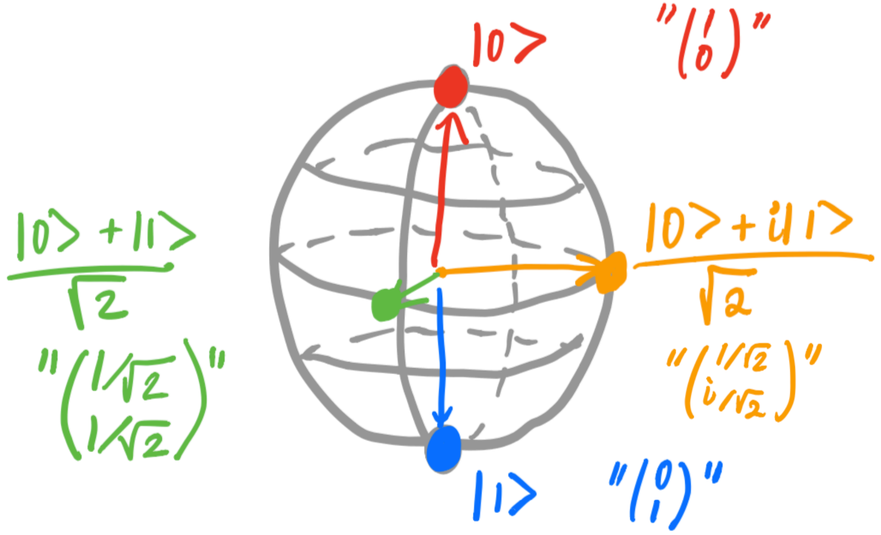

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- **Many qubits, big Hilbert space** $\mathscr{H}' = \mathscr{H} \otimes \mathscr{H} \ldots \otimes \mathscr{H}$

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

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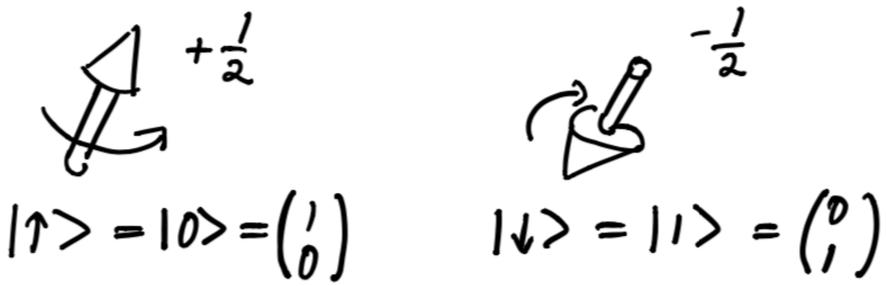

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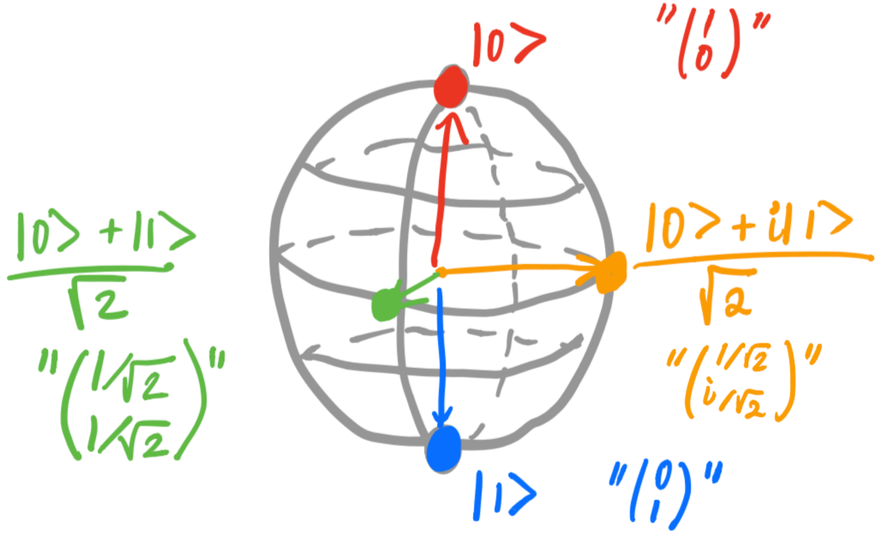

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$$\begin{pmatrix}a_0\\b_0\end{pmatrix} \otimes \begin{pmatrix}a_1\\b_1\end{pmatrix} = \begin{pmatrix}a_0a_1\\a_0b_1\\b_0a_1\\b_1a_1\end{pmatrix}$$

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

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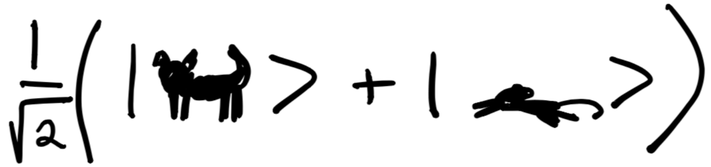
- **Power of quantum: superposition of information**

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



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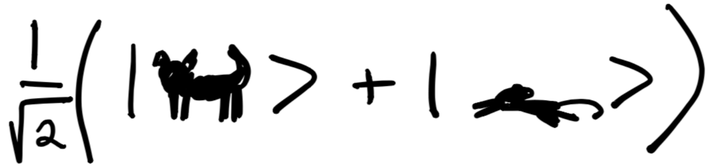

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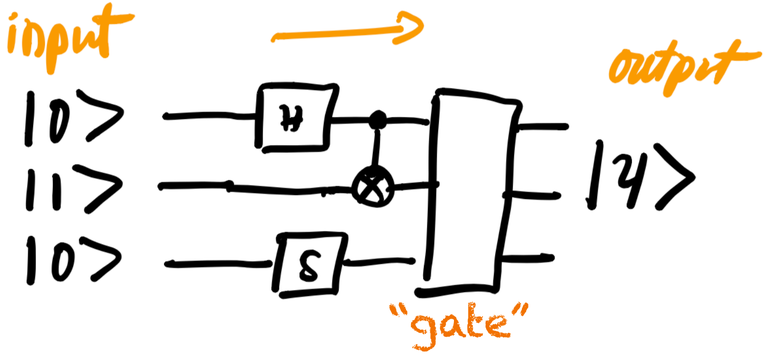

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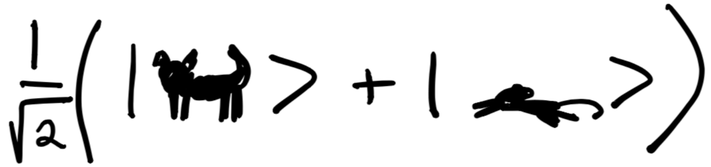

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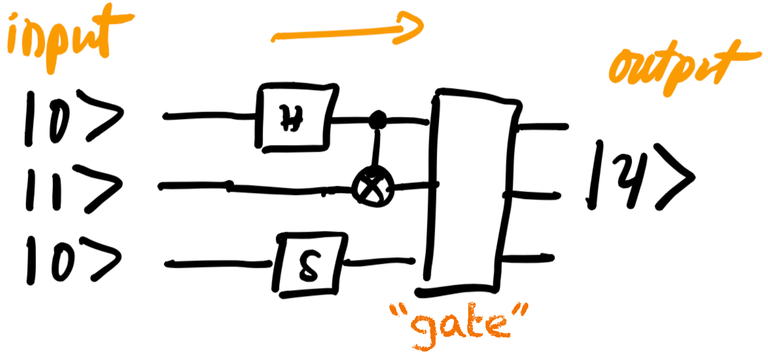

classically, think "matrix multiplication"
(matrix size grows exponential)

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

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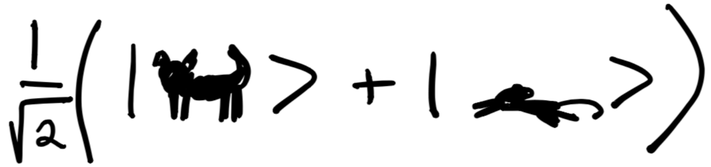

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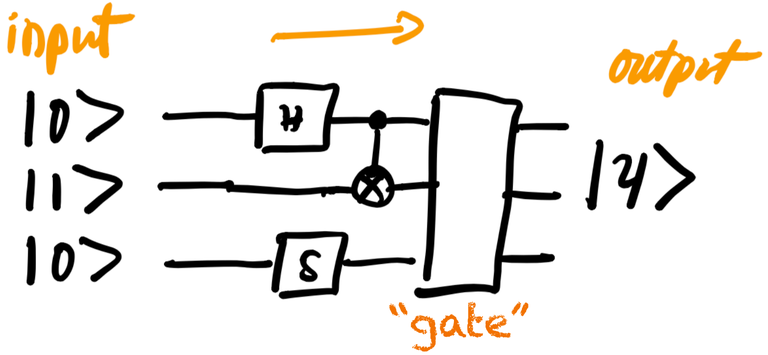

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- **Quantum parallelism** $x = 001001110, \qquad f(x)?$

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

Basics - Quantum 101

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- **Information can be entangled**

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|01\rangle + |10\rangle \Big)$$

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

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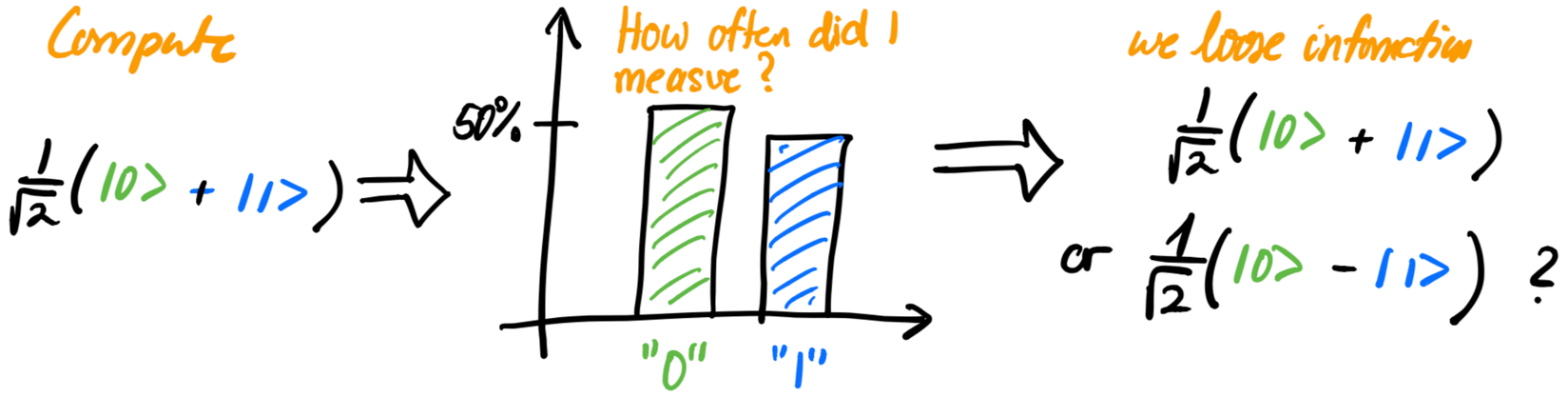
- **Quantum Mechanics: Extract Information via Measurement**



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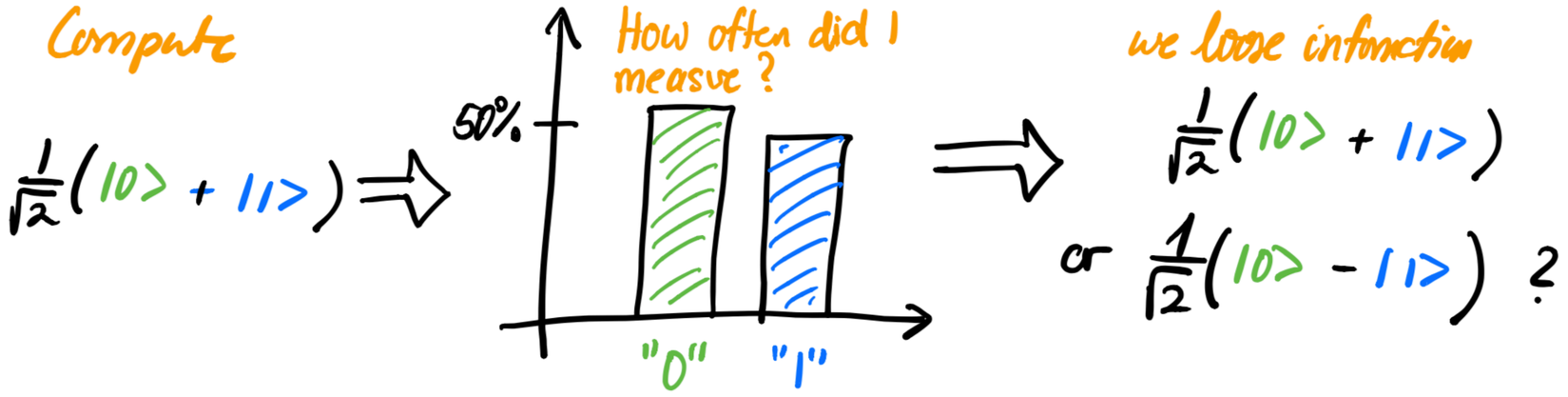

- **Extracting answer from Quantum Computer: subtile issue**

Quantum Computation for Physics

Challenges

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 $N = 197$)

Quantum Computation for Physics

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

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

$$i\hbar\partial_t |\psi\rangle = H|\psi\rangle$$

$$H = \sum_i \frac{\hat{p}^2}{2m} + \sum_{ij} V_{ij} + \sum_{ijk} V_{ijk} + \ldots$$

(Hamiltonian operator)

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(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

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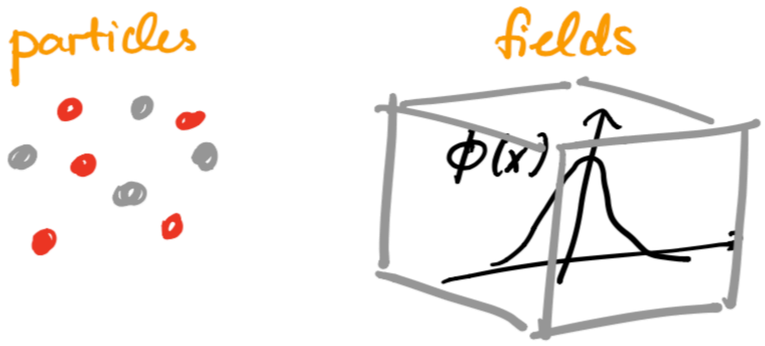
- **Quantum Many-Body Theory → Quantum Field Theory**



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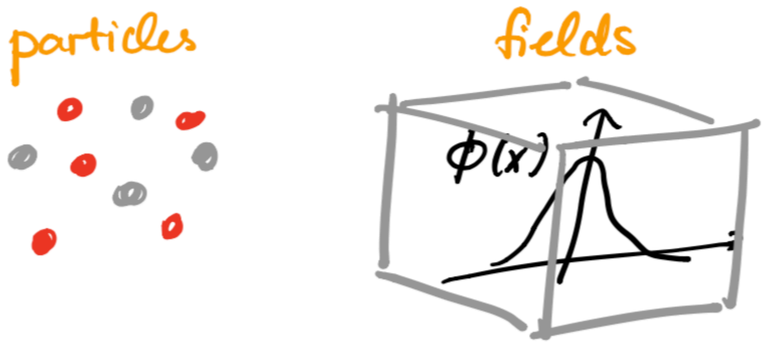

- **Example (Quantum) Electrodynamics**

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

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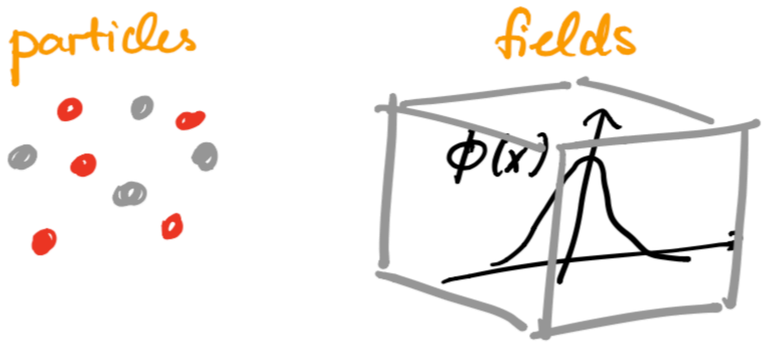

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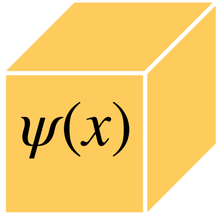
- **Every x labels one quantum mechanical degree of freedom.**

Infinitely many dof's in any volume V!



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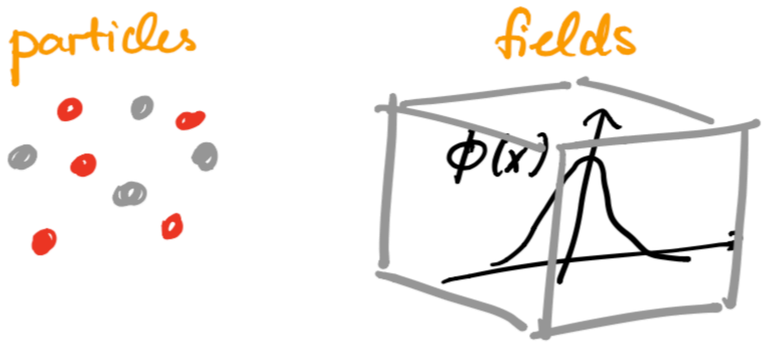

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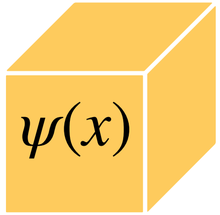

Ψ "Heisenberg field operator"

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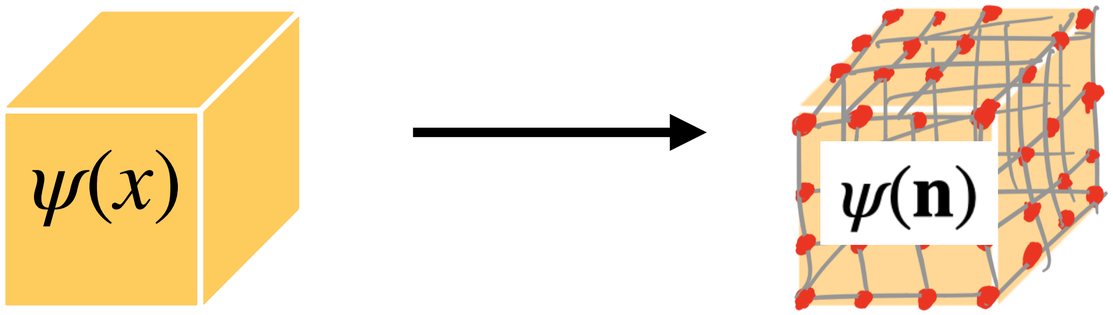
- **Quantum Field Theory→ Lattice Quantum Field Theory**



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

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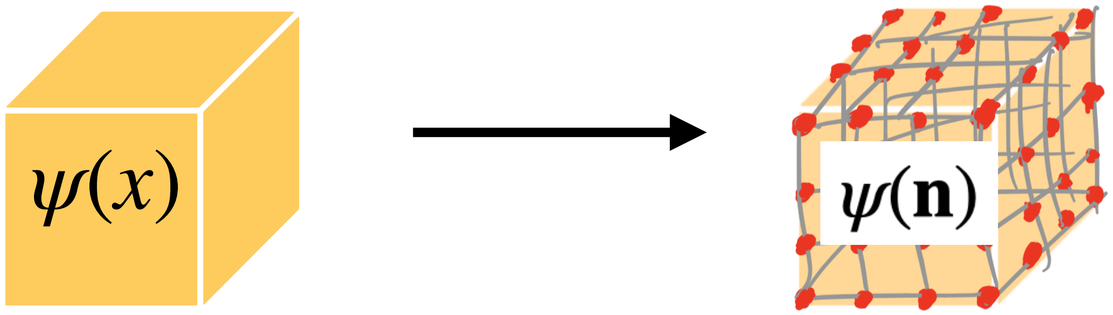

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- **Lattice Quantum Field Theory ~ Quantum Many Body Theory**

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- **Gauge Theories (e.g. QED)**

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

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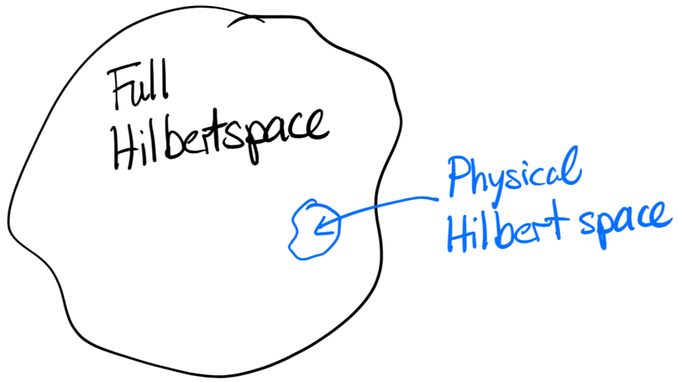
- **Redundancy, not all dofs are physical!**



Quantum Computation for Physics

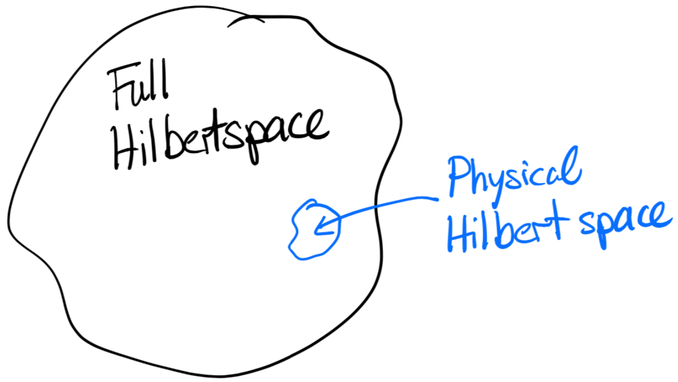
Challenges

- **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!

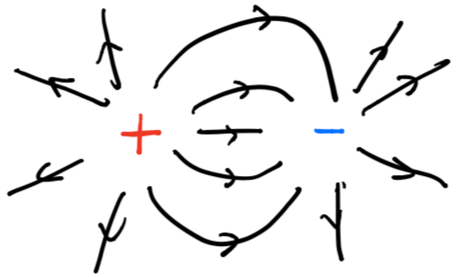
- **Redundancy, not all dofs are physical!**



- **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

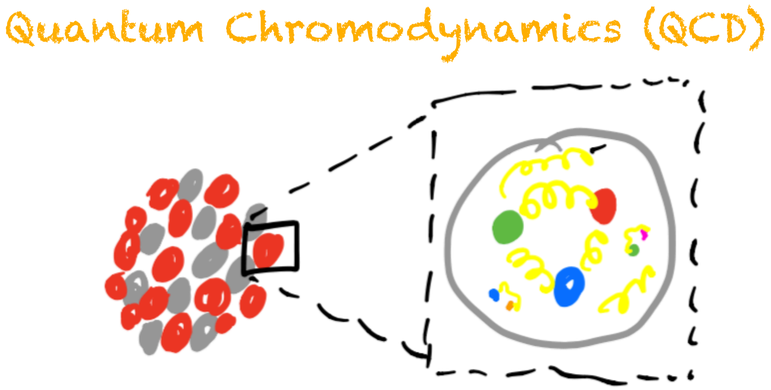
Quantum Computation for Nuclear Physics

Lattice QCD simulations

- **From Hamiltonian to Lagrangian**

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

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



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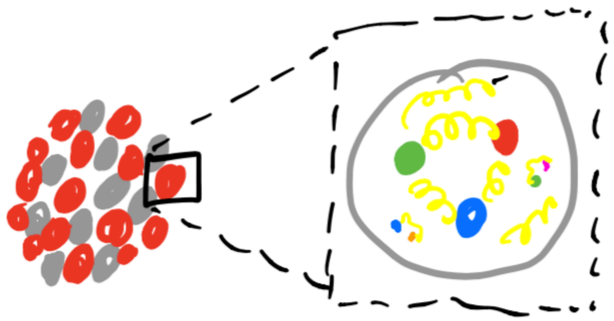
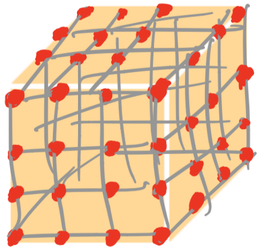
Quantum Chromodynamics (QCD)



- **… to path integral**

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



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

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

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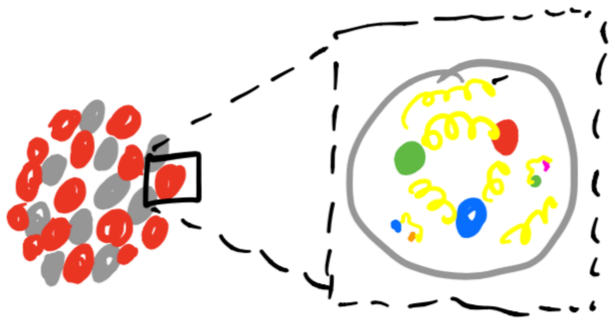

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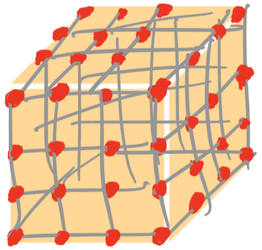

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- **In Euclidean Spacetime: statistical mechanics problem**

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

Lattice Monte-Carlo simulations work in many dimensions!

Quantum Computation for Nuclear Physics

Lattice QCD simulations

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

Quantum Computation for Nuclear Physics

Lattice QCD simulations

- **Very expensive**

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- Do not work for various interesting problems (*)!

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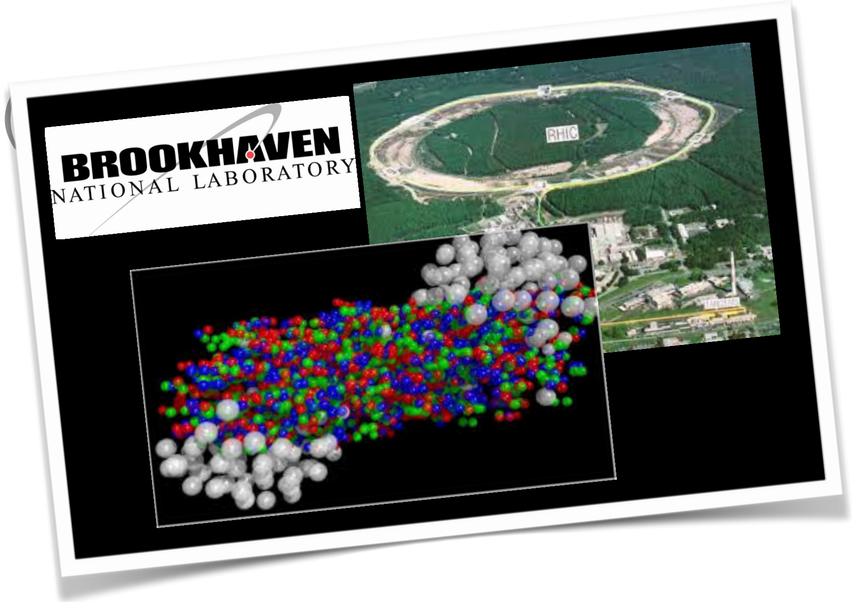

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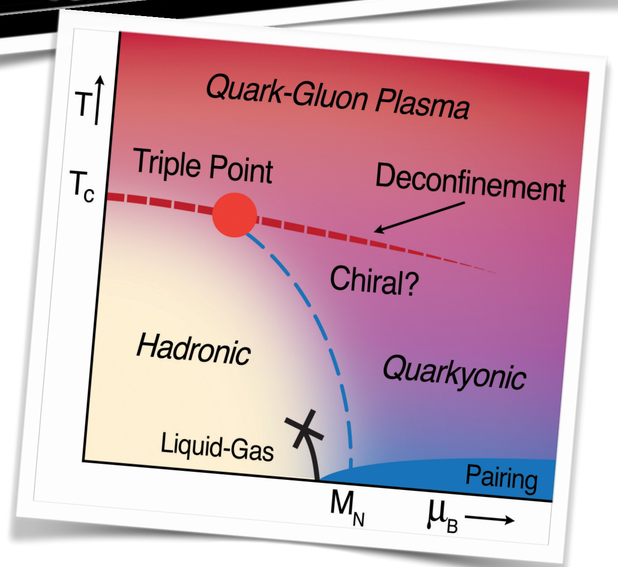

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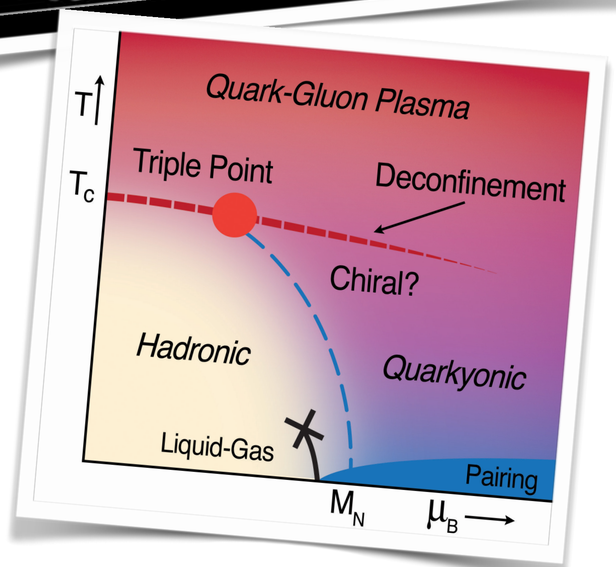

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How to do it?

Step 1: Digitization

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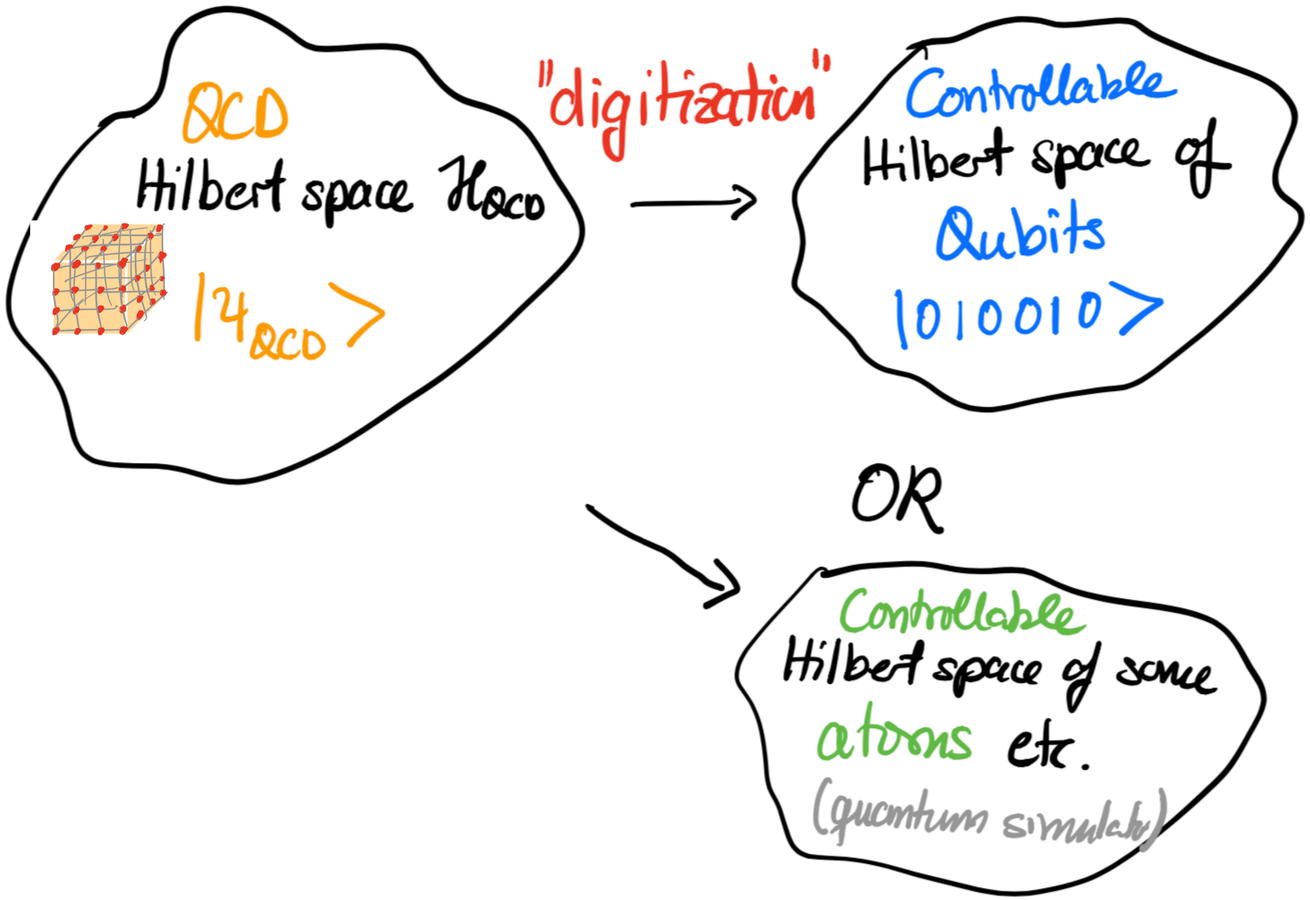

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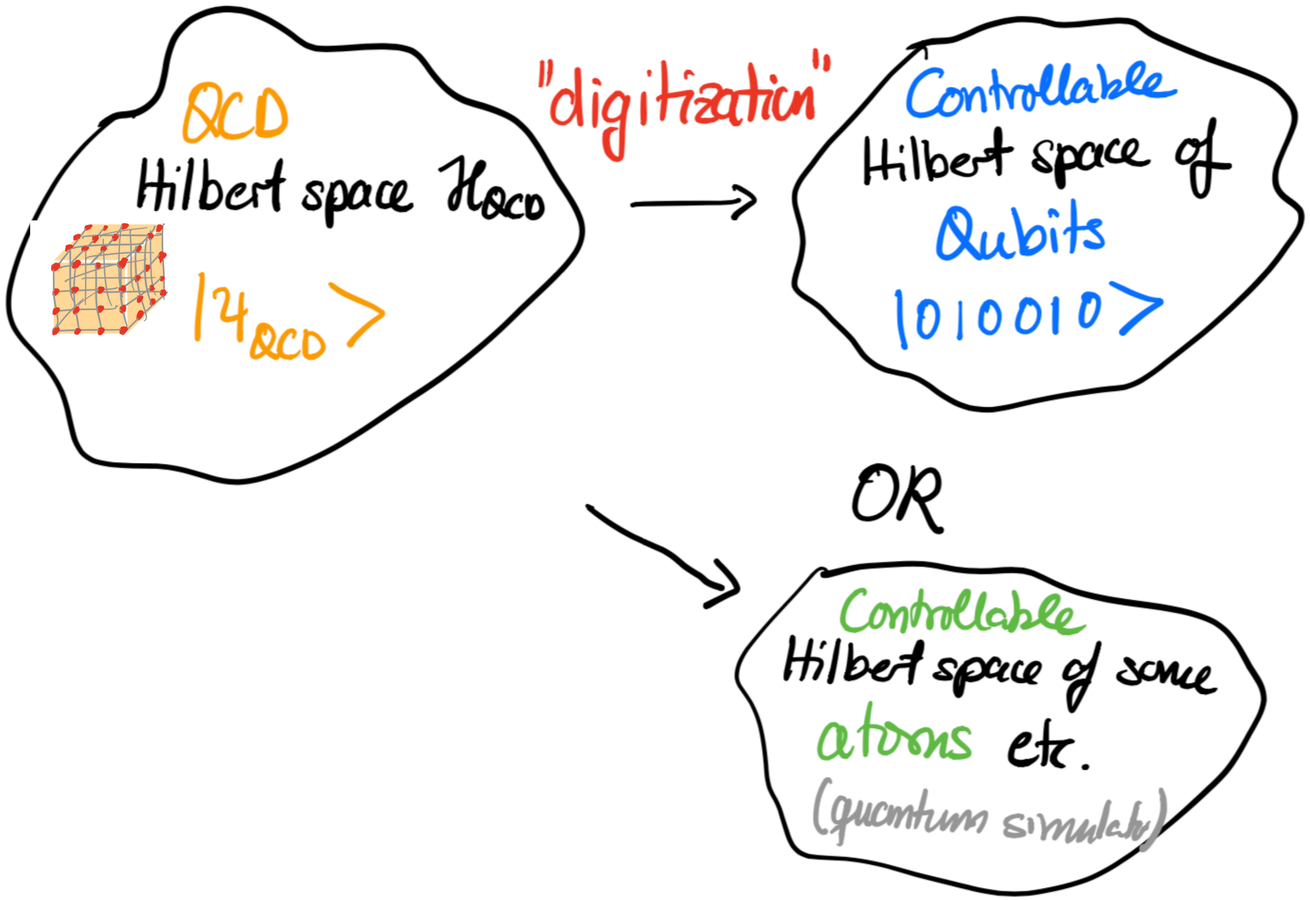

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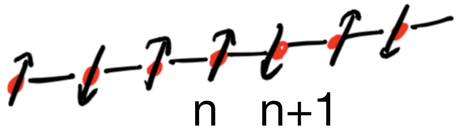

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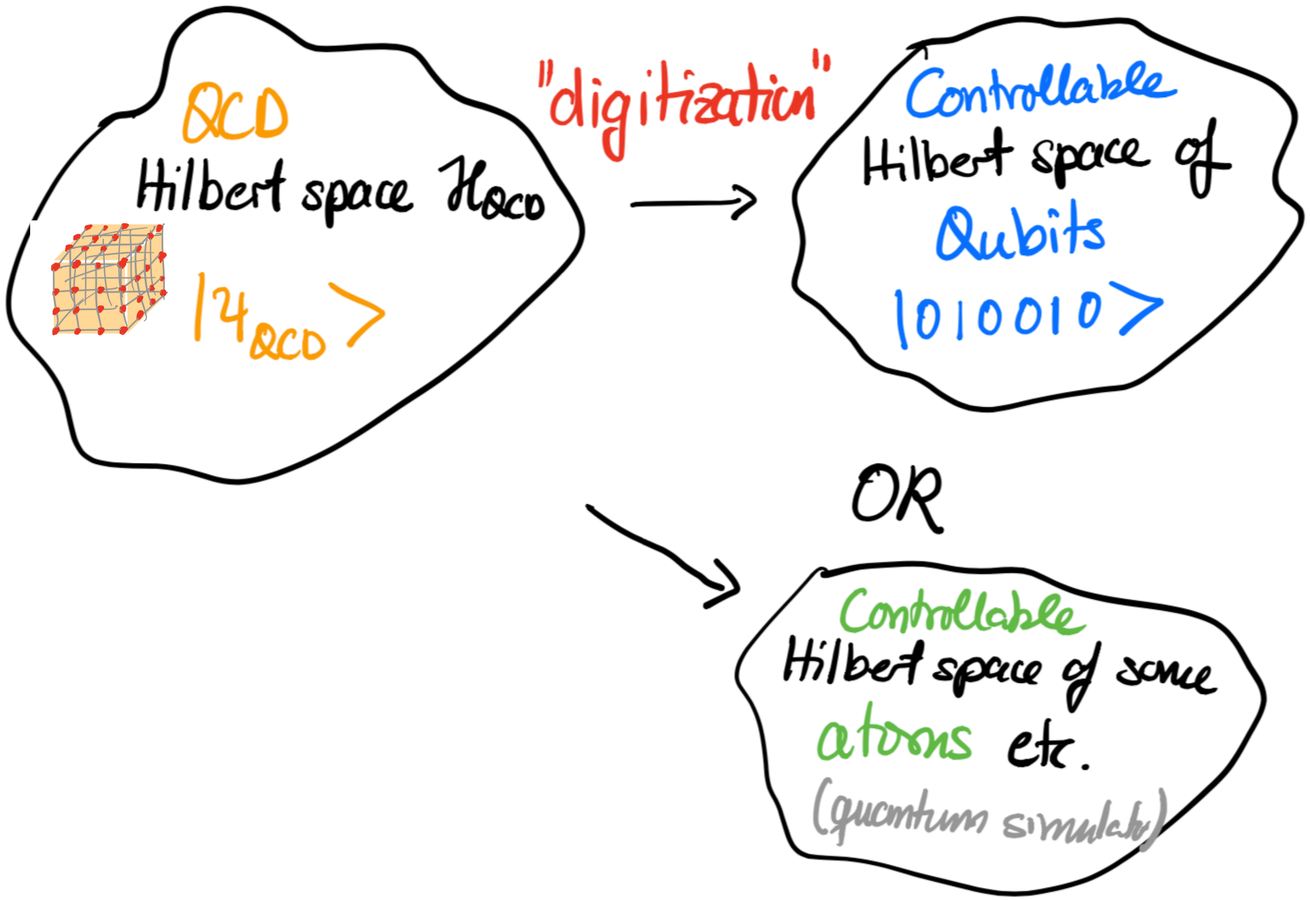

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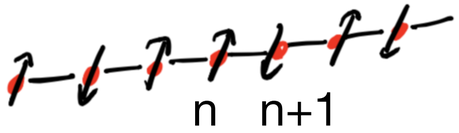

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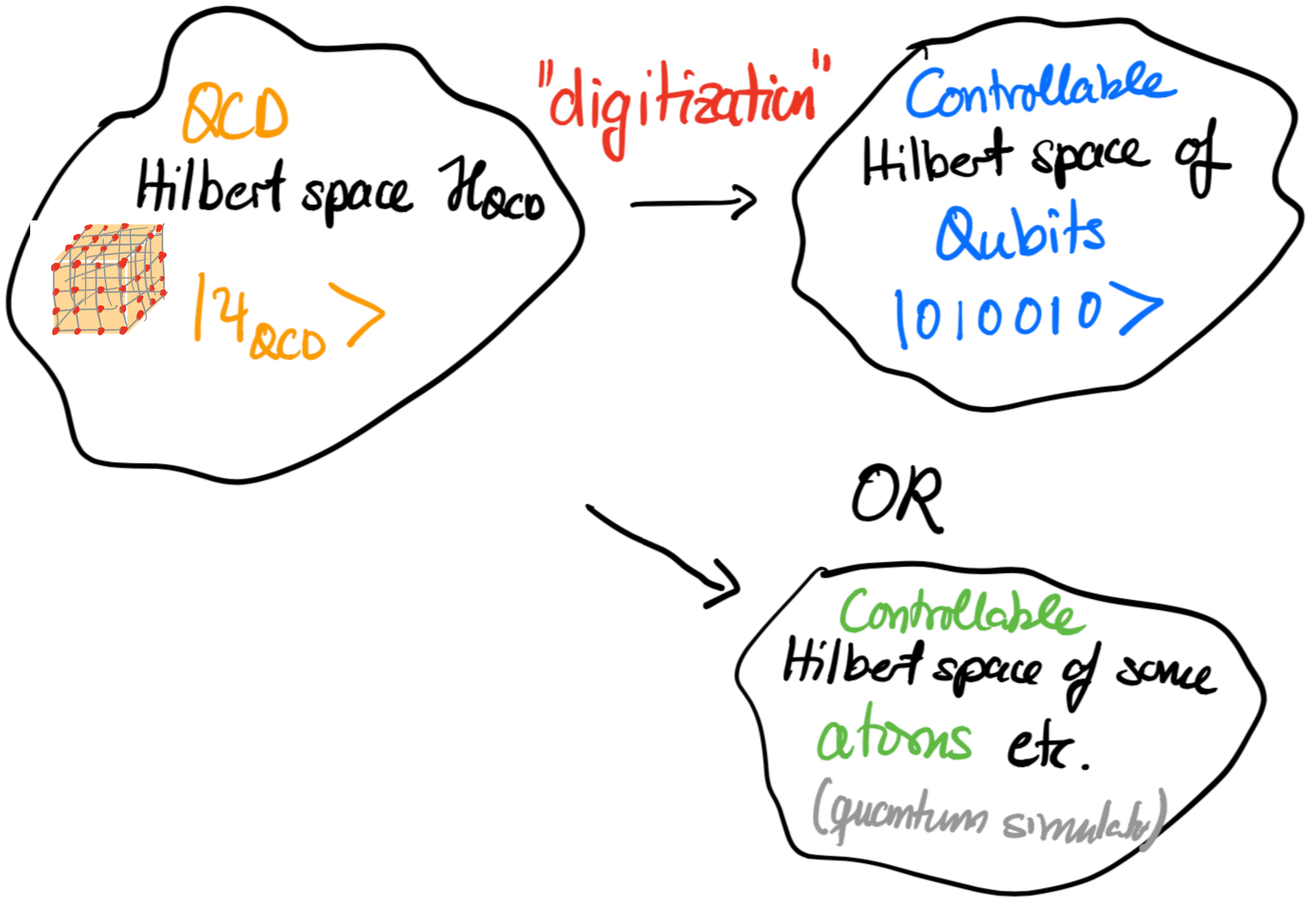

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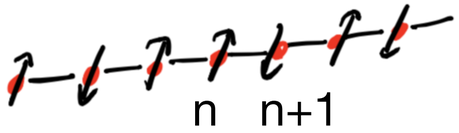

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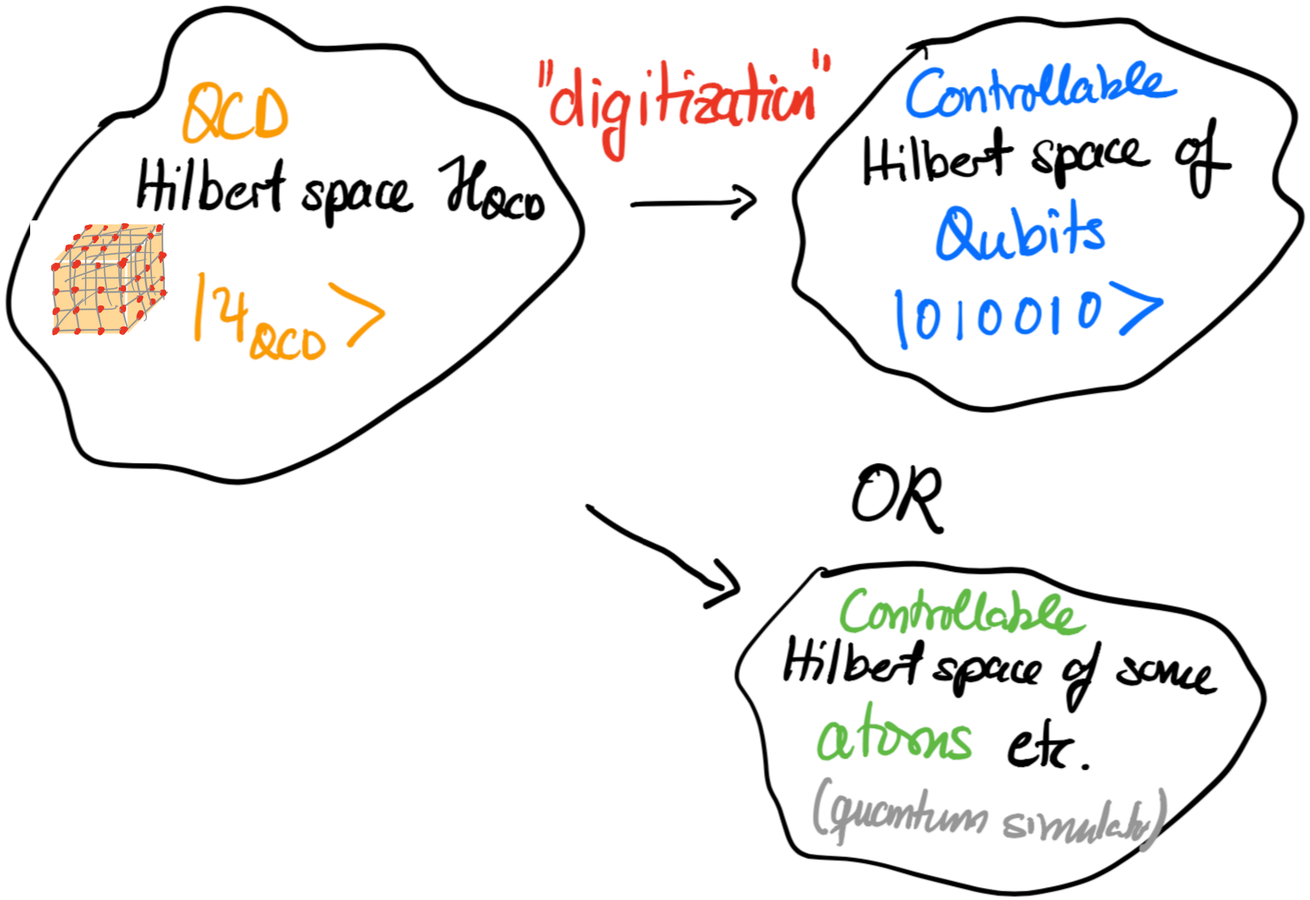

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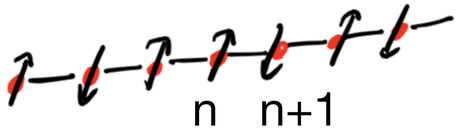

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$$\mathcal{H}^{\text{fermions}} \leftrightarrow \mathcal{H}^{\text{qubits}}$$

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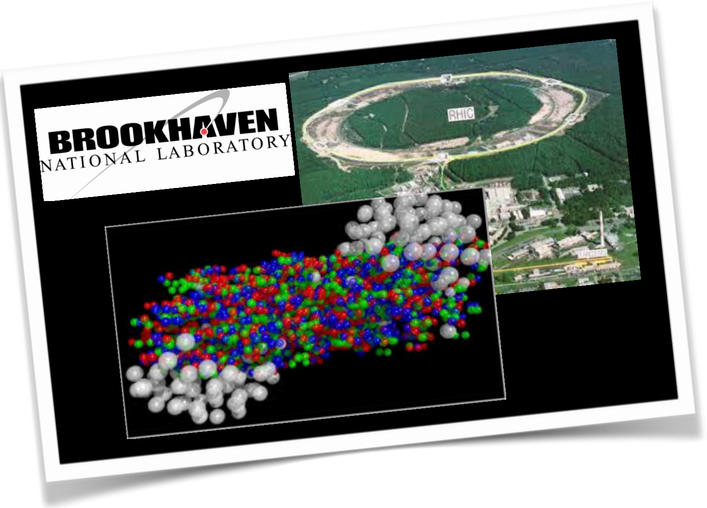

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How does state $|\psi\rangle$ evolve over time?

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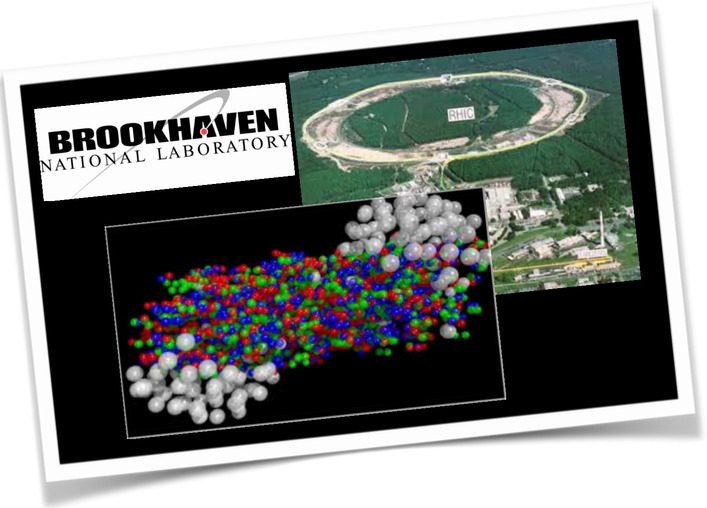

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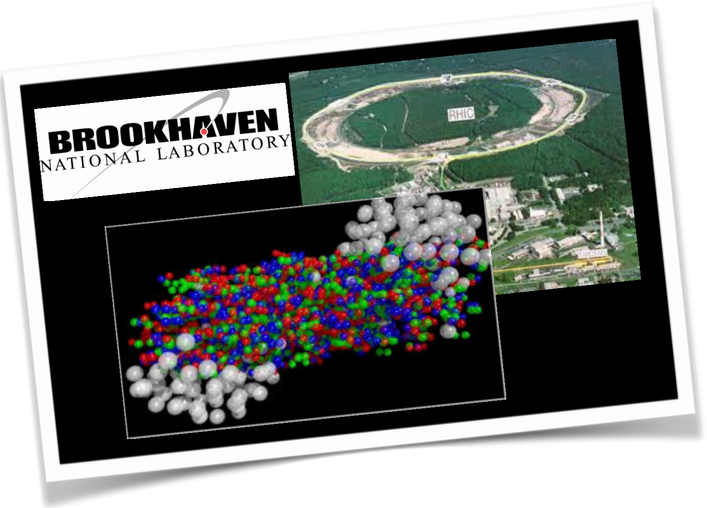

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final state

initial state

time evolution operator

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

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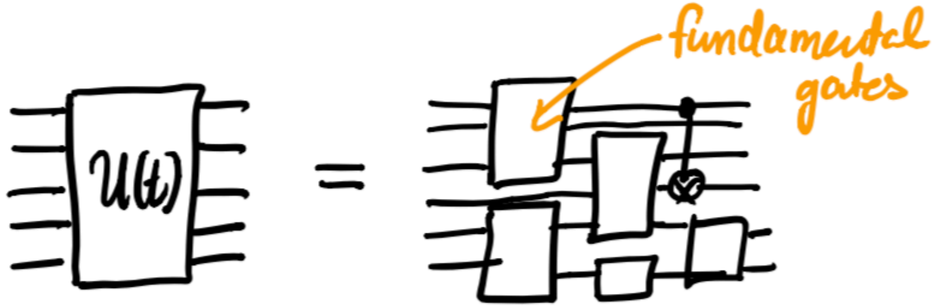
- **Decompose *U(t)* into circuit**



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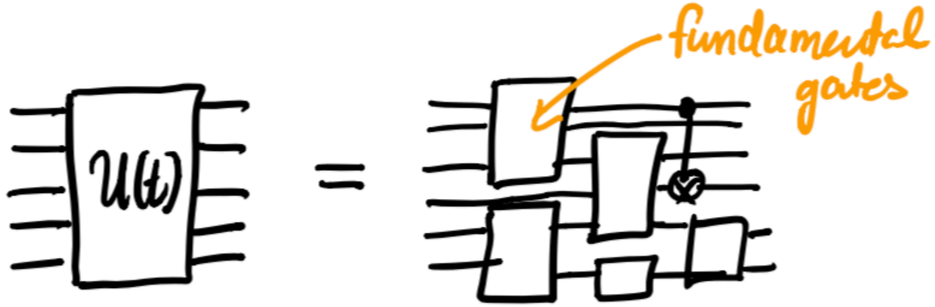

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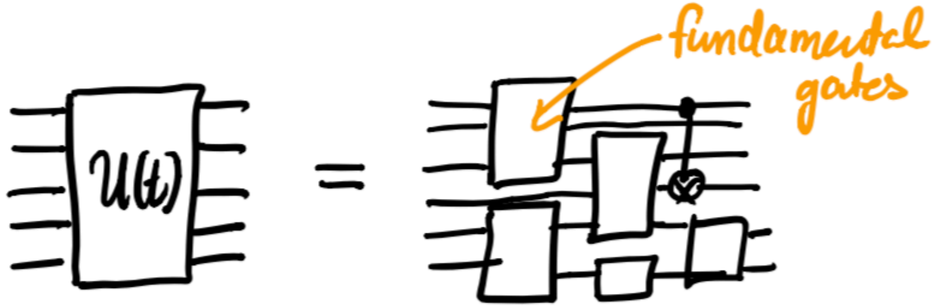

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- **Figure out how to set up** $|\psi\rangle$

- **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.

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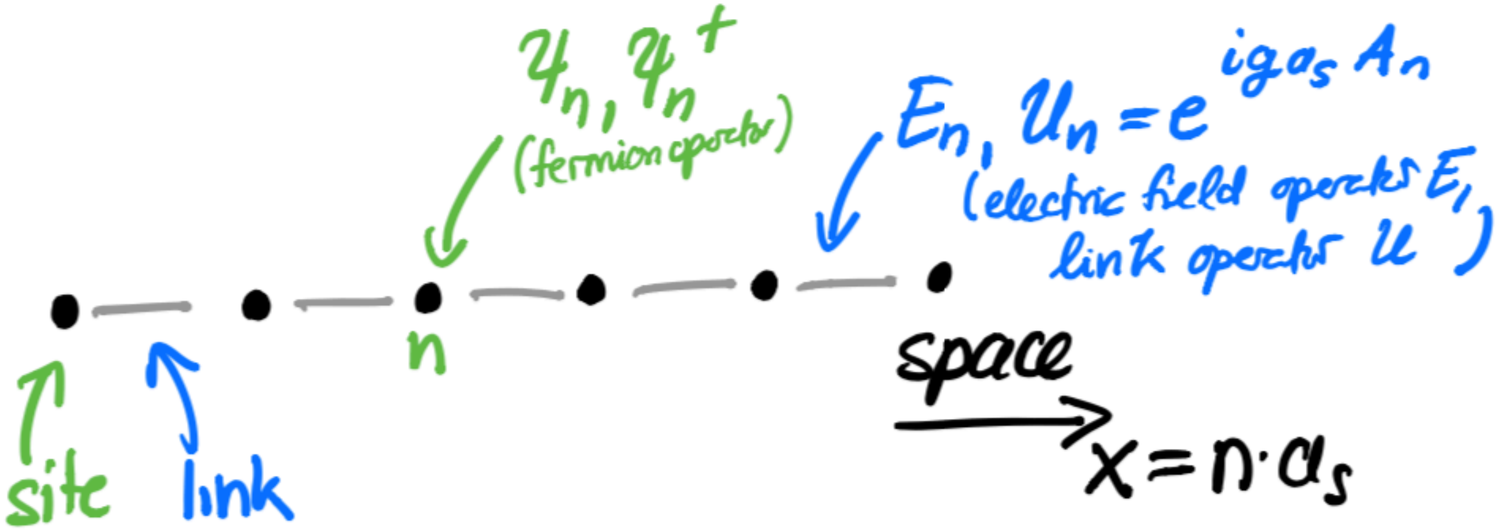

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→ map onto qubits (✓)

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gauge sector: infinitely many states (✗)

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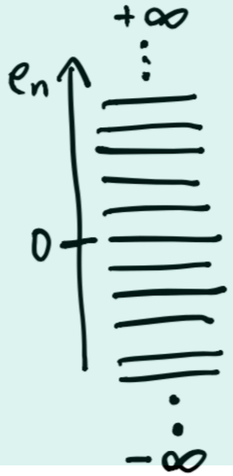

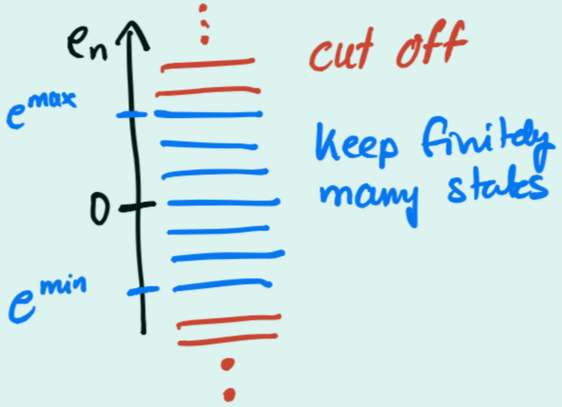

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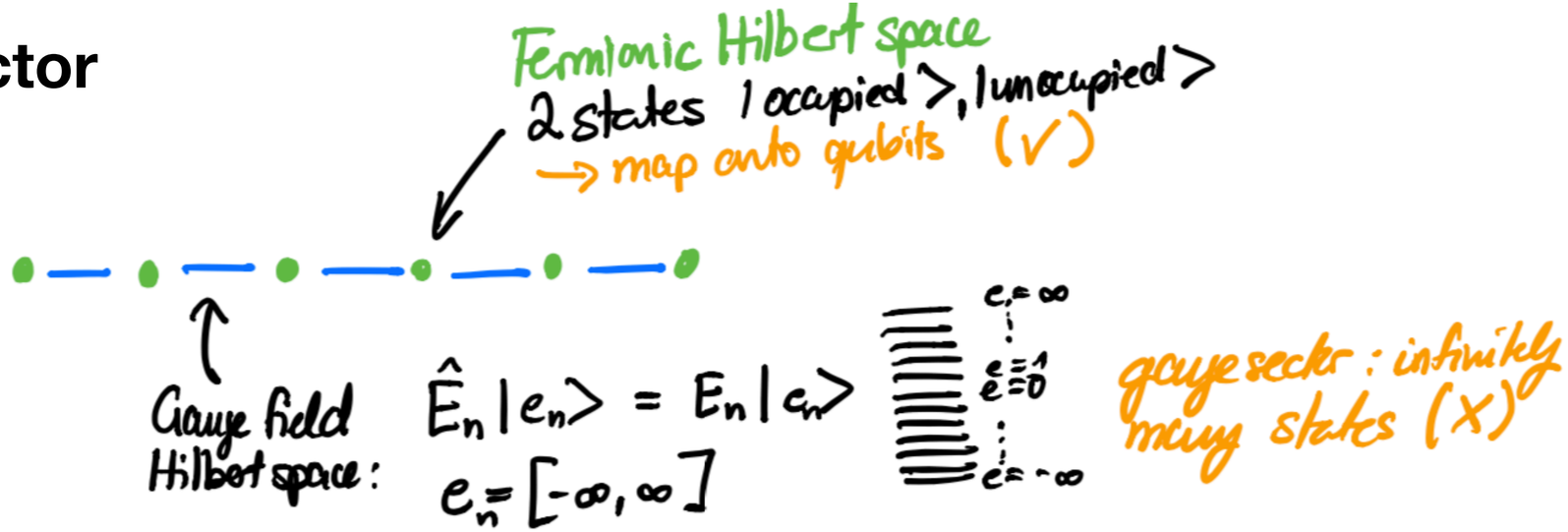

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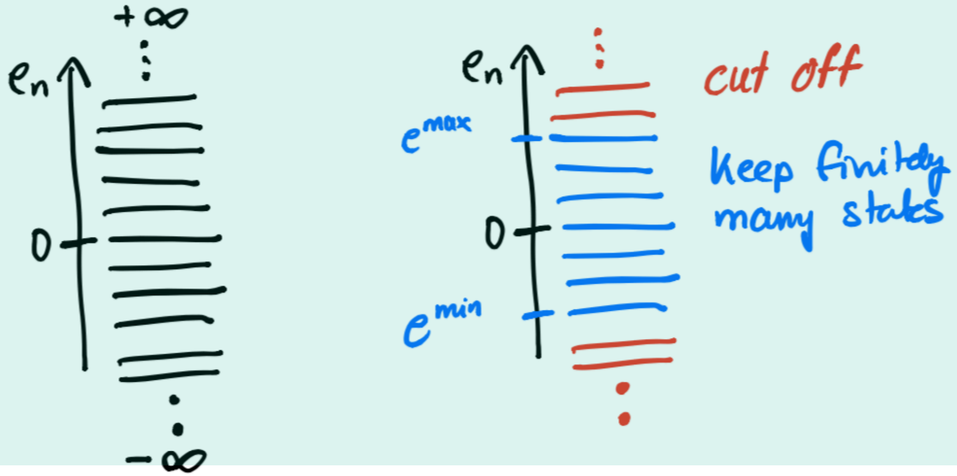

- **Map onto qubits**

Operator formulation of Lattice Gauge Theory

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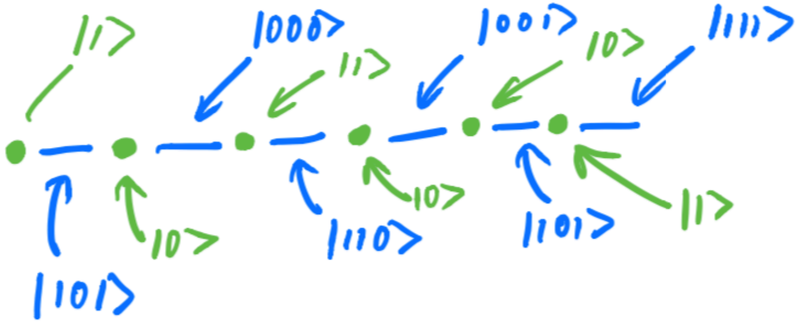
- **A state of the full theory**



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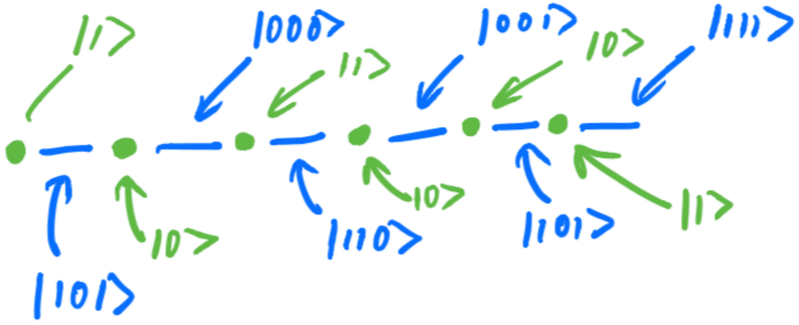

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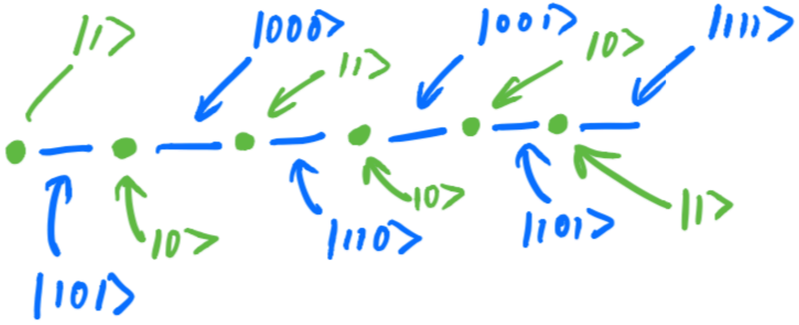

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- **Hamiltonian commutes with Gauss law**
  $[H, G_n] = 0$ If initial state is physical, it will stay physical

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

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Operator formulation of Lattice Gauge Theory

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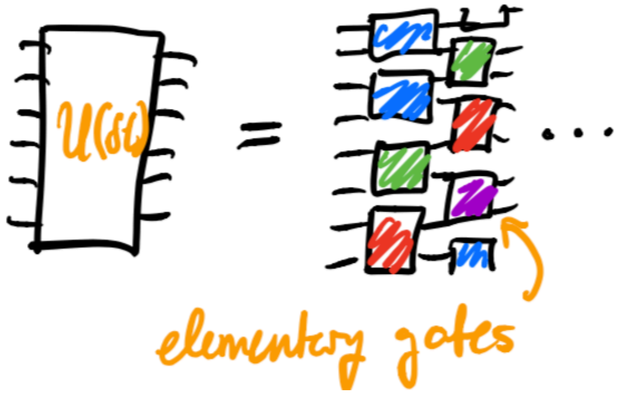
- $U(t) = \prod_t U(\delta t)$

"Trotterization"

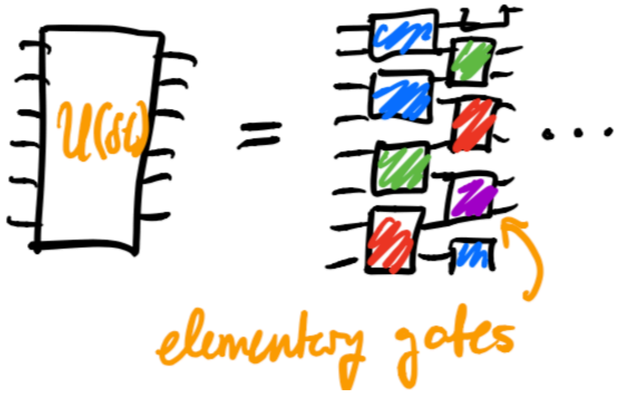


Operator formulation of Lattice Gauge Theory

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

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

"Trotterization"

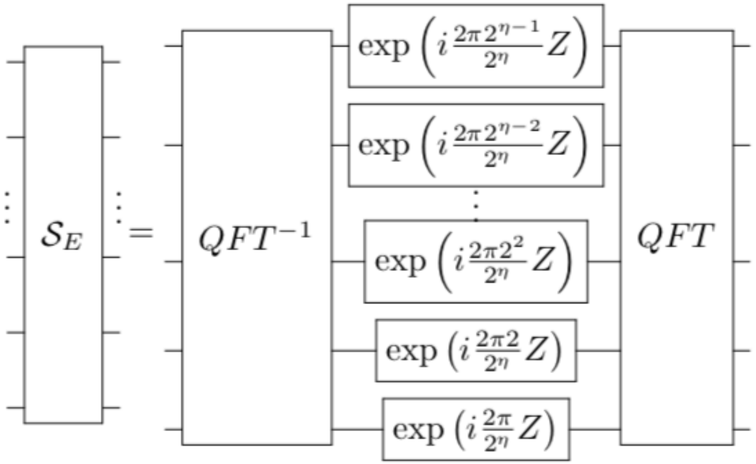


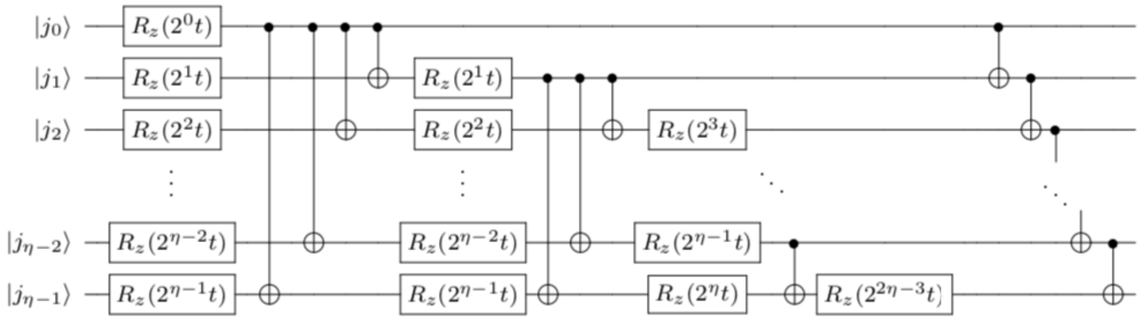
Trapped ions:

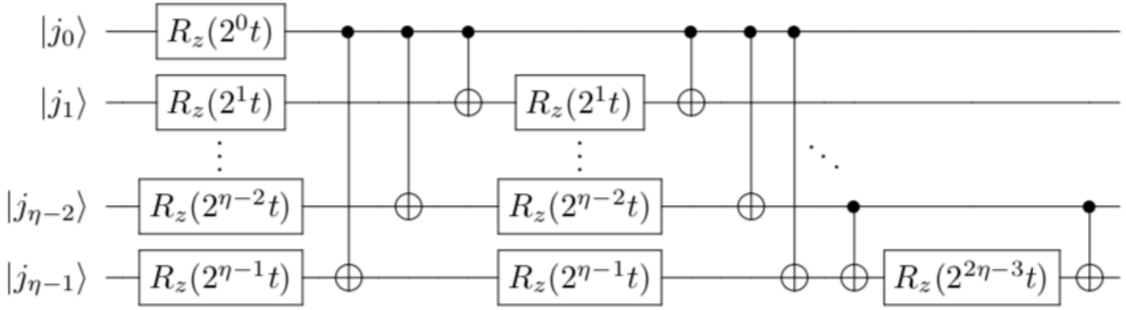
Martinez et al, Nature 534 (2016) 516

- **Take a look at e.g. 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

Quantum Computation for the Electron Ion Collider

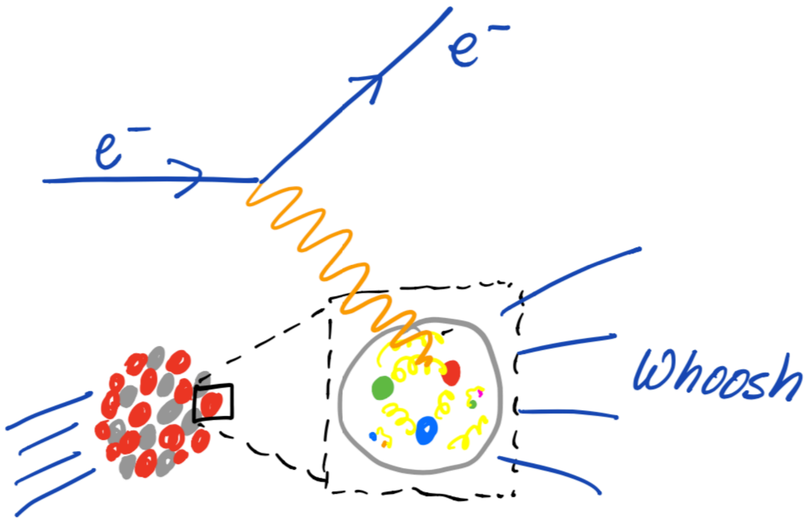
FYI
SCIENCE POLICY NEWS FROM AIP
Bulletin

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** $|P\rangle$?

New Ideas

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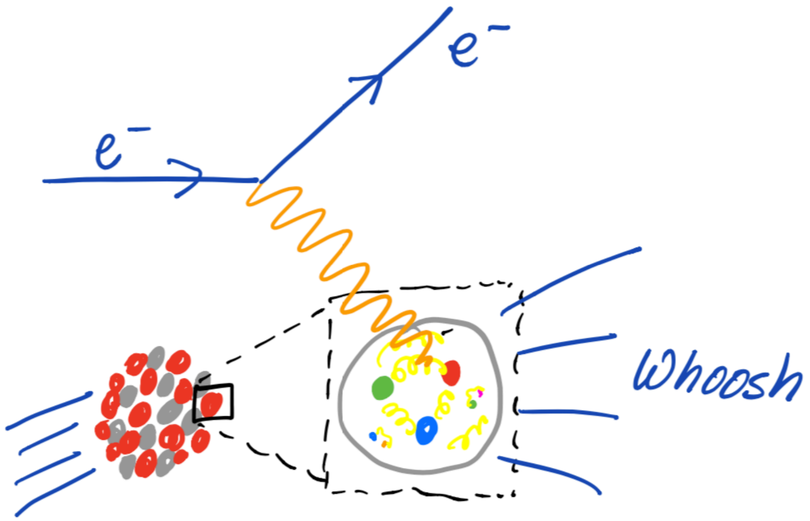

- **Measured are "real-time correlation functions"** $\langle P | J_\mu(x) J_\nu(0) | P \rangle$
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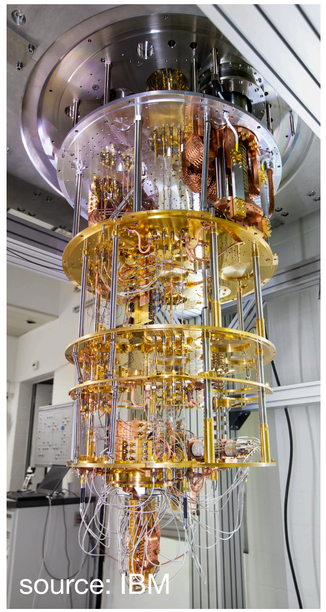
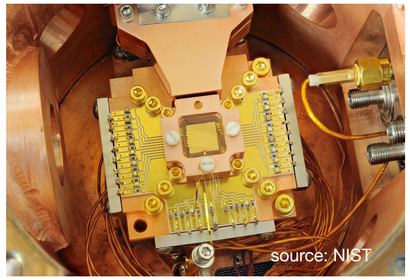
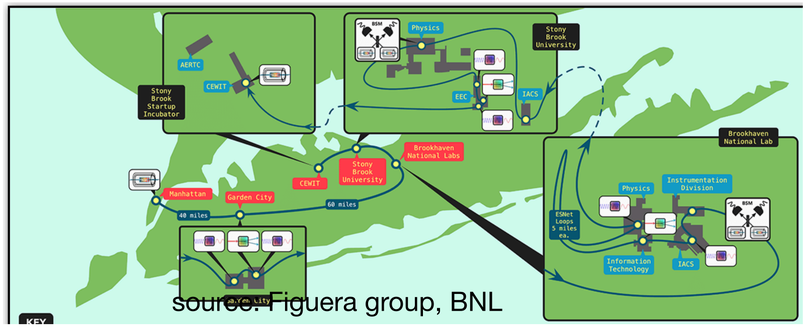
Quantum computers can go where classical computing fails!

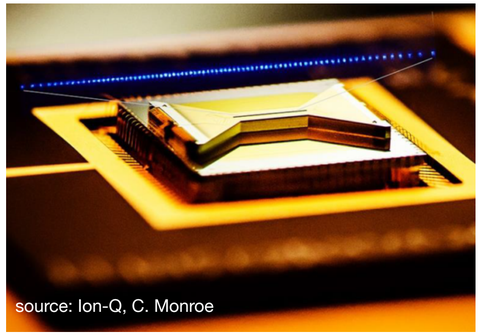
Summary

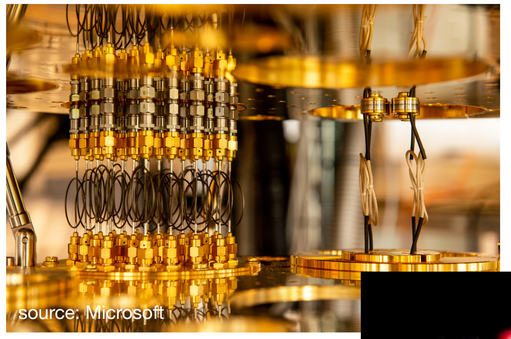
Very exciting times ahead! - (Second) Quantum Revolution!

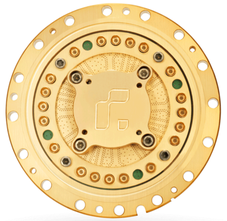


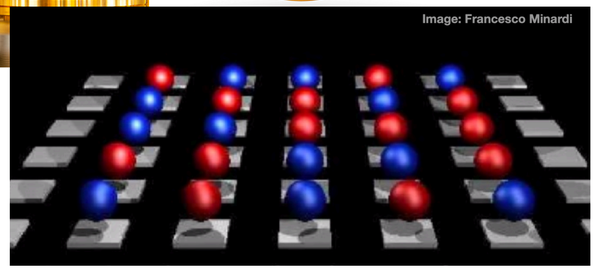


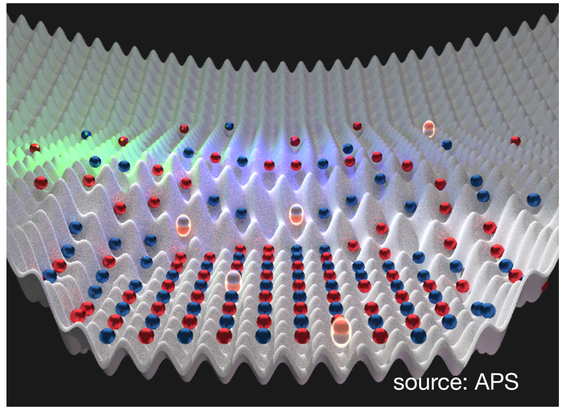












Enjoy thinking differently about problem? Go quantum!

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)

BROOKHAVEN NATIONAL LABORATORY

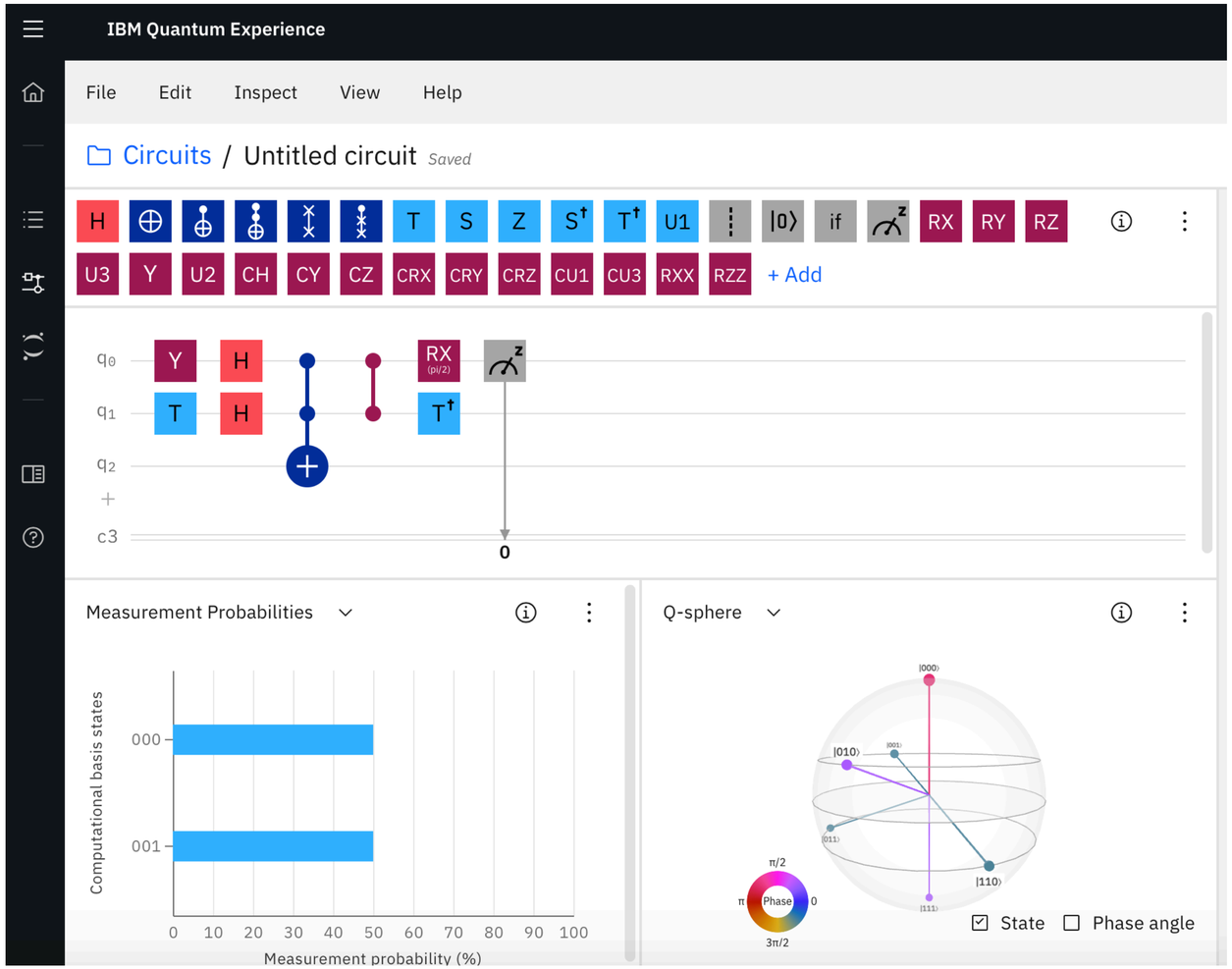
→

UNIVERSITY OF MARYLAND 1856

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

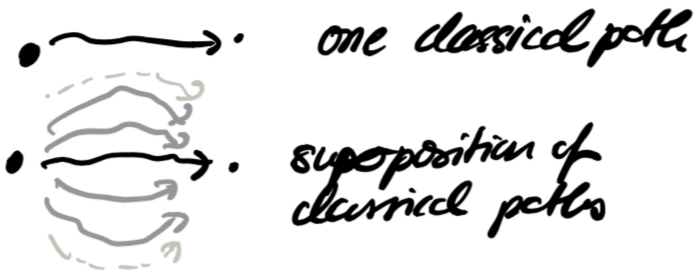
Backup: What is a path integral?

Backup: What is a path integral?

- Path integral for single particle

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

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



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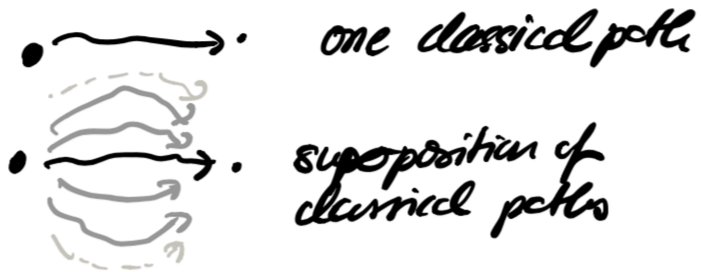
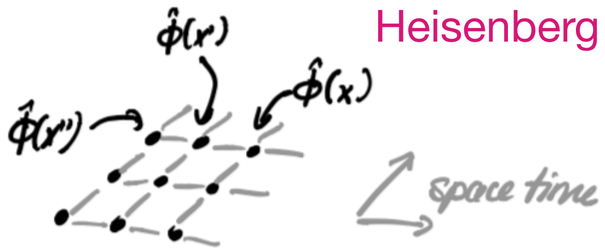


- Path integral for many body theory:
  (Quantum) Field Theory

Heisenberg Field Operator



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

$$\hat{\phi}(x)|\phi_x\rangle = \phi(x)|\phi_x\rangle$$

eigenvalue at x.

$$\hat{\pi}(x)|\pi_x\rangle = \pi(x)|\pi_x\rangle$$

$$\mathcal{H} = \bigotimes_x \mathcal{H}_x$$

$$\mathcal{H}_x = \text{span}\{|\phi_x\rangle\} = \text{span}\{|\pi_x\rangle\}$$

- path integral: $\langle\phi_B|e^{-iHt}|\phi_A\rangle$

Quantum mechanically superposition of a "paths".

Backup: What is a path integral?

not so crucial
to understand now!

Backup: What is a path integral?

- Path Integral = Representation of quantum mechanical amplitude

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

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

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

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

"weighted average over field operator eigenvalue"

not so crucial to understand now!

Backup: Whiteboard space

Backup: Whiteboard space

Backup: Whiteboard space