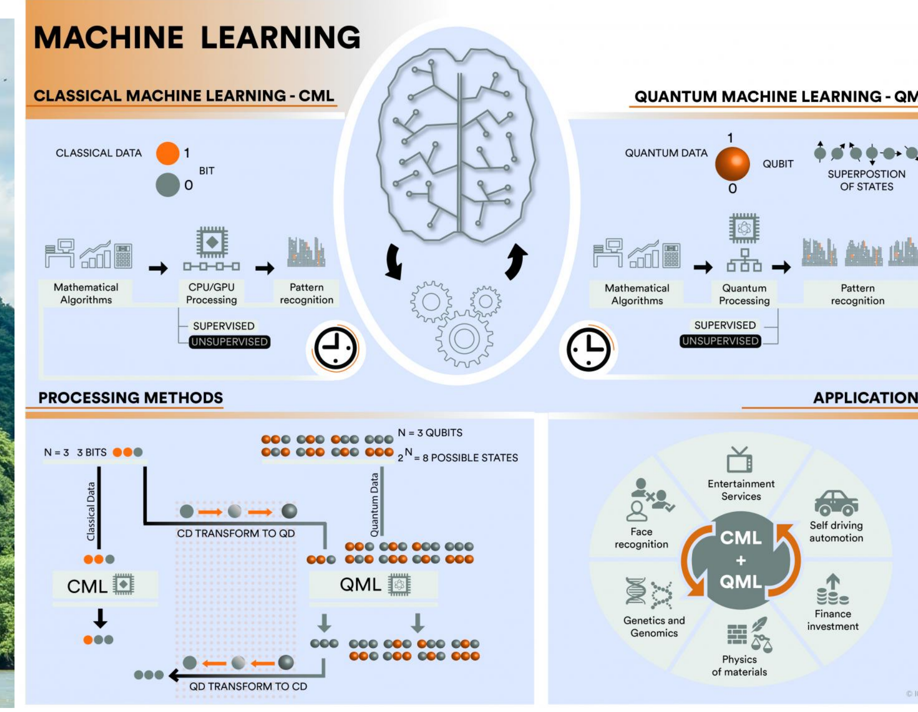
I Hear And I Forget.

I See And I Remember.

I Do And I Understand.

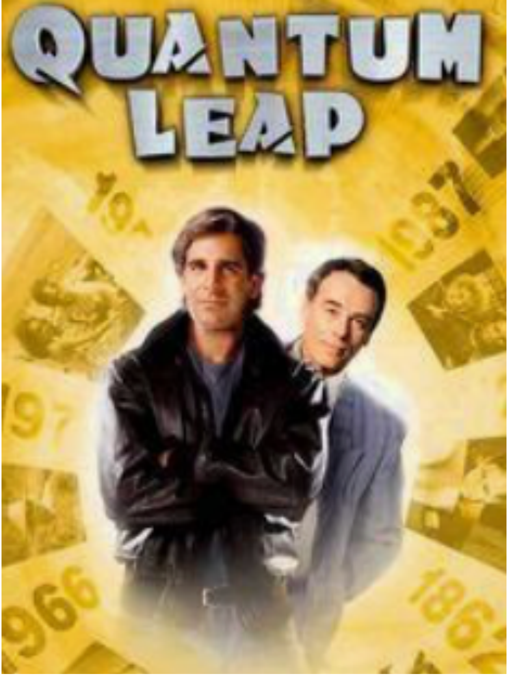
Confucius



Quantum Computing and Quantum Machine Learning

Michael Spannowsky

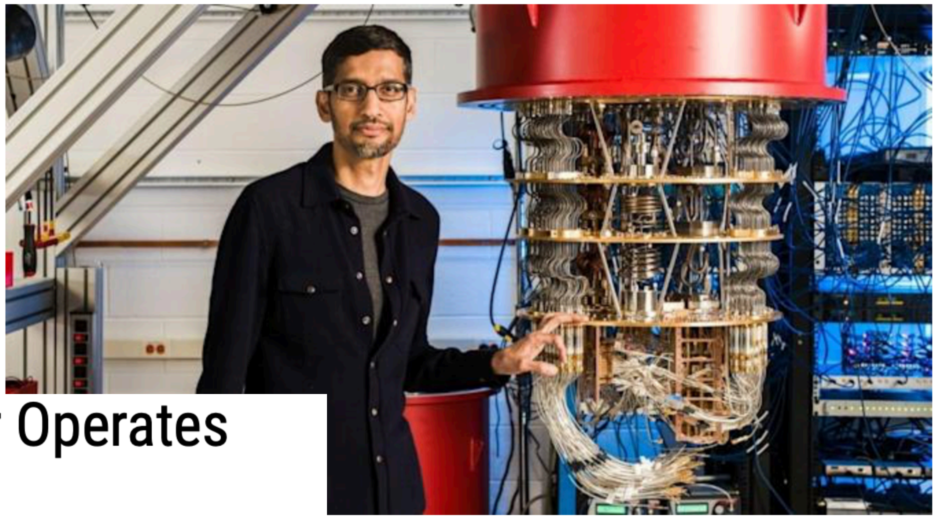
IPPP, Durham University



The Morning After: Google claims 'quantum supremacy'

And a controversial 'Ghost in the Shell' trailer.

R. Lawler
@Rjcc
October 24th, 2019



Master in Elektrotechnik, Informatik, Robotik, Maschinenwesen o. ä. (w/m/d)
German Aerospace Center (DLR) · Oberpfaffenhofen, Bavaria, Germany (On-site)
4 company alumni

Professor Cyber Security im Online Fernstudium (m/w/d)
IU International University of Applied Sciences · Germany (Remote)
Actively recruiting

Expertin für Post-Quanten-Kryptographie (w/m/d)
Deutsche Bahn · Frankfurt, Hesse, Germany (On-site)
Actively recruiting

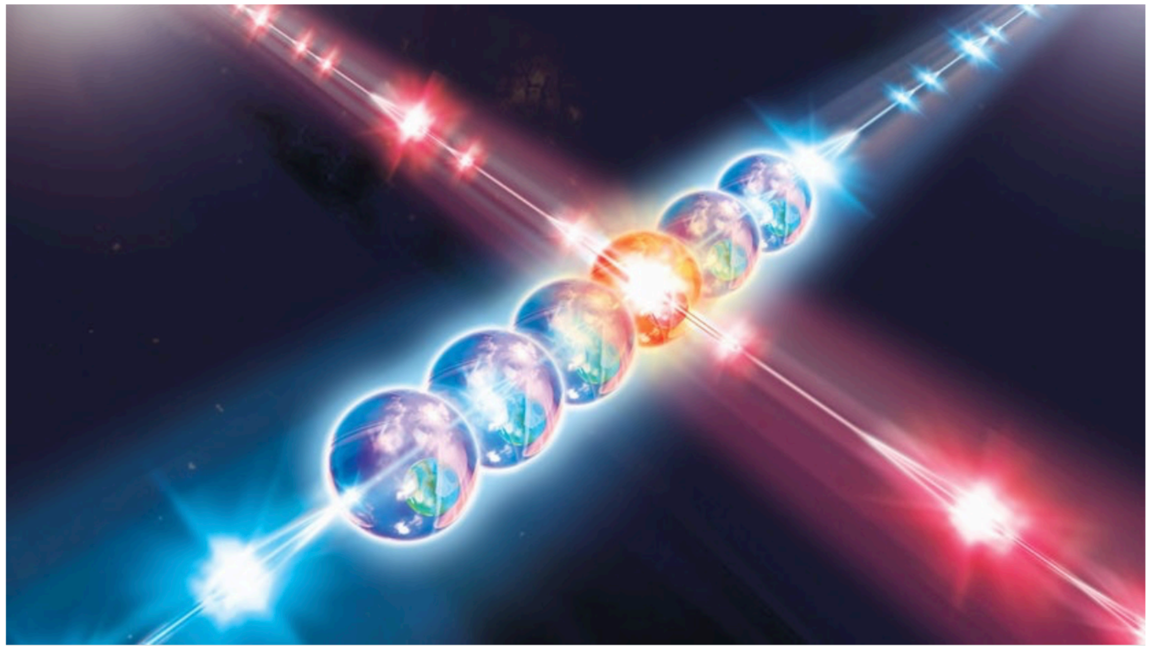
Master Thesis: Design of digitally enhanced power management circuits for Future Quantum Computers
Forschungszentrum Jülich · Jülich, North Rhine-Westphalia, Germany (On-site)
1 company alum

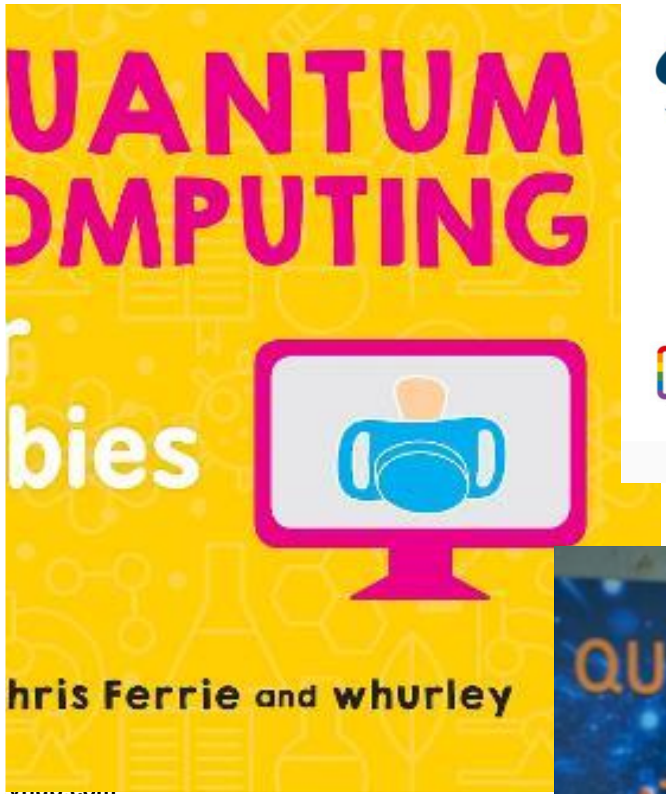
Expertin für Quantenkommunikation (w/m/d)
Deutsche Bahn · Frankfurt, Hesse, Germany (On-site)
Actively recruiting

First Quantum Computer Simulator Operates The Speed Of Light

Share

Kristen Philipkoski
Published 10 years ago: September 2, 2011 at 7:02 am - Filed to: COMPUTING





uantum Computers Will Be Incredibly Useful For

Computers don't exist in a vacuum. They serve to solve problems, and the type of problems they can solve are influenced by their hardware. Graphics processors are specialized for rendering images; artificial intelligence processors for AI; and quantum computers designed for... what? While the power of quantum computing is impressive, it does not mean that existing ...

Futuristic News
208 followers

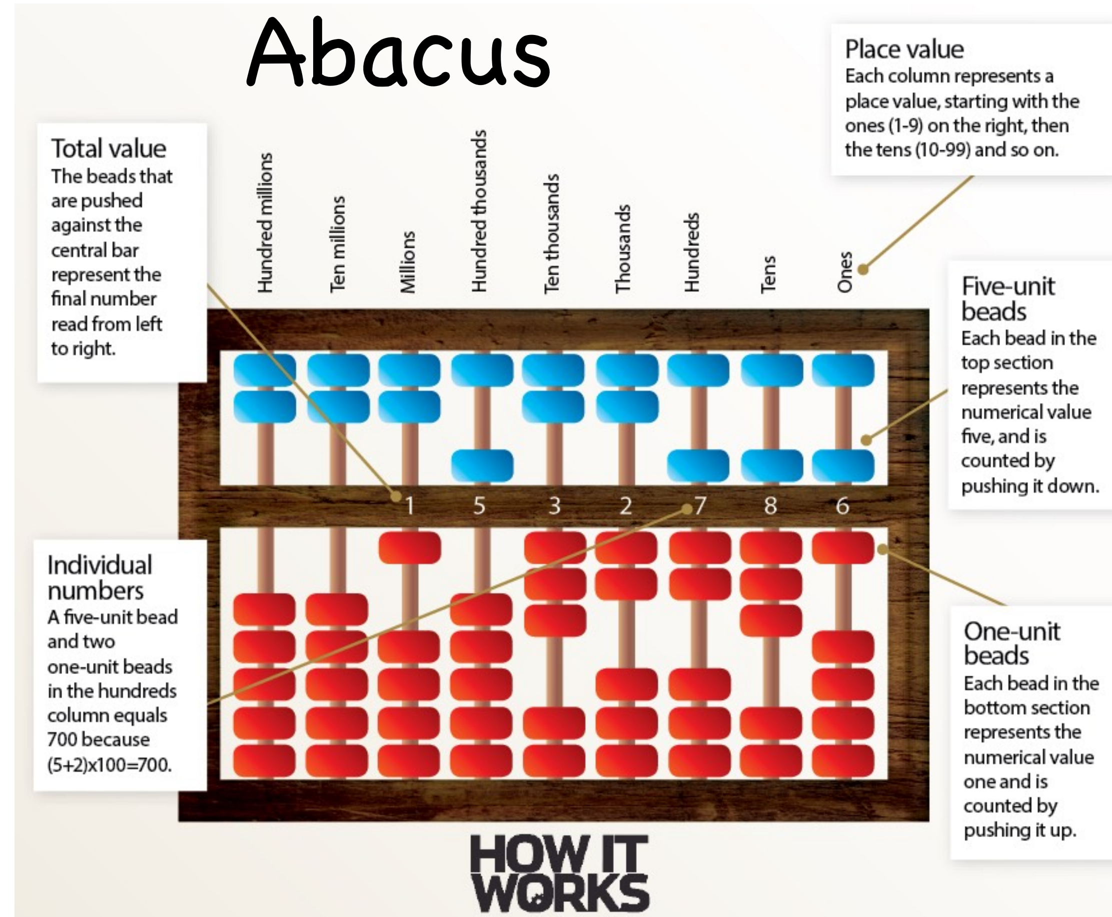
"Nature is quantum [...] so if you want to simulate it, you need a quantum computer" - Richard Feynman (1982)

Easily said ... so how do we do that?

Beginning of a scientific journey that accelerated in recent years tremendously....

Pre-digital age computing:

- express values in combinations and positions of beads
- manipulate beads mechanically
- convert position and combination of beads back into value



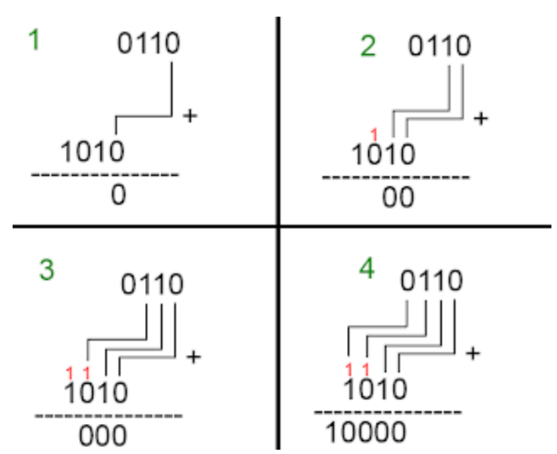
Digital age computing:

convert into different representation	define algebraic procedure on new representation	obtain result in new representation	convert back

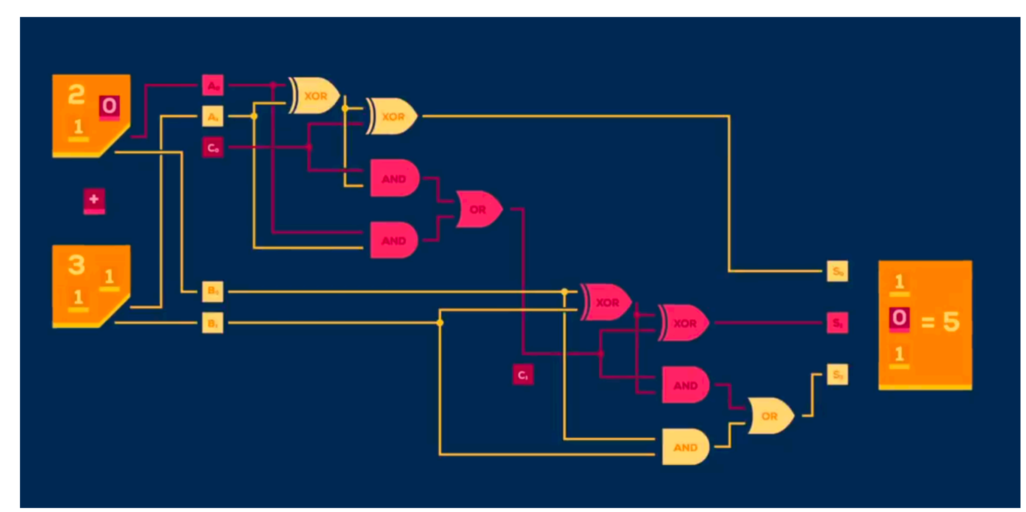
6+10 → Binary

```
  0110
+ 1010
-----------
 10000
```

→



→ 10000 → 16

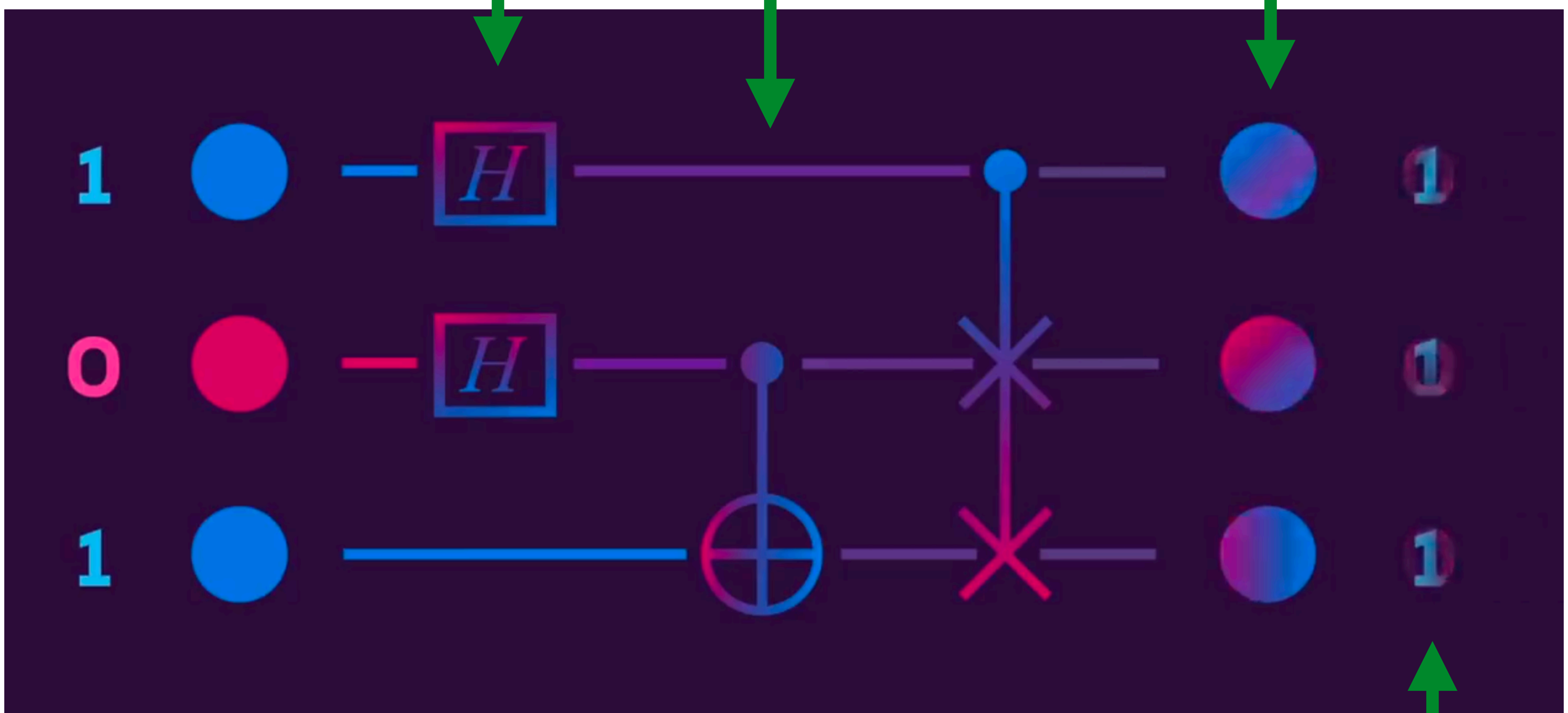


Quantum Age computing

(quantum) operations on qubits

initialisation

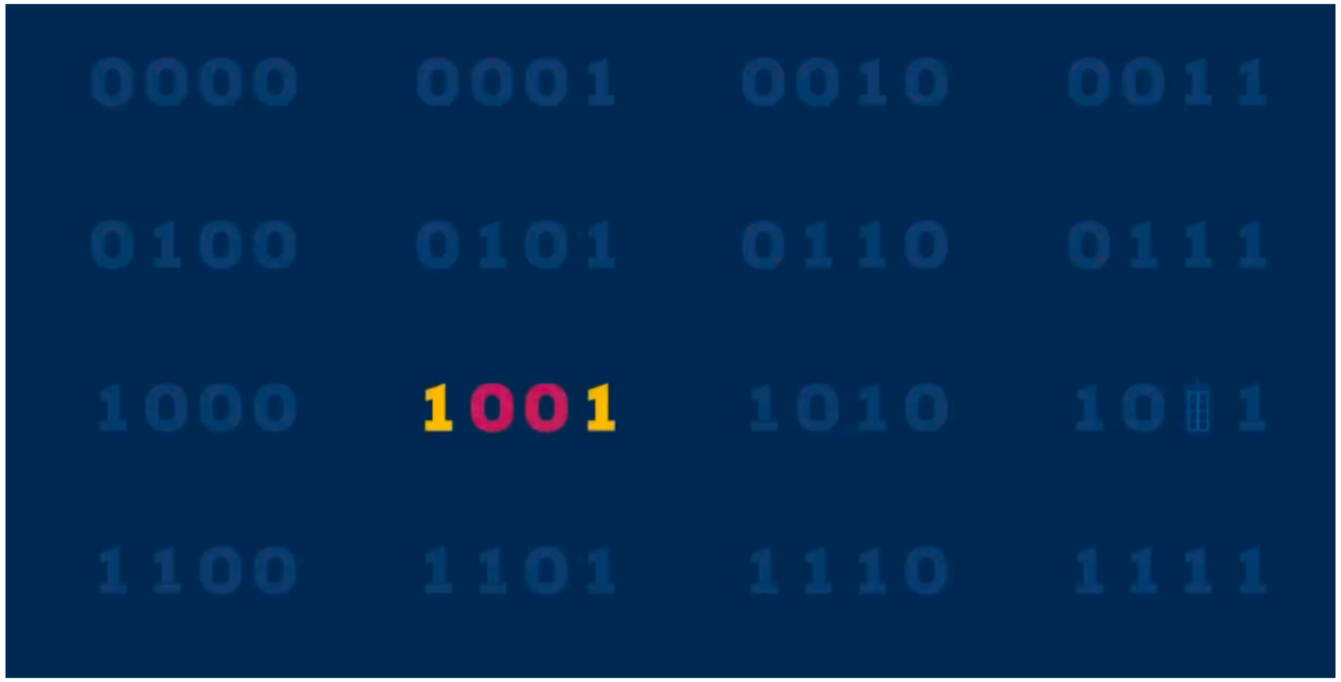
results in output of superpositions



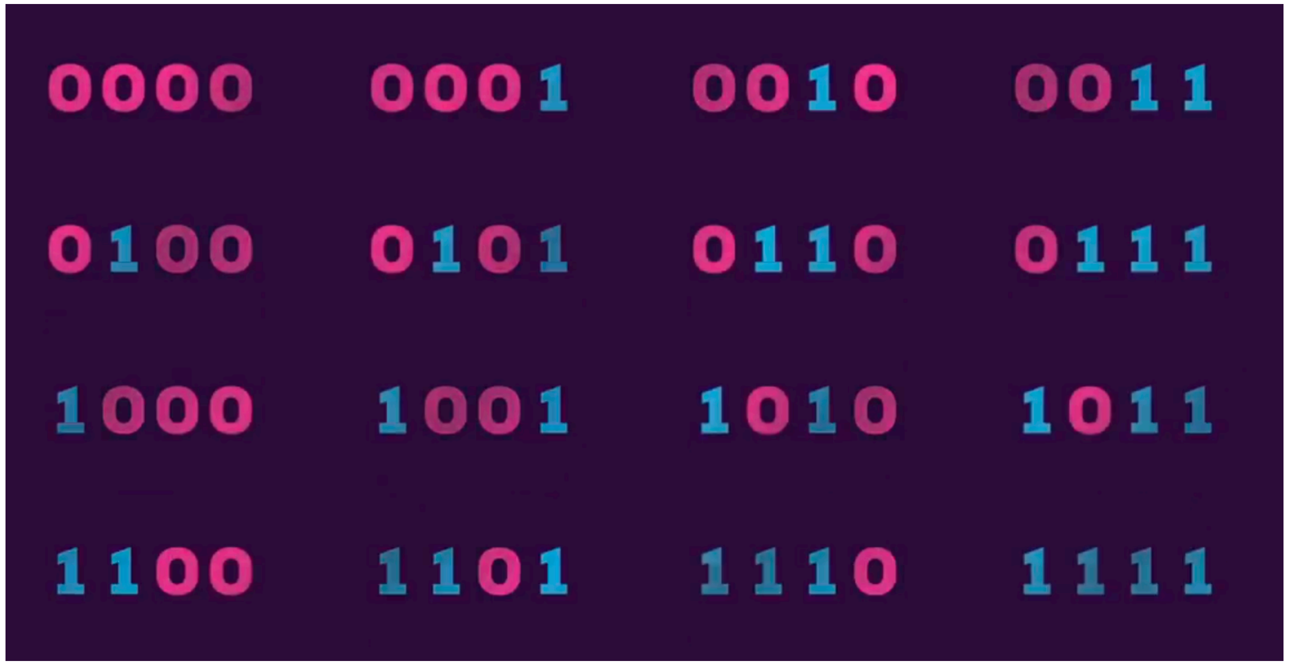
We then measure one specific outcome. Have to repeat measurement to statistically evaluate how likely each outcome is (by calculating and measuring several times). Since we work only with probabilities, we measure only probabilities

How can these quantum principles help to improve computations?

classical
system is in one state out of 16

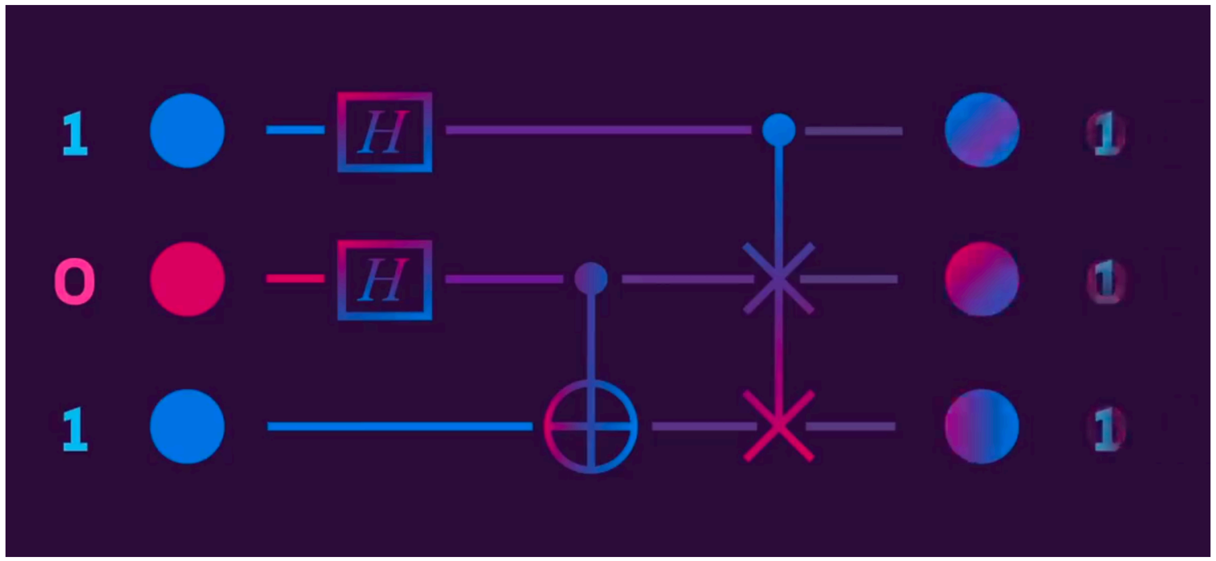


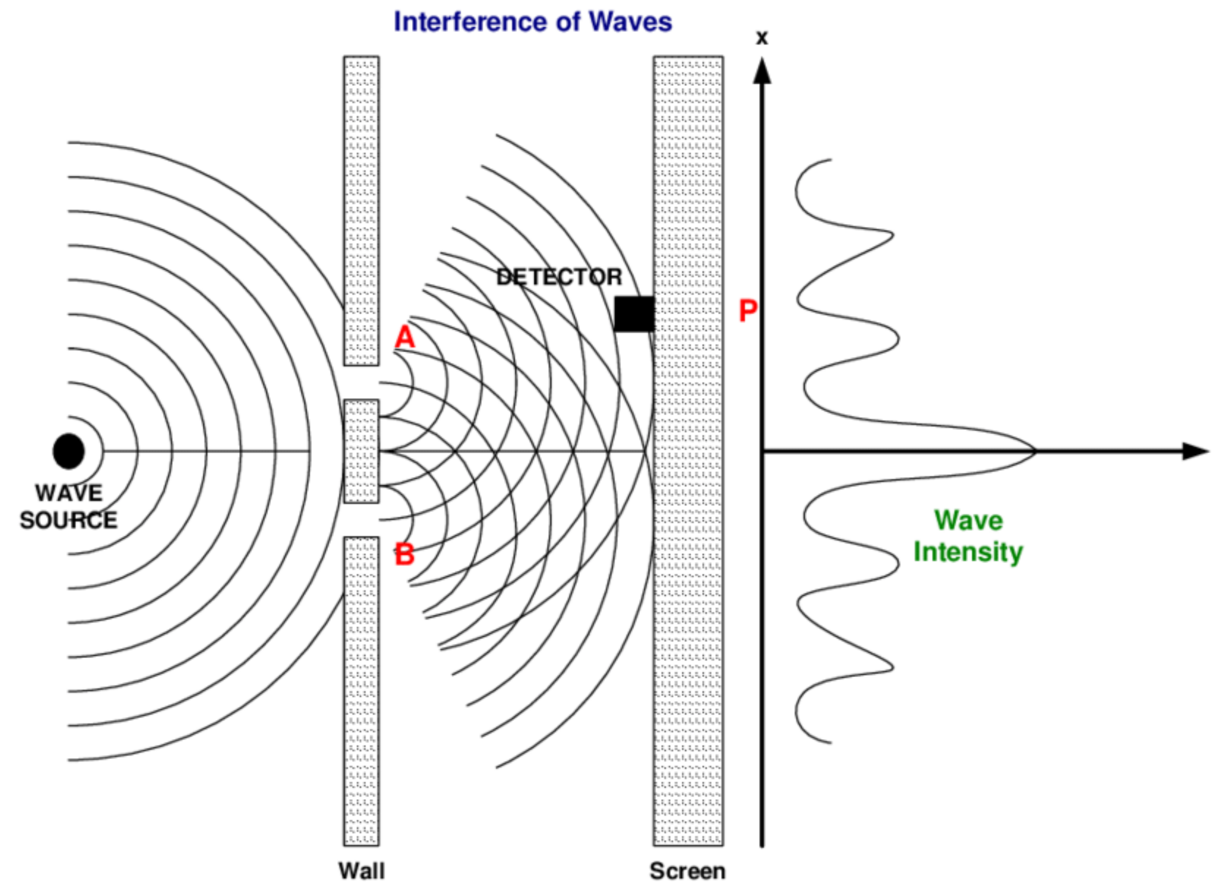
quantum (superposition)
can be in all states at same time



- Configuration space here 16=2^4 states.
- Computations can be performed simultaneously on the whole configuration space. **-> can be much faster than classically**
- A measurement of the quantum system after the computations are performed results in the observation of one of these configurations, with a probability that corresponds to the computational processes

Quantum Gate

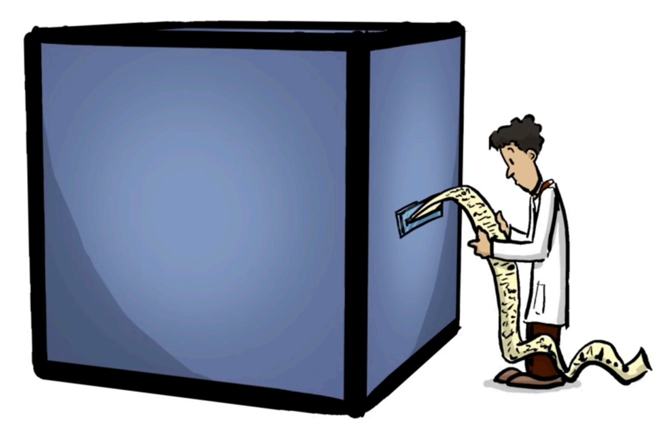




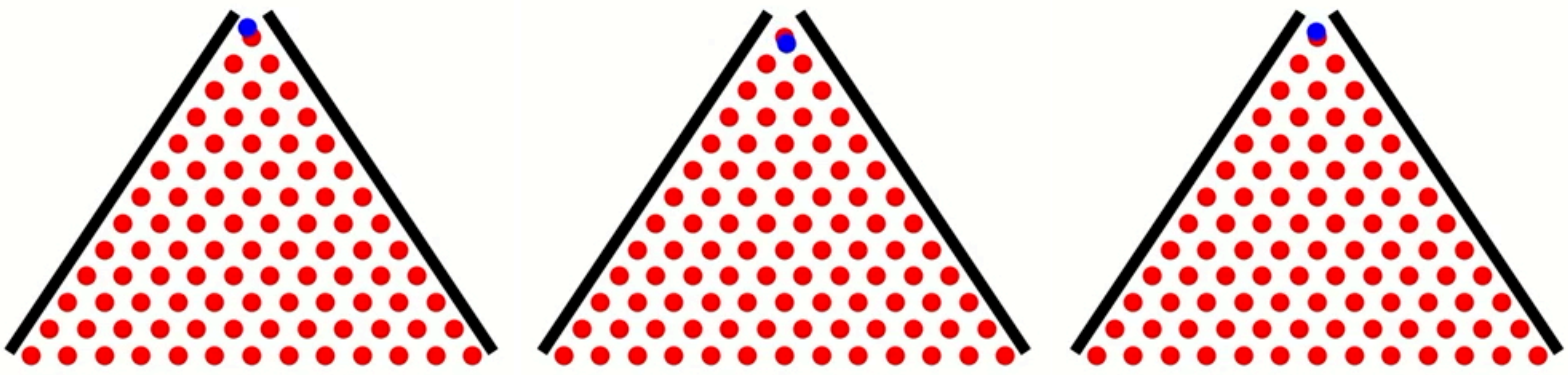
quantum gate and multi slit experiment are conceptually identical

While operating one cannot see how the gate works. Only at the end one can measure the outcome (box is closed during operations)

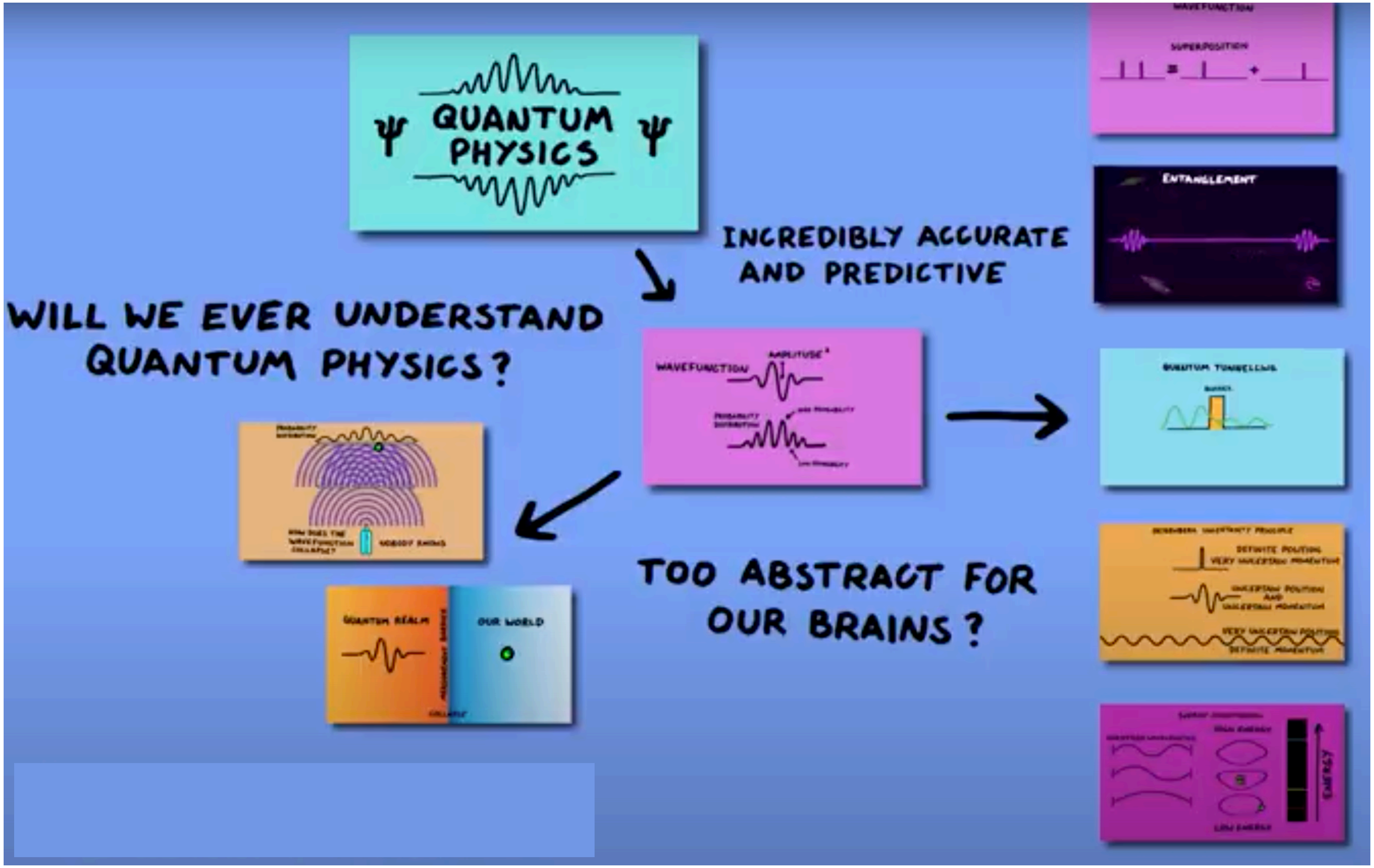
It's a secret computation...



Galton Board as analogy for Quantum Computer



The quantum mechanical principles on which the algorithms have to rely to have a chance for a quantum advantage are



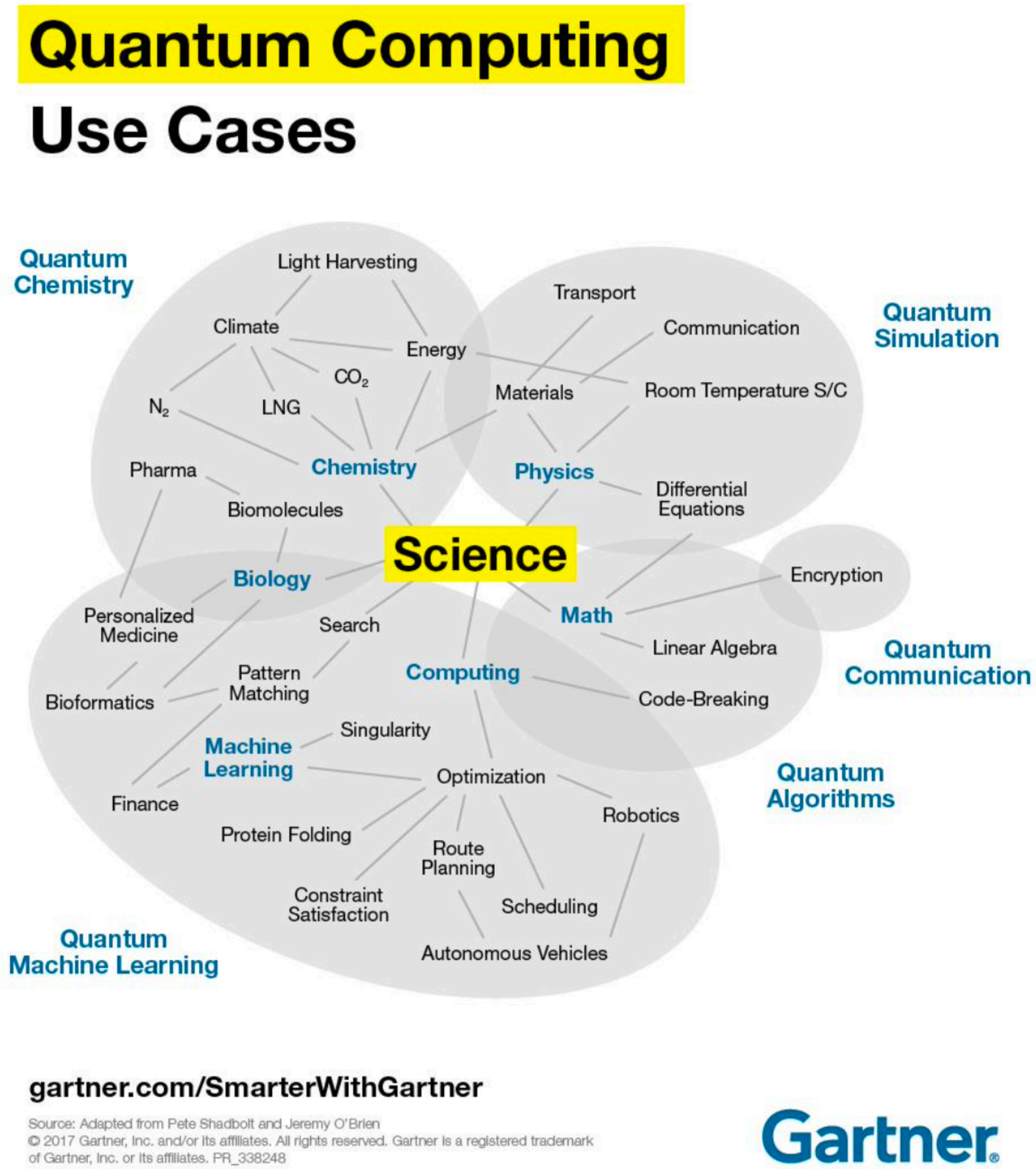
- Superposition
- Entanglement
- Tunneling
- Heisenberg principle
- Quantisation
- Configuration space sampling

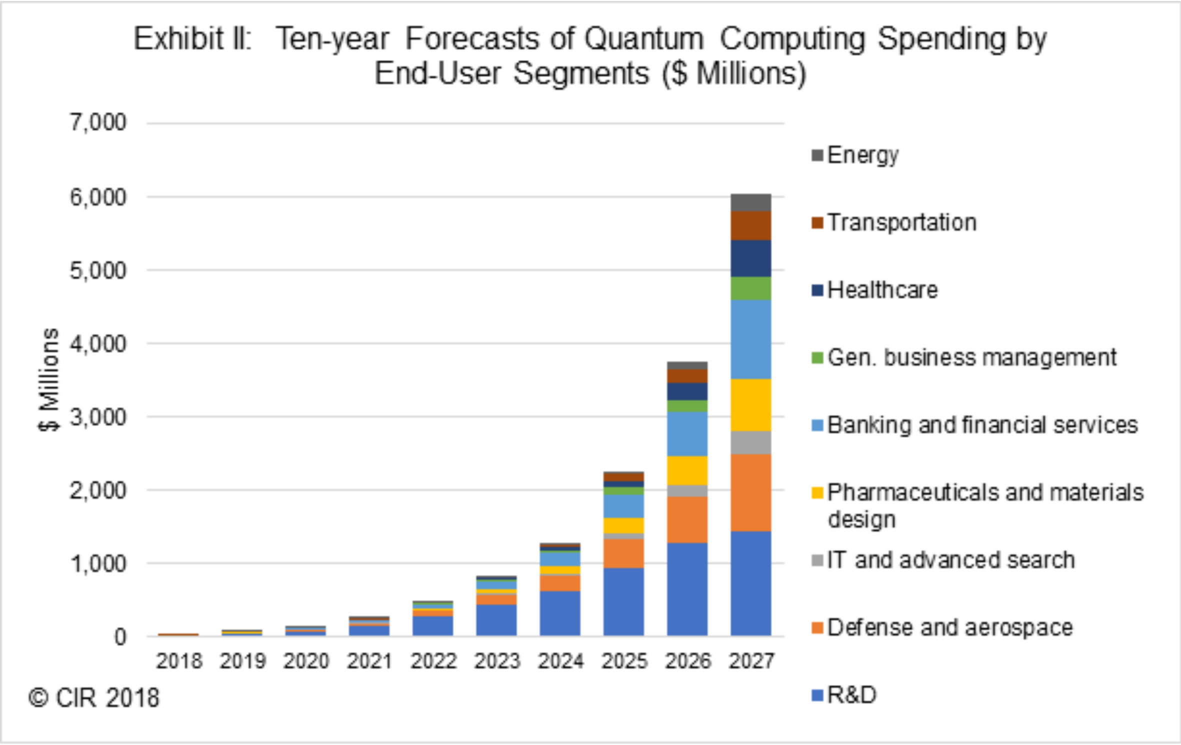
→ Required to go beyond classical computing

What are the potential advantages of Quantum Devices?

- Quantum Simulation: Simulating genuine quantum systems, e.g. molecules
  Medical applications, Chemistry applications, HEP etc
- Quantum Cryptography and Security: Encryption and decryption, e.g. emails, RSA
- Quantum Information Science: Transformation, storage and transmission of information, e.g. databases, teleportation, networks etc
- Quantum Sensing and Quantum Metrology: High-precision measurements, Quantum Imaging, Quantum Navigation/Timing
- Quantum Machine Learning and Optimisation: Learning and optimisation based on quantum algorithms
- Speed and efficiency: Simple classical tasks performed faster or with less electricity consumption etc

Private and Public Sector is placing big bets on Quantum Computing





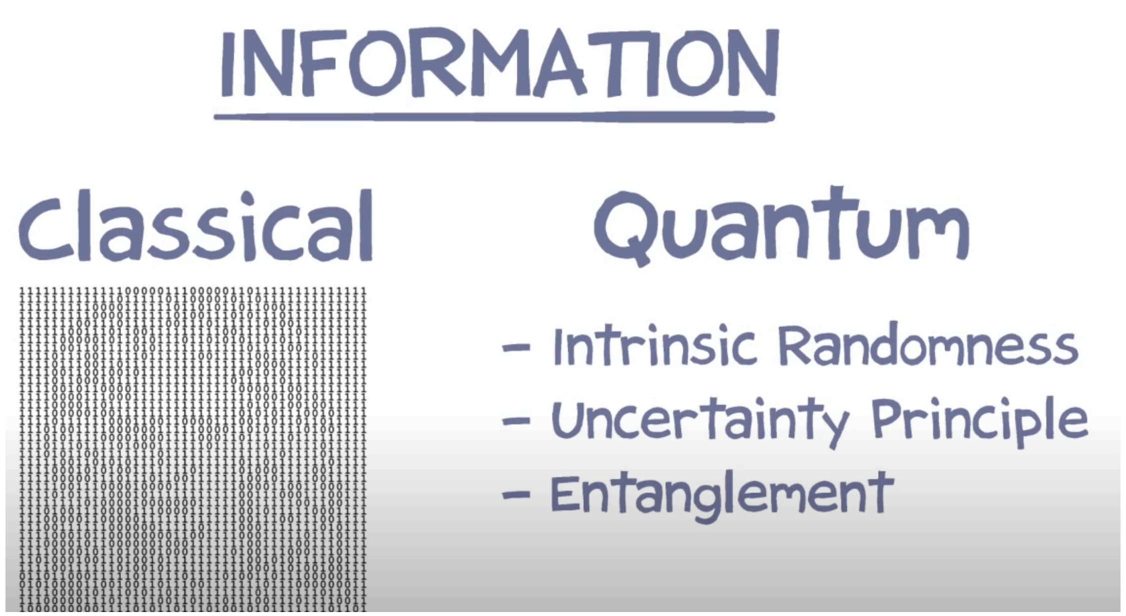
Significant financial investment expected across many sectors

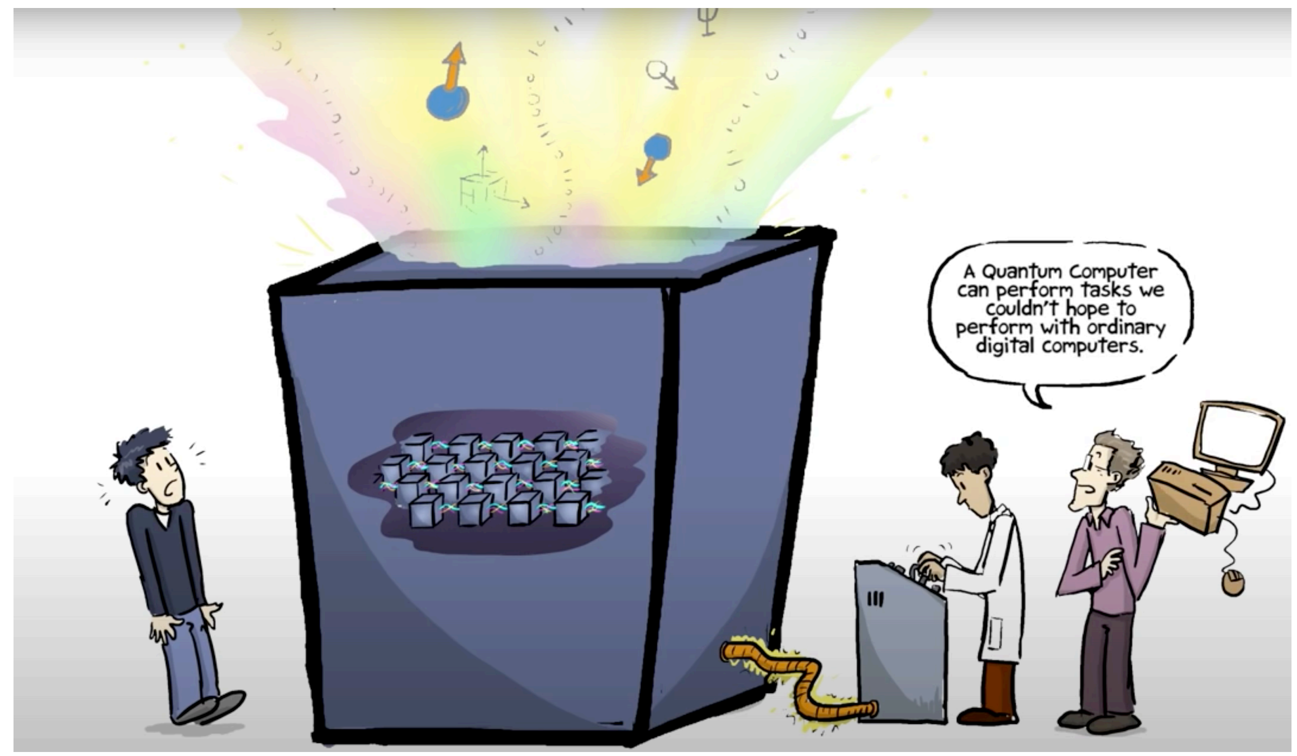
In US, already now higher financial investment from private than public sector

All national and international labs have QC programmes (Fermilab, BNL, LBNL, CERN, ...)

Basic motivation for Quantum Computing

"Can we take the quantum mechanical properties of microscopic objects and scale them up to larger quantum systems while harnessing their quantum prowess?"





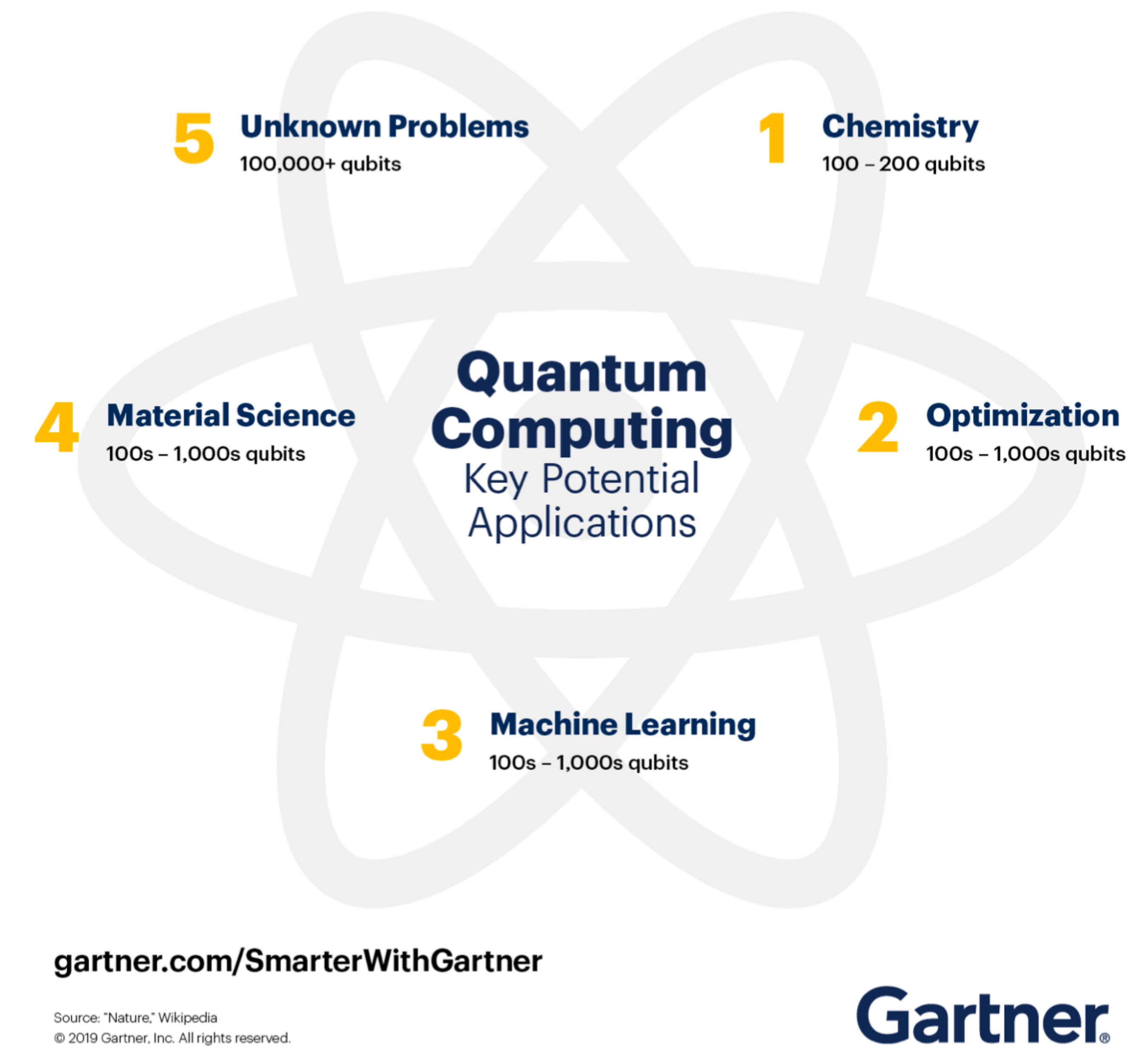
For some specialised task quantum supremacy has been shown

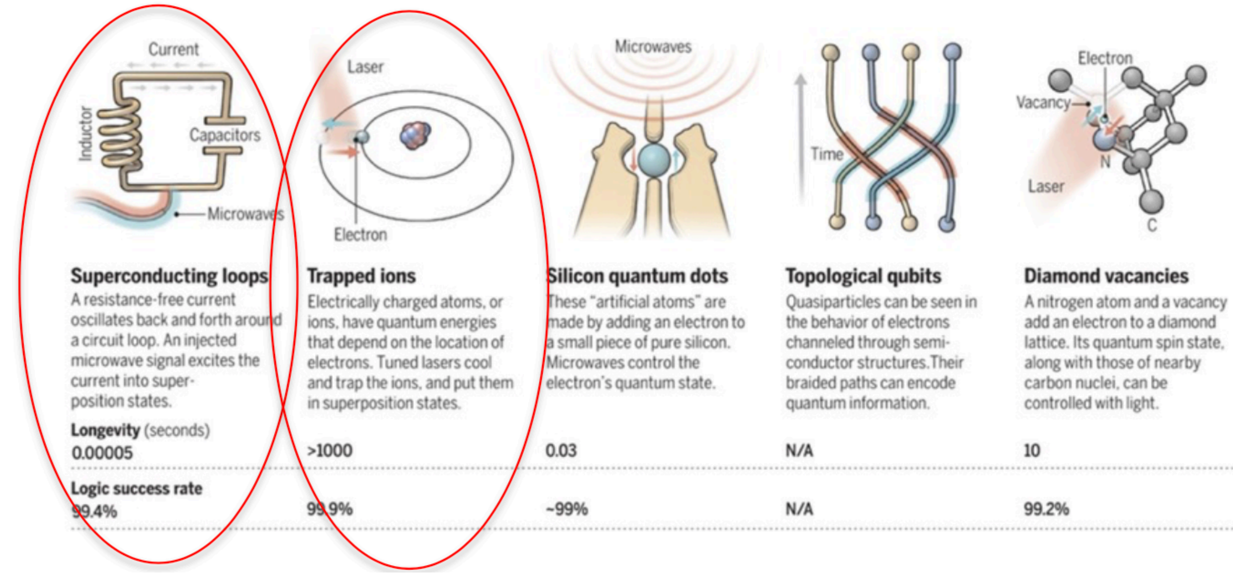
Disclaimer: nobody today thinks that quantum computers will universally replace classical computers

Technical challenges of a quantum computer

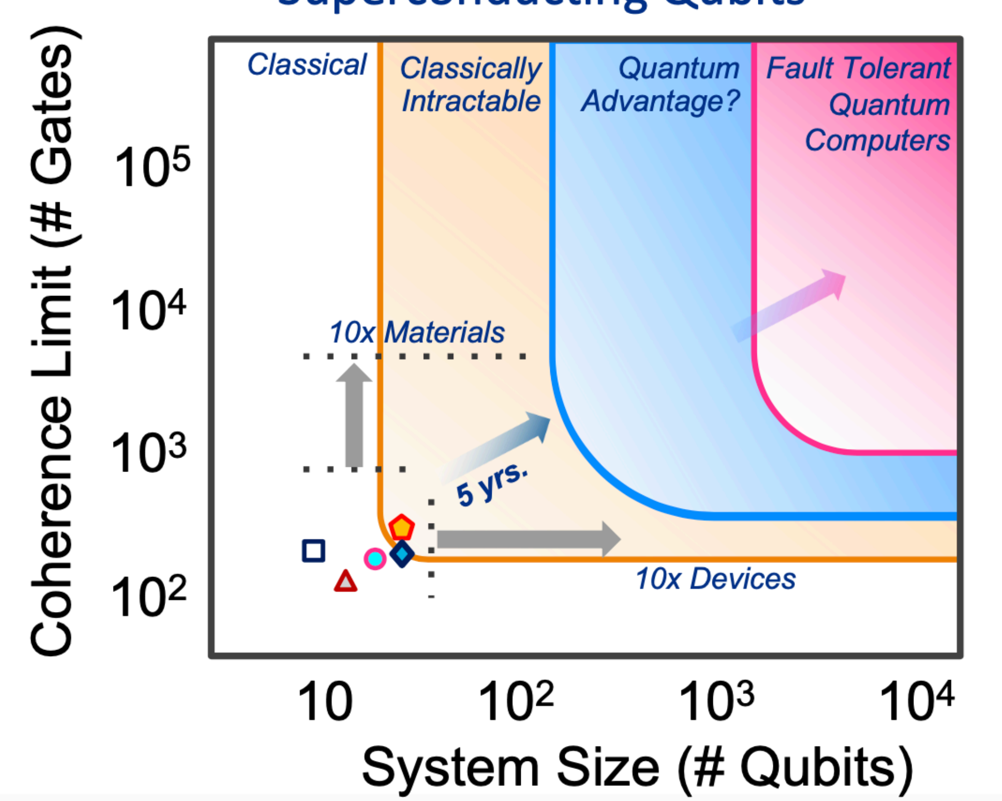
- Many quantum paradigms require system to be perfectly isolated (shielded from outside) to maintain coherence - for as long as the algorithm takes

The road to Quantum Advantage





Qubit technologies overview. From: Forbes, [*Quantum Computer Battle Royale: Upstart Ions Versus Old Guard Superconductors*]



IBM 400 qubits in 2022

IBM 1000 qubits in 2023

Quantum Information & Physics

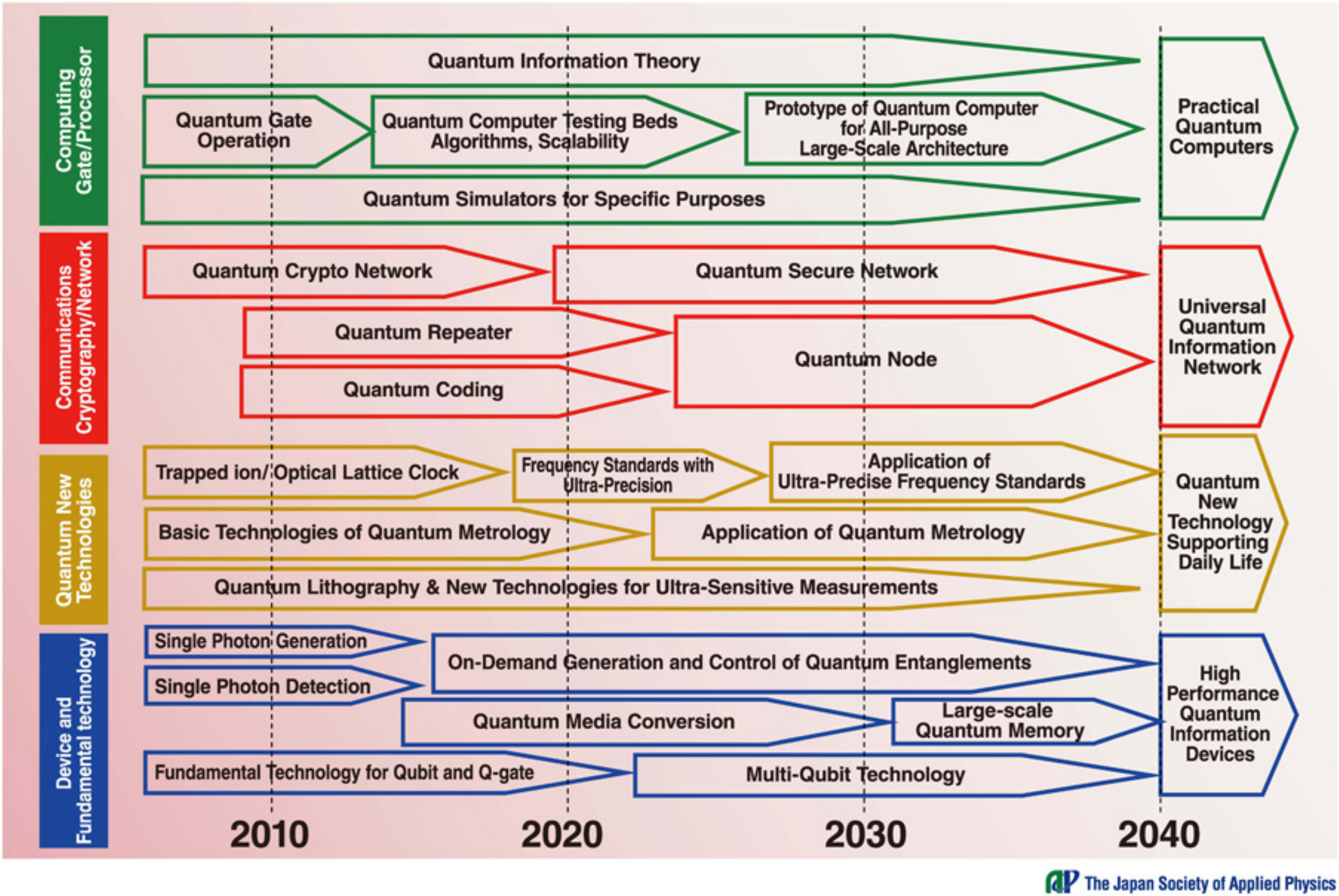
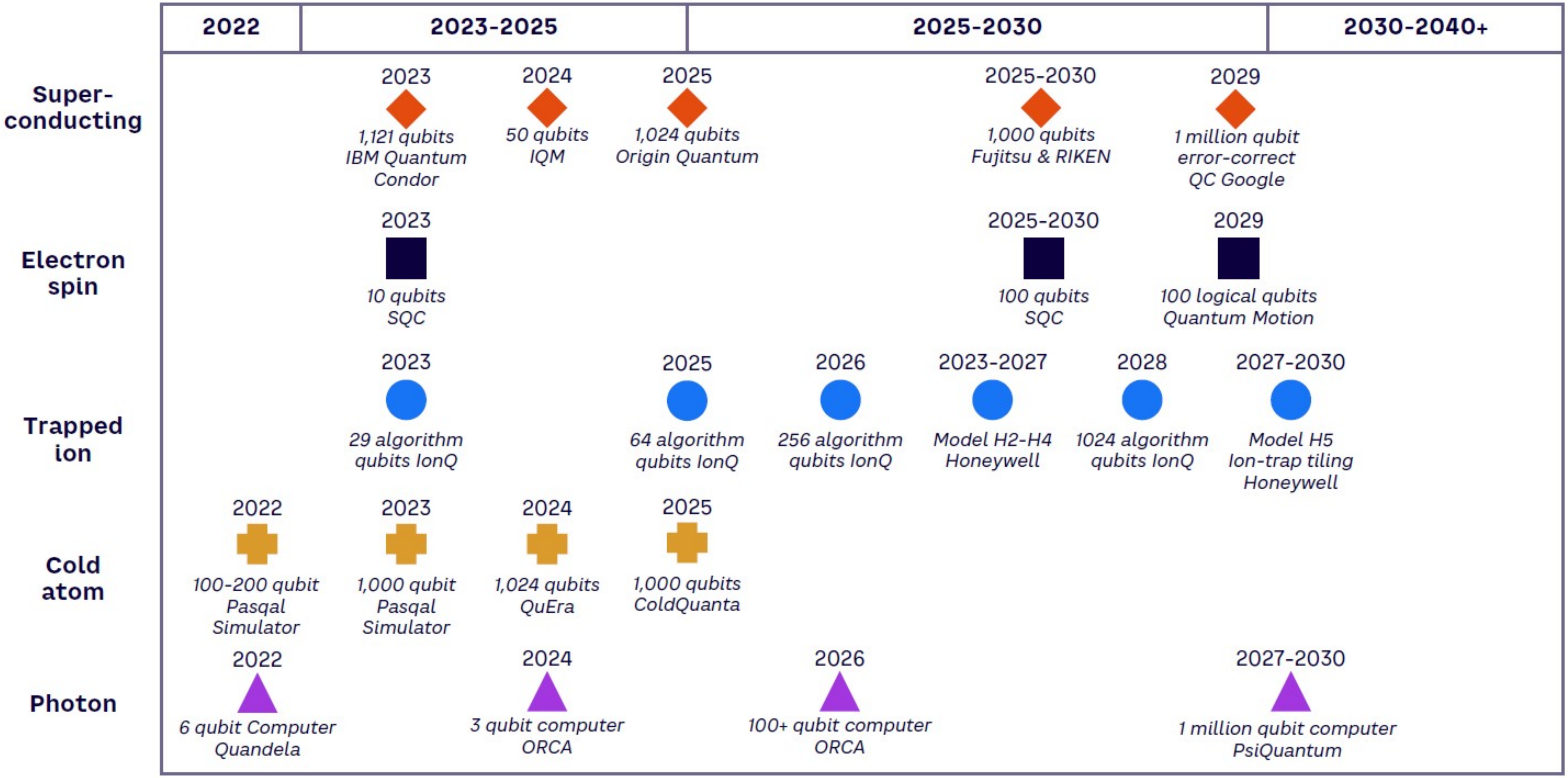


Figure 2. Quantum computing prototypes announced on vendor roadmaps



Source: Arthur D. Little, Olivier Ezratty

Analog vs Digital Quantum Computing

Analog and digital quantum computing are two different approaches to quantum computing, each with its own advantages and disadvantages.

Analog Quantum Computing (AQC):

- Based on the principle of quantum evolution of a quantum system, e.g. quantum annealing
- The system uses its intrinsic quantum dynamics, following the Schroedinger Equation
- Ground state represents the solution to the problem at hand
- Not always universal, but often well-suited for optimisation problems

Example: D-Wave Systems. The D-Wave quantum annealer uses a network of qubits that can collectively tunnel through the solution space to find the global minimum of a given function.

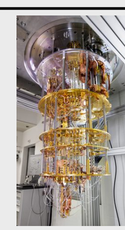
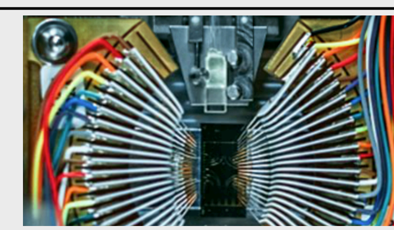
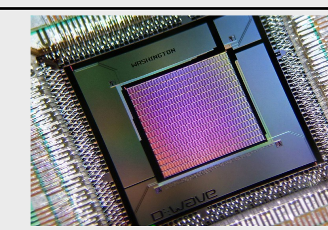
Digital Quantum Computing (DQC):

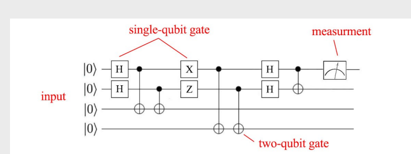
- Digital quantum computing, also known as gate-based quantum computing
- Uses quantum logic gates to perform operations on qubits
- Considered to be more versatile than analog computing.
- However, might require higher level of control over the quantum system, which can be challenging

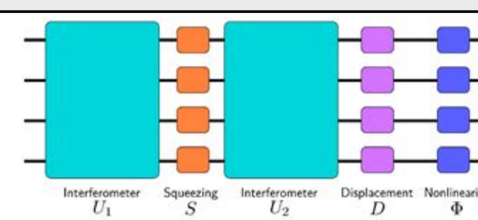
Example: IBM's and Google's quantum computers use the gate-based model of quantum computing.

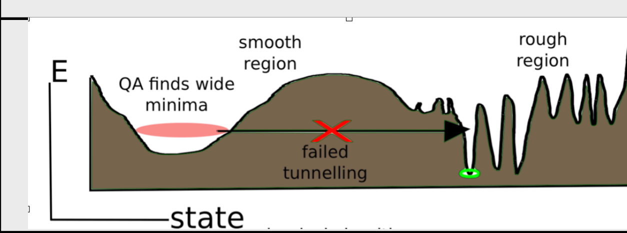
Popular Quantum Computing paradigms

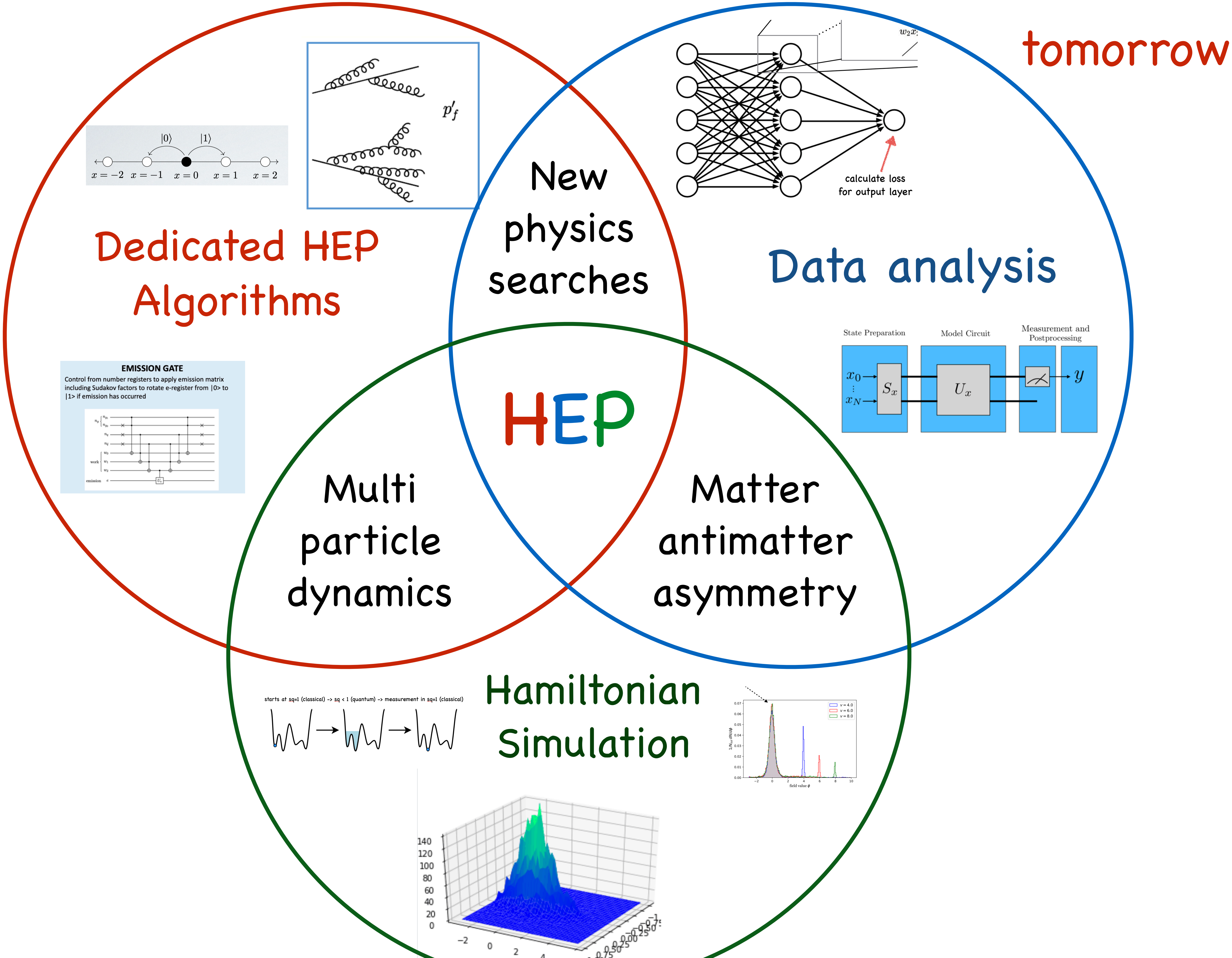
Quantum computing has long and distinguished history but is only now becoming practicable.

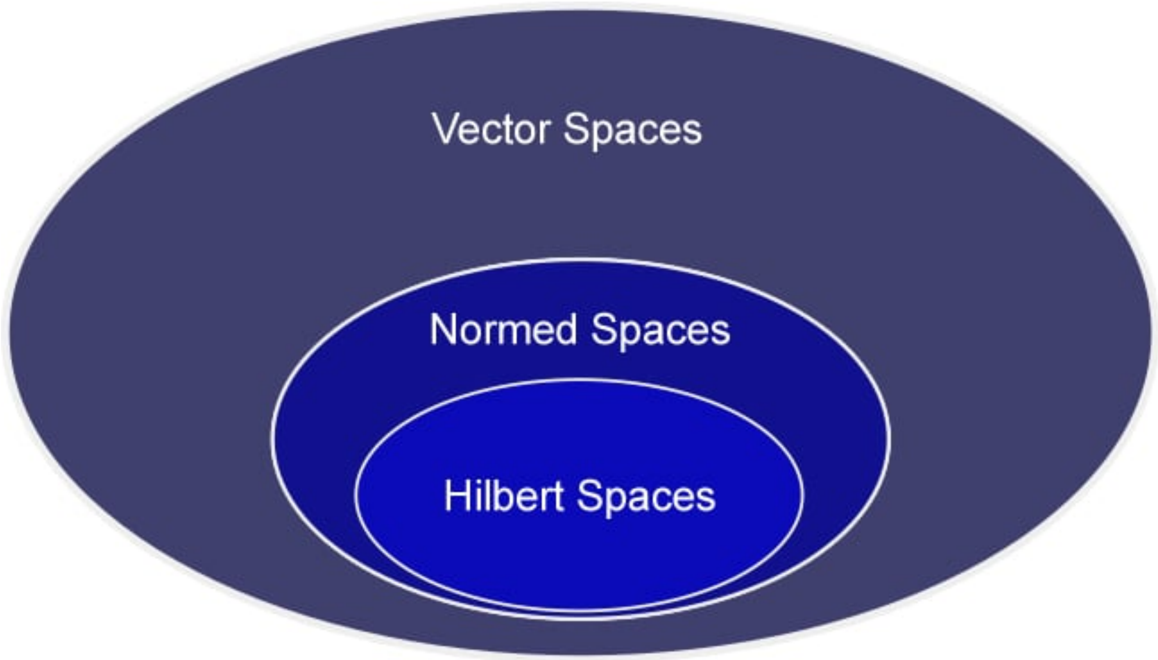
Type	Discrete Gate (DG)	Continuous Variable (CV)	Quantum Annealer (QA)
Property	Universal (any quantum algorithm can be expressed)	Universal - GBS non-Universal	Not universal — certain quantum systems
Advantage	most algorithms and tech support	uncountable Hilbert (configuration) space	continuous time quantum process
How?	IBM - Qiskit ~ 100 Qubits	Xanadu	DWave - LEAP ~7000 Qubits
What?			

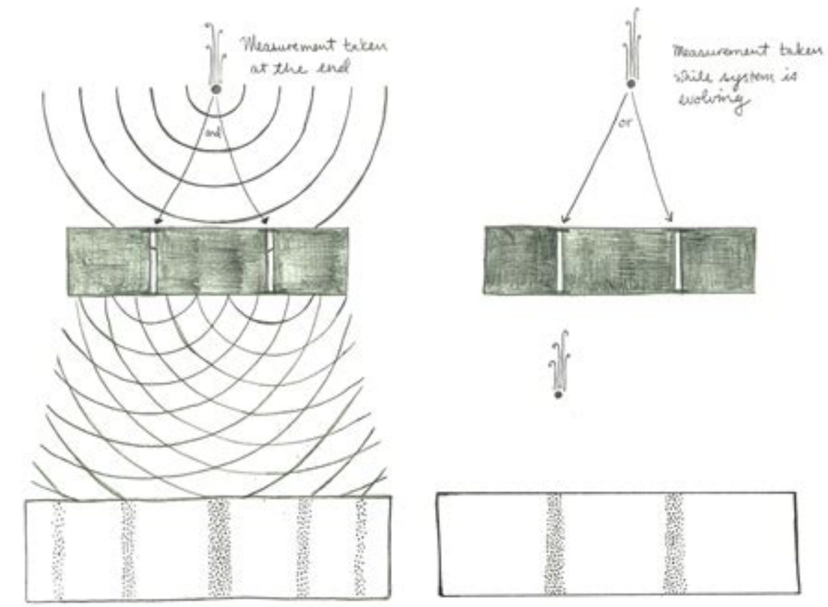




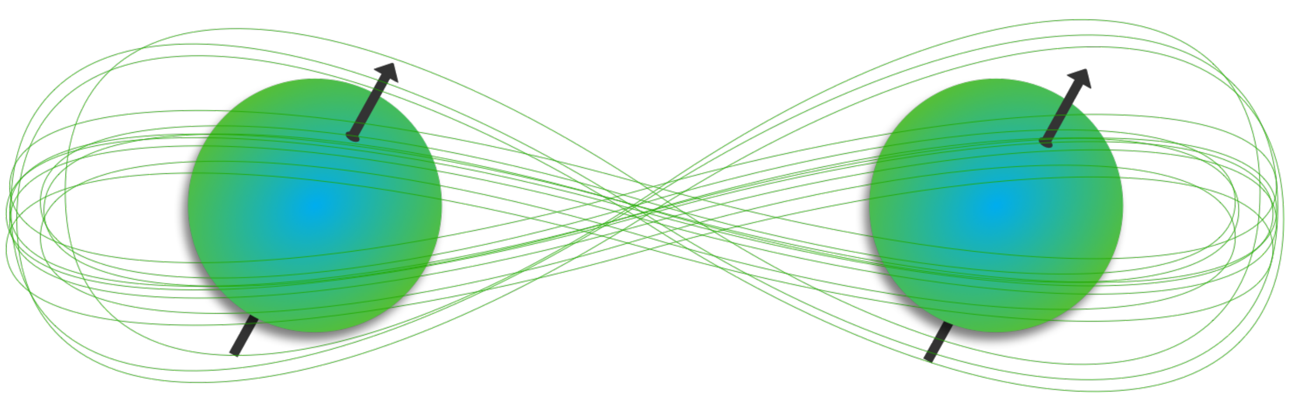


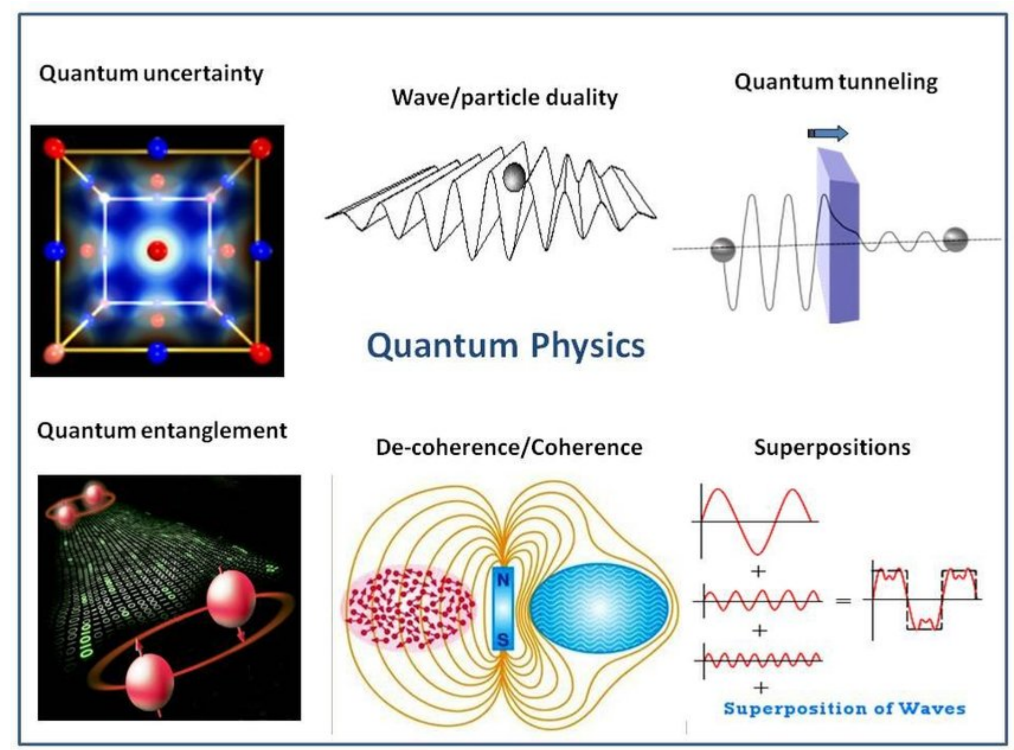

tomorrow
Dedicated HEP Algorithms
New physics searches
Data analysis
HEP
Multi particle dynamics
Matter antimatter asymmetry
Hamiltonian Simulation
calculate loss for output layer
State Preparation
Model Circuit
Measurement and Postprocessing
EMISSION GATE
Control from number registers to apply emission matrix including Sudakov factors to rotate e-register from |0> to |1> if emission has occurred
starts at sq=1 (classical) -> sq < 1 (quantum) -> measurement in sq=1 (classical)





Quantum Mechanics Basics





Phenomenological observations:

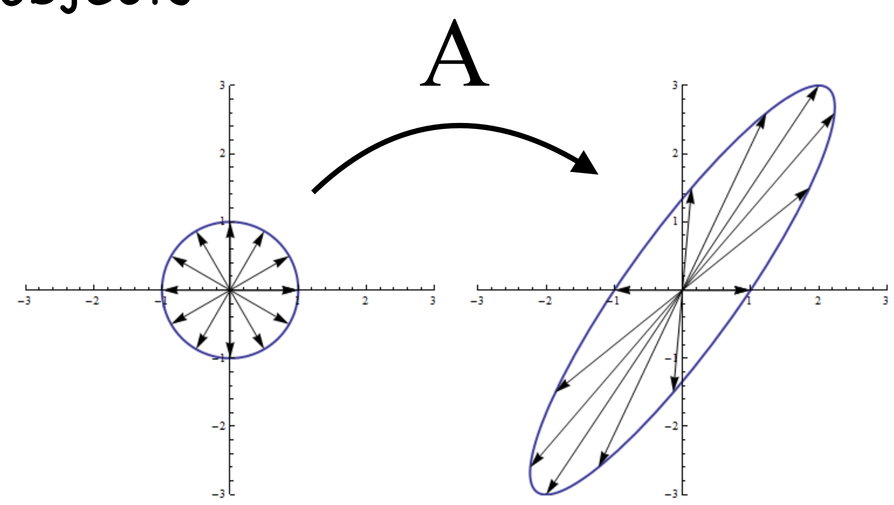
- **Randomness of measurement outcomes:** Repeated measurements of the same physical quantity (observable) A in the same physical conditions (state) produce different results.

- **Post-measurement state:** Let ψ be the physical state of the considered quantum system. If we perform a measurement process on the system to measure the observable A and the obtained outcome is $a \in R$ then the state of the system, after the measurement, is ψ_a.

- **Incompatible observables:** There are pairs of observables that cannot be simultaneously measured by an experiment.

Mathematical description of QM for QC

- Define and work in **Hilbert space** → Superposition principle
  → Distance and similarity measure
  → composition and transformation of objects



- Physical states are elements of Hilbert space
- States are manipulated through linear operators $A(\alpha\psi + \beta\varphi) = \alpha A\psi + \beta A\varphi$
- Physical quantities are expressed through self-adjoint operators, that have real eigenvalues $\lambda\langle\psi|\psi\rangle = \langle\psi|A\psi\rangle = \langle A\psi|\psi\rangle = \lambda^*\langle\psi|\psi\rangle$
- The eigenvalues of unitary operator are complex numbers with unit modulus, also called phases: for φ eigenvector of unitary operator U with eigenvalue μ, $\langle\varphi|\varphi\rangle = \langle U\varphi|U\varphi\rangle = \mu^*\mu\langle\varphi|\varphi\rangle = |\mu|^2\langle\varphi|\varphi\rangle$, then $|\mu|^2 = 1$, so $\mu = e^{i\varphi}$ with $\varphi \in R$
- Spectral Theorem: If $A \in \mathbf{B}(H)$ is normal, that is, $AA^\dagger = A^\dagger A$, if and only if there exists an orthonormal basis of H made by eigenvectors of A.
  → any **self-adjoint operator** is **diagonalisable** and admits a **spectral decomposition**
  → **Functional calculus** for bounded (and unbounded) operators

- Composite quantum systems:

  Let H_A and H_B be Hilbert spaces and $\psi \in H_A$, $\varphi \in H_B$.

  The **tensor product of** ψ **and** φ is defined by: $\psi \otimes \varphi(x, y) := \langle \psi | x \rangle_A \langle \varphi | y \rangle_B \quad x \in \mathrm{H}_A, y \in \mathrm{H}_B$

  The tensor product of Hilbert spaces $H_A \otimes H_B$ consists of all such tensor products equipped with the inner product: $\langle \psi \otimes \varphi | \psi' \otimes \varphi' \rangle := \langle \psi | \psi' \rangle_A \cdot \langle \varphi | \varphi' \rangle_B \quad \psi, \psi' \in \mathrm{H}_A \ \varphi, \varphi' \in \mathrm{H}_B$

  The **tensor product of operators** $A \in \mathbf{B}(H_A)$ and $B \in \mathbf{B}(H_B)$ is: $(A \otimes B)(\psi \otimes \varphi) := A\psi \otimes B\varphi$

  If dim H_A = n and dim H_B = m then dim($H_A \otimes H_B$) = n·m.

For example:

- for $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ and $|\phi\rangle = \gamma|0\rangle + \delta|1\rangle$ we get

$$|\psi\rangle \otimes |\phi\rangle = \alpha\gamma|0\rangle \otimes |0\rangle + \alpha\delta|0\rangle \otimes |1\rangle + \beta\gamma|1\rangle \otimes |0\rangle + \beta\delta|1\rangle \otimes |1\rangle$$

- for operators $A|\psi\rangle = a|\psi\rangle$ and $B|\phi\rangle = b|\phi\rangle$ we have:

$$(A \otimes B)(|\psi\rangle \otimes |\phi\rangle) = (A|\psi\rangle) \otimes (B|\phi\rangle) = a|\psi\rangle \otimes b|\phi\rangle = ab(|\psi\rangle \otimes |\phi\rangle)$$

- $$A = \begin{pmatrix} a_{11} & \cdot & \cdot & \cdot & a_{1n} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ a_{n1} & \cdot & \cdot & \cdot & a_{nn} \end{pmatrix} \quad B = \begin{pmatrix} b_{11} & \cdot & \cdot & \cdot & b_{1m} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ b_{m1} & \cdot & \cdot & \cdot & b_{mm} \end{pmatrix} \rightarrow A \otimes B = \begin{pmatrix} a_{11}B & \cdot & \cdot & \cdot & a_{1n}B \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ a_{n1}B & \cdot & \cdot & \cdot & a_{nn}B \end{pmatrix}$$

- Some states cannot be written as a direct tensor product, e.g.

$$|\psi\rangle_{AB} = |\psi\rangle_A \otimes |\psi\rangle_B \quad \neq \quad \frac{1}{\sqrt{2}}|0\rangle_A|0\rangle_B + \frac{1}{\sqrt{2}}|1\rangle_A|1\rangle_B \quad \text{Bell states}$$

So, using the language of states and their tensor products is not be sufficient.

$$|\psi_x\rangle \longrightarrow \rho = \sum_x p_x |\psi_x\rangle\langle\psi_x|$$

Density matrix:

Consider a quantum system with state space C^d. A density matrix, commonly denoted as ρ , is a linear operator $\rho \in L(C^d, C^d)$ such that:

1. $\rho \geq 0$, and
2. $tr(\rho) = 1$.

The density matrix is a representation of a system's statistical state

- Concepts **pure** vs **mixed states**, **coherent** vs **incoherent superposition**

- **Entanglement**

The density operator $\rho \in \mathbf{S}(H_A \otimes H_B)$ is said to be separable if it can be written as a statistical mixture of product states:

$$\rho = \sum_i \lambda_i \rho_i^{(A)} \otimes \rho_i^{(B)}$$

where $\lambda_i \geq 0$ and $\sum_i \lambda_i = 1$. Otherwise it is said to be **entangled**.

Example: $$|\Psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$ Bell state

Assume the Bell state could be written into product of two states

$$|\Psi\rangle = |a\rangle \otimes |b\rangle = (\alpha|0\rangle + \beta|1\rangle) \otimes (\gamma|0\rangle + \delta|1\rangle) = \alpha\gamma|00\rangle + \alpha\delta|01\rangle + \beta\gamma|10\rangle + \beta\delta|11\rangle$$

Condition for Bell state: $\alpha\delta|01\rangle + \beta\gamma|10\rangle = 0 \quad \text{and} \quad \alpha\gamma|00\rangle = \beta\delta|11\rangle = \frac{1}{\sqrt{2}}$

$$\alpha\delta = 0 \quad \text{and} \quad \beta\gamma = 0$$

both conditions cant hold

doesnt work

Bell state cant be written as product

Let's reconsider the phenomenological evidence list:

Randomness of measurement outcomes:
The possible experimental values of the observable A are the element of its spectrum $\sigma(A)$.

Given a pure state $|\psi\rangle \in H$, the probability of measuring the value $a \in \sigma(A)$ is:

$$\mathbb{P}_\psi(a) = \langle \psi | P_a \psi \rangle$$

where $\{P_a\}_{a\in\sigma(A)}$ is the spectral measure or projection value measure (PVM) of A. If we consider repeated measurements of the observable A in the same physical conditions represented by the state $|\psi\rangle$, the expectation value of A on the state $|\psi\rangle$ is the mean of the outcomes:

$$\langle A \rangle_\psi := \sum_{a\in\sigma(A)} a\,\mathbb{P}_\psi(a) = \langle \psi | A\psi \rangle$$

Post-measurement state: Let $|\psi\rangle \in H$ be the state of the considered quantum system. If we perform a measurement process of A with outcome $a \in \sigma(A)$, then the state of the system, after the measurement, is:

$$|\psi_a\rangle = \frac{P_a|\psi\rangle}{\sqrt{\langle\psi|P_a\psi\rangle}}$$

In the presented mathematical formulation of quantum mechanics the measurement process of the observable A is completely described by the PVM $\{P_a\}_{a\in\sigma(A)}$ which determines the probability distribution of the outcomes and the post-measurement state.

Compatible and incompatible observables: A and B are compatible when they commute:

$$[A, B] := AB - BA = 0$$

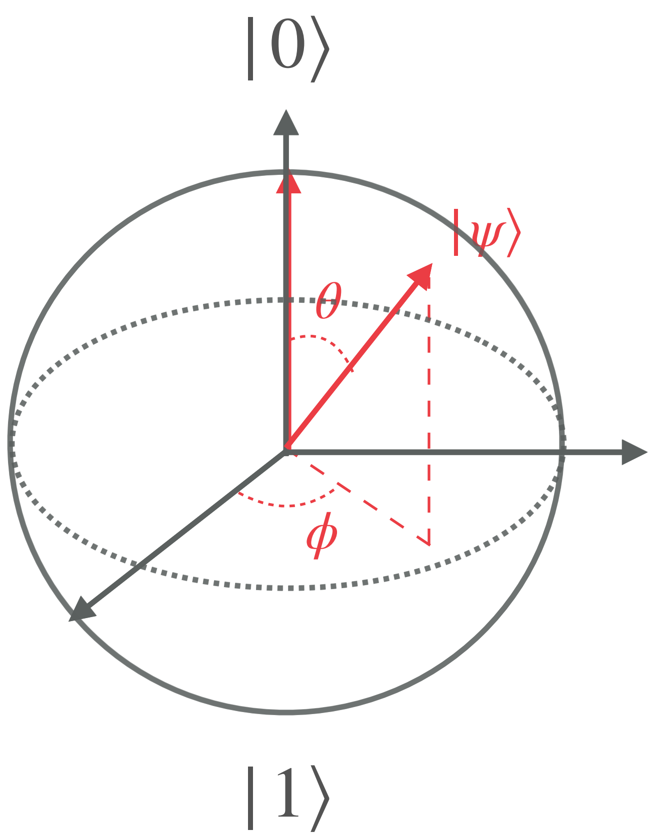
in this case: $P_a^A P_b^B = P_b^B P_a^A$ $\forall a \in \sigma(A)$ and $\forall b \in \sigma(B)$, so the following probability is well-defined:

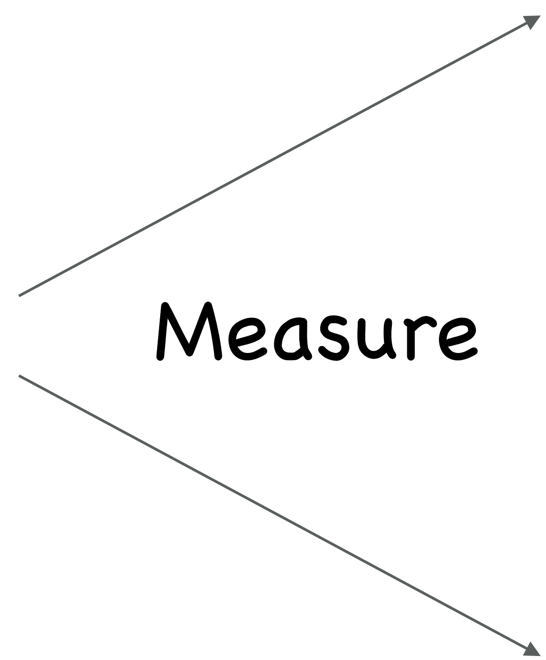
$$\mathbb{P}_\psi(A = a \wedge B = b) = \langle\psi|P_a^A P_b^B\psi\rangle = \langle\psi|P_b^B P_a^A\psi\rangle$$

Rotation about the Bloch Sphere and state parametrisation

$|0\rangle$

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}$$





$|1\rangle$ Prob$\left(|1\rangle\right) = \left(e^{i\phi}\sin\frac{\theta}{2}\right)^2$

$|0\rangle$ Prob$\left(|0\rangle\right) = \left(\cos\frac{\theta}{2}\right)^2$

Apply Unitary rotation $U_3|0\rangle$: $U_3(\theta,\phi,\lambda) = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -e^{i\lambda}\sin\left(\frac{\theta}{2}\right) \\ e^{i\phi}\sin\left(\frac{\theta}{2}\right) & e^{i(\phi+\lambda)}\cos\left(\frac{\theta}{2}\right) \end{pmatrix}$

$|1\rangle$

Extending this to a system of N qubits forms a 2^N-dimensional Hilbert Space

Quantum dynamics

The time evolution of an isolated quantum system is mathematically described by a one-parameter group of unitary operators $\{U_t\}_{t\in R}$ defined by:

$$U_t := \sum_{\lambda\in\sigma(\mathcal{H})} e^{-i\frac{t}{\hbar}\lambda} P_h \equiv e^{-i\frac{t}{\hbar}\mathcal{H}}$$

where $\hbar$ is the reduced Planck constant, H is the Hamiltonian operator which represents the observable total energy of the considered system and $\{P_h\}_{h\in\sigma(H)}$ is the spectral measure of H.

If the state at time t = 0 is $|\psi_0\rangle \in H$ then the state at time t > 0 is:

$$|\psi_t\rangle = U_t|\psi_0\rangle = e^{-i\frac{t}{\hbar}\mathcal{H}}|\psi_0\rangle$$

Taking the time derivative obtains the Schroedinger equation:

$$i\hbar\frac{d}{dt}|\psi_t\rangle = \mathcal{H}|\psi_t\rangle$$

In case of a time-dependent Hamiltonian, H must be replaced by a one-parameter family of self-adjoint operators $\{H(t)\}_{t\in R}$ and the Schroedinger equation assumes the form:

$$i\hbar\frac{d}{dt}|\psi_t\rangle = \mathcal{H}(t)|\psi_t\rangle$$

Hamiltonian simulation

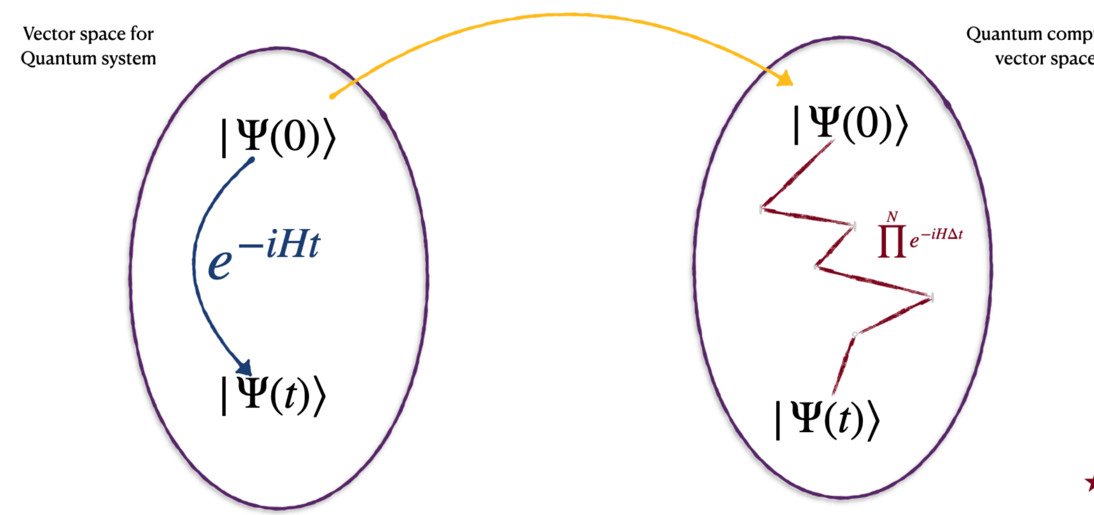
Recall Schroedinger Equation and time evolution equation

$$|\psi(t)\rangle = \hat{U}(t)\,|\psi(0)\rangle \quad \rightarrow \quad \frac{\partial \hat{U}(t)}{\partial t} = -\,iH\hat{U}(t) \rightarrow \hat{U}(t) = e^{-iHt}$$

If $H = H^\dagger$ (Hermitian) then $\hat{U}(t)$ is unitary

$$e^{-iHt}e^{iHt} = 1 \quad \text{and} \quad e^{-iHt} = (e^{iHt})^\dagger$$

$$e^{-iHt} = \sum_{j=0}^{\infty} \frac{(-iHt)^j}{j!}$$



[2111.00627]

[2301.00560]

Pauli Operators

Tensor products of Pauli operators {I, X, Y, Z} form a basis for the vector space of 2^n x 2^n complex matrices, which are used to represent quantum states and operators in a system of n qubits.
Thus, our hermitian matrix H can be decomposed into Pauli operators

Trotterisation

For commuting self-adjoint operators $[S,T]=0$ we find

$$e^{S+T}\xi = e^S e^T \xi, \quad \xi \in D(S)\cap D(T)$$

However, if S and T do not commute this doesnt hold.
Surprisingly the Trotter Product Formula comes to the rescue:

$$\operatorname*{s-lim}_{n\to\infty}\left(e^{-i\frac{t}{n}S}e^{-i\frac{t}{n}T}\right)^n = e^{-it(S+T)}.$$

Consequently

$$e^{A+B} \approx \left(e^{A/N}e^{B/N}\right)^N \approx \left[\left(I+\frac{A}{N}\right)\left(I+\frac{B}{N}\right)\right]^N = \left[I+\frac{A}{N}+\frac{B}{N}+\frac{AB}{N^2}\right]^N \approx \left[I+\frac{A+B}{N}\right]^N$$

→ If N too large causes numerical instabilities, but must be sufficiently large

→ Trotterization error, important error for quantum algorithms (Hamiltonian simulation, time evolution etc)

Trotterization tells us the error we make when writing H as a sum of H_i

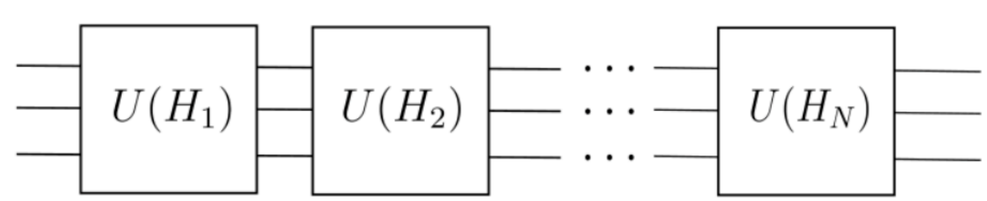
$$H = H_1 + H_2 + H_3 + \cdots + H_N \quad \text{for} \quad U(H, t) = e^{-iHt/\hbar}$$

Thus we implement an approximated time evolution where the H_i are compositions of Pauli matrices

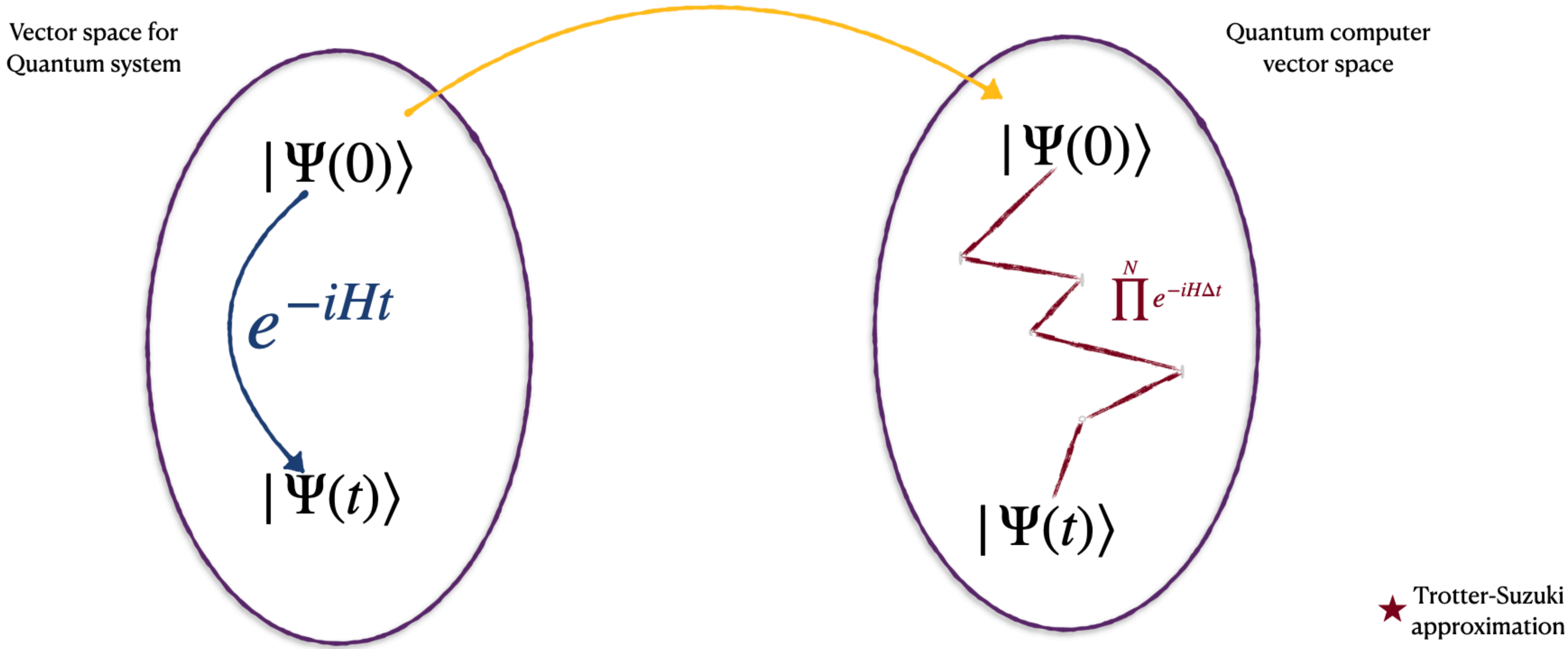
$$U(H,t,n) = \prod_{j=1}^{n} \prod_{k} e^{-iH_k t/n} \qquad H = \sum_k H_k,$$

Each piece remains unitary, and H_i is hermitian

$$H = H_1 + H_2 + \cdots + H_N$$



Task is to convert each piece into gate operations



Trotterization error needs to be assessed, e.g. by reducing time steps

From QM to QFT

- Extend QM to systems with variable particle numbers (quantum many-body problems)
- Promote classical fields to operator-valued functions, acting on states in Fock space

$$\mathscr{F} = \bigoplus_{n=0}^{\infty} \mathscr{H}^{\otimes n}$$

- Second Quantisation Programme
- Time Evolution Operator: $|\Psi(t)\rangle = \hat{U}(t,t_0)|\Psi(t_0)\rangle, \quad \hat{U}(t,t_0) = \mathcal{T}\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t')dt'\right)$

perturbative approach

e.g. scatting in weak coupling regime

➡ Interaction picture (split Hamiltonian into free and interaction H)
➡ define Dyson series: perturbative expansion, suitable if coupling is small
➡ Wick contractions, Feynman diagrams
➡ S-Matrix, LSZ theorem

non-perturbative approach

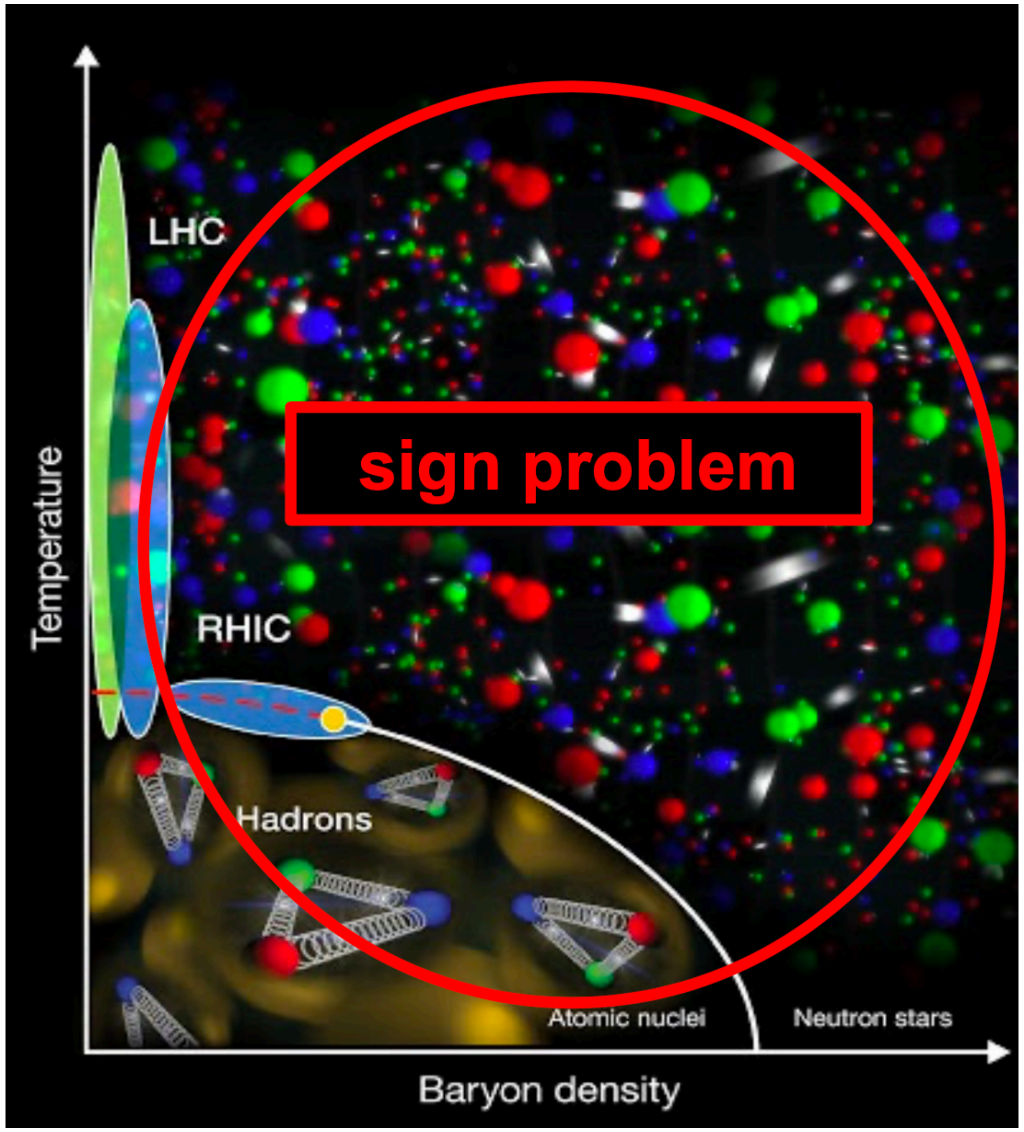
e.g. Real-time time evolution suitable for large couplings

➡ One usually works in the Schroedinger picture (states are time-dependent and operators are time-independent (unless they are explicitly time-dependent))
➡ Latticisation, Kogut-Susskind programme

Why Hamiltonian simulation? → The infamous sign problem

- Sign problem - profound challenge for simulation of field theories

- Can arise in presence of chemical potential, topological terms, multi-particle dynamics, ...



- Example chemical potential $\mu\bar{\psi}\gamma^0\psi$

$$Z = \int \mathscr{D}\bar{\psi}\mathscr{D}\psi\mathscr{D}A \; e^{-S[\bar{\psi},\psi,A]} \quad \text{(partition function)}$$

$$S = \int_0^{1/T} d\tau \int d^3x \left[\bar{\psi}(\gamma^\mu D_\mu + m)\psi + \frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu} + \mu\bar{\psi}\gamma^0\psi \right]$$

and integration over fermion fields and Wick rotation (imaginary time)

$$Z = \int \mathscr{D}A e^{-S_{\text{gauge}}[A]} \cdot \det(\gamma^\mu D_\mu + m + \mu\gamma^4) \longrightarrow$$ For $\mu \neq 0$ complex phases don't cancel

The infamous sign problem

- Importance sampling

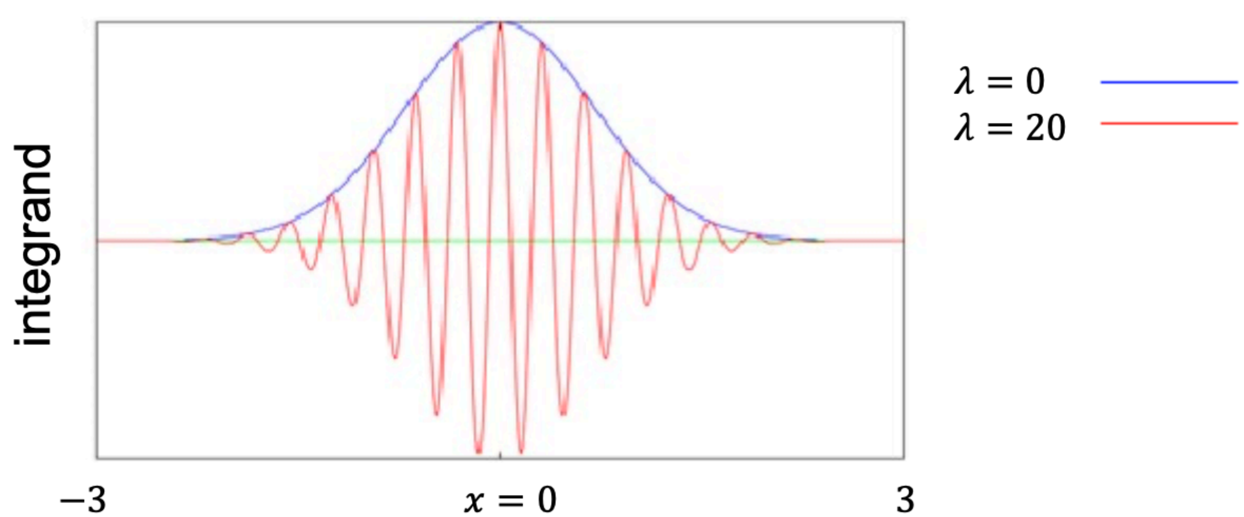
  Interpretation of $e^{-S_{\text{gauge}}} \det(M)$

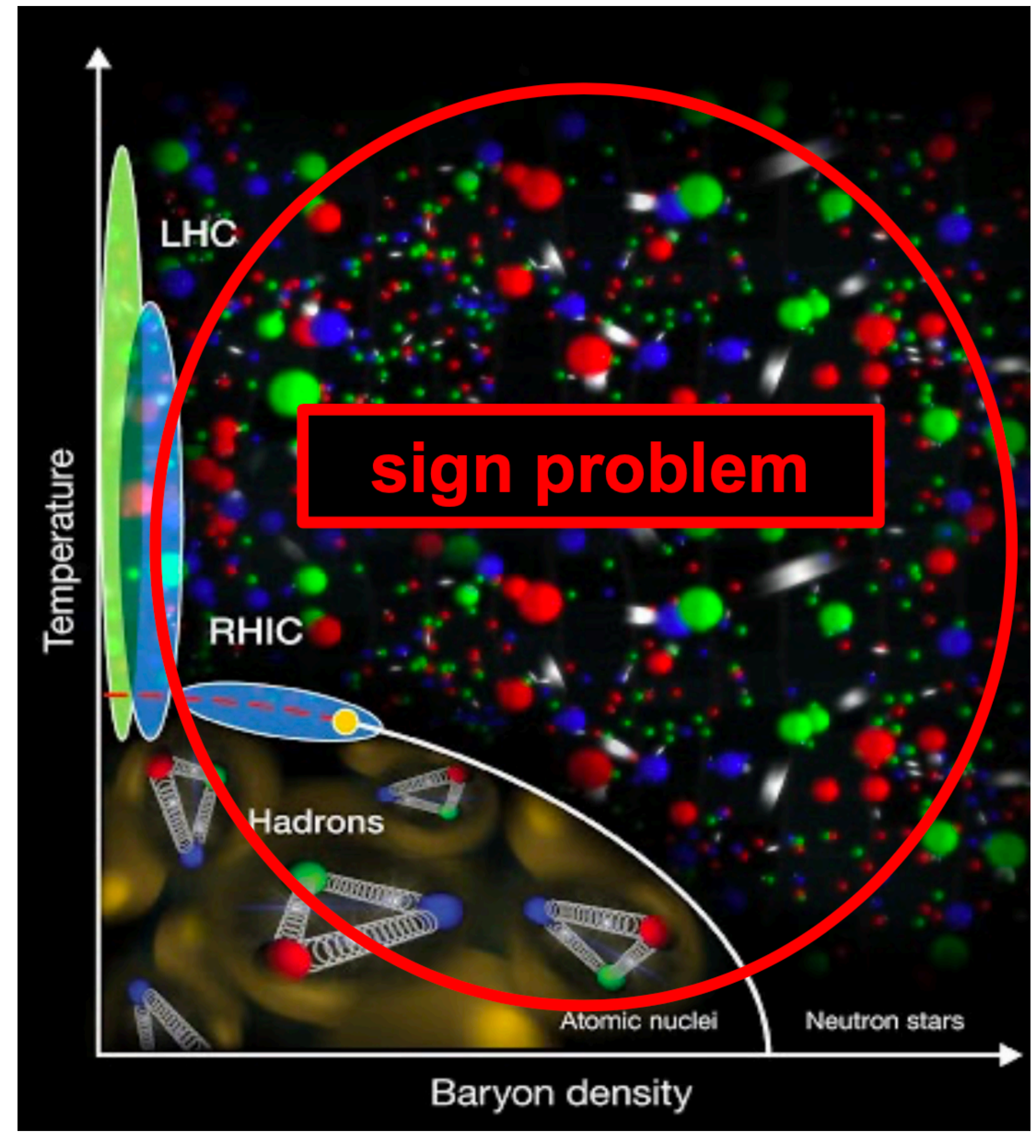
  as probability weight

- Highly oscillatory integrands

$$\langle O \rangle = \frac{\int \mathscr{D}A e^{-S_{\text{gauge}}} \, O \, |\det[M(A)]| \, e^{i\phi(A)}}{\int \mathscr{D}A e^{-S_{\text{gauge}}} |\det[M(A)]| \, e^{i\phi(A)}}$$

near cancellation of pos and neg contribs



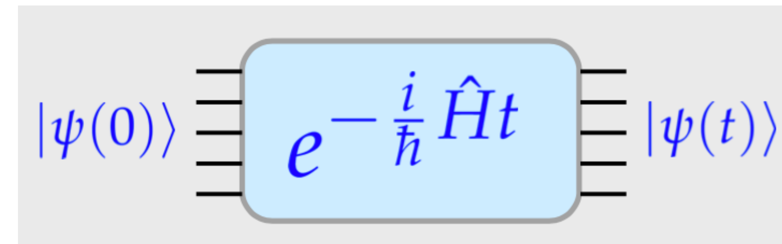


[de Forcrand '10]

$$\int dx \exp(-x^2 + i\lambda x) \to \int dx \exp(-x^2)\cos(\lambda x)$$

HEP application focused quantum simulations

- Real-time evolution on quantum computer can avoid sign problem



- Continuous field theories $\phi(x)$ describe particle phenomenology

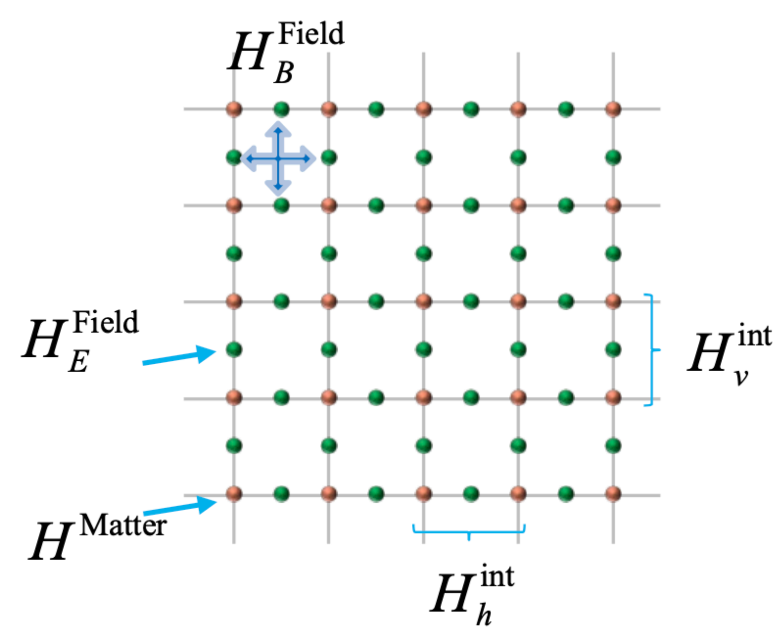
-> infinite dimensional 'matrices'

$$\left| \left\langle X(T) \middle| U(T,-T) \middle| pp(-T) \right\rangle \right|^2$$

- Needs discretisation irrespective of classical or quantum computation

Kogut-Susskind formulation

[Kogut, Susskind '74]



Steps to Hamiltonian Simulation on the lattice (Kogut-Susskind)

We consider a non-Abelian gauge theory with fermionic matter fields. The gauge group is general and denoted as $SU(N)$

The Lagrangian density is given by $$\mathcal{L} = -\frac{1}{4} F^a_{\mu\nu} F^{\mu\nu a} + \bar{\psi} \left(i\gamma^\mu D_\mu - m \right) \psi$$

where:

ψ: Fermion field

m: Fermion mass

γ^μ: Gamma matrices satisfying Clifford algebra

structure constant of gauge group

$F^a_{\mu\nu}$: Field strength tensor $$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g f^{abc} A^b_\mu A^c_\nu$$

D_ψ: Covariant derivative $$D_\mu \psi = \left(\partial_\mu - i g T^a A^a_\mu \right) \psi$$

generators of gauge group

Deriving the Hamiltonian density

Gauge fields A_μ^a:

$$\pi^{a\mu} = \frac{\partial \mathcal{L}}{\partial(\partial_0 A_\mu^a)} = -F^{0\mu a}$$

electric field components

spatial components $\pi^{ai} = -F^{0ia} = E^{ia}$

temporal component $(\mu = 0)$ $\pi^{a0} = 0$

Fermion fields $\psi, \bar{\psi}$:

$$\pi_\psi = \frac{\partial \mathcal{L}}{\partial(\partial_0 \psi)} = i\psi^\dagger \qquad \pi_{\bar{\psi}} = \frac{\partial \mathcal{L}}{\partial(\partial_0 \bar{\psi})} = 0$$

$\bar{\psi}$ does not have a canonical momentum
associated with it -> primary constraint
thus, it is not an independent dynamical variable
Hamlitonian needs to be constructed carefully to
take constraint into account

Legendre transformation:

Hamiltonian density $\mathcal{H} = \pi^{a\mu}\partial_0 A_\mu^a + \pi_\psi \partial_0 \psi - \mathcal{L}$

replace the ∂_0 component in terms of conjugate momenta (Hamilton approach)

Gauge field: $\pi^{ai} = -F^{0ia} = -\left(\partial^0 A^{ia} - \partial^i A^{0a} + g f^{abc} A^{0b} A^{ic}\right) \longrightarrow \partial^0 A^{ia} = -\pi^{ai} - D^i A^{0a}$

with $D^i A^{0a} = \partial^i A^{0a} - g f^{abc} A^{ib} A^{0c}$

Fermion field: $\partial_0 \psi = -i\left(\alpha \cdot \boldsymbol{D} - \beta m\right)\psi - g A_0^a T^a \psi$ with Dirac matrices α and β

$$\begin{aligned}\mathcal{H} &= \pi^{ai}\left(-\pi^{ai} - D^i A^{0a}\right) + i\psi^\dagger\left(-i\left(\alpha \cdot \boldsymbol{D} - \beta m\right)\psi - g A_0^a T^a \psi\right) - \mathcal{L} \\ &= \frac{1}{2}\pi^{ai}\pi^{ai} + \frac{1}{4}F_{ij}^a F^{ija} + \psi^\dagger\left(-i\alpha \cdot \boldsymbol{D} + \beta m\right)\psi + A_0^a G^a\end{aligned}$$

Electric Energy Term — Magnetic Energy Term — Fermion Energy Term — Gauss's law operator $G^a = D_i \pi^{ai} - g\psi^\dagger T^a \psi$

Physical states $\left|\Psi\right\rangle$ must satisfy $G^a\left|\Psi\right\rangle = 0$ to ensure gauge invariance (Gauss's law)

The continuous Hamiltonian operator H is $H = \int d^3x\, \mathcal{H}$ with $\mathcal{H} = \frac{1}{2}\pi^{ai}\pi^{ai} + \frac{1}{4}F_{ij}^a F^{ija} + \psi^\dagger\left(-i\alpha \cdot \boldsymbol{D} + \beta m\right)\psi + A_0^a G^a$

Discretisising Space: Introducing the lattice

Spatial lattice: Lattice sites defined by integer coordinates $\mathbf{n} = (n_x, n_y, n_z)$

Lattice spacing defined by the value a (fixed distance between neighbouring sites)

⟶ serves as UV cutoff

The time remains continuous to retain the Hamiltonian formulation

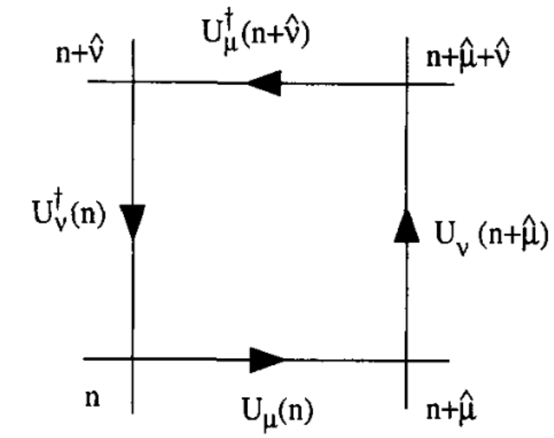
Link variables: When discretising a gauge theory onto a lattice, we replace the continuous space-time with a discrete set of points (sites). The gauge fields $A_\mu(x)$, which live on continuous space-time, need to be represented in a way that preserves gauge invariance on the lattice
-> variables U are introduced such that they maintain gauge invariance

defined as $U_i(\mathbf{n}) = e^{iagA_i^a(\mathbf{n})T^a}$

The link variable $U_i(\mathbf{n})$ represents the **parallel transporter** (also known as the **Wilson line**) along the link from site $\mathbf{n}$ to site $\mathbf{n} + \hat{i}$. It encodes the phase factor acquired by a particle moving through the gauge field along that link.

Fermion Fields: $\psi(\mathbf{n})$ placed at the lattice sites, representing matter fields at each space point

Define plaquette operator $U_{\mu\nu}(\mathbf{n}) = U_\mu(\mathbf{n})U_\nu(\mathbf{n}+\hat{\mu})U^\dagger_\mu(\mathbf{n}+\hat{\nu})U^\dagger_\nu(\mathbf{n})$



The plaquette operator is a measure of the curvature (field strength) of the gauge field over the area of the plaquette. In the limit of small lattice spacing a, $U_{\mu\nu}(\mathbf{n})$ approximates the exponential of the field strength tensor integrated over the plaquette area.

For small a we have $U_\mu(\mathbf{n}) = e^{iagA^a_\mu(\mathbf{n})T^a} \simeq 1 + iagA^a_\mu(\mathbf{n})T^a - \dfrac{a^2g^2}{2}(A^a_\mu(\mathbf{n})T^a)^2 + \mathcal{O}(a^3)$

Calculating the plaquette for small a

with $A^b_\nu(\mathbf{n}+\hat{\mu}) = A^b_\nu(\mathbf{n}) + a\partial_\mu A^b_\nu(\mathbf{n}) + \mathcal{O}(a^2)$

$$
\begin{aligned}
U_{\mu\nu}(\mathbf{n}) &= \left(1 + iagA^a_\mu(\mathbf{n})T^a\right)\left(1 + iagA^b_\nu(\mathbf{n}+\hat{\mu})T^b\right) \\
&\quad \times \left(1 - iagA^c_\mu(\mathbf{n}+\hat{\nu})T^c\right)\left(1 - iagA^d_\nu(\mathbf{n})T^d\right) + \mathcal{O}(a^3) \\
&= 1 + ia^2gF^a_{\mu\nu}(\mathbf{n})T^a + \mathcal{O}(a^3)
\end{aligned}
$$

With the plaquette we can express the latticised magnetic energy term H_B as the trace over the plaquete:

$$
H_B = \frac{1}{g^2}\sum_{\mathbf{n},i<j}\left(N_c - \mathrm{Re}\,\mathrm{Tr}\left[U_{ij}(\mathbf{n})\right]\right) \approx \frac{a^4}{2}\sum_{\mathbf{n},i<j} F^a_{ij}(\mathbf{n})F^a_{ij}(\mathbf{n})
$$

↑ gauge invariant quantity

Electric energy term $$H_E = \frac{g^2}{2}\sum_{\mathbf{n},i,a}[E_i^a(\mathbf{n})]^2$$

Fermion energy term $H_F = H_K + H_M$

Kinetic term: $$H_K = \frac{1}{2a}\sum_{\mathbf{n},i}\left[\psi^\dagger(\mathbf{n})\alpha^i U_i(\mathbf{n})\psi(\mathbf{n}+\hat{i}) - \psi^\dagger(\mathbf{n}+\hat{i})\alpha^i U_i^\dagger(\mathbf{n})\psi(\mathbf{n})\right]$$

Mass term: $$H_M = m\sum_{\mathbf{n}}\psi^\dagger(\mathbf{n})\beta\psi(\mathbf{n})$$

Ensure gauge invariance of H on the lattice

group element at site $\mathbf{n}$

Local gauge transformations at each site $\mathbf{n}$ $\psi(\mathbf{n}) \to G(\mathbf{n})\psi(\mathbf{n})$ and Link $U_i(\mathbf{n}) \to G(\mathbf{n})U_i(\mathbf{n})G^\dagger(\mathbf{n}+\hat{i})$

→ Electric energy term $[E_i^a(\mathbf{n})]^2$ is gauge invariant

→ Trace of plaquette variable $\mathrm{Tr}[U_{ij}(\mathbf{n})]$ is gauge invariant

→ The combination $\psi^\dagger(\mathbf{n})U_i(\mathbf{n})\psi(\mathbf{n}+\hat{i})$ is gauge invariant

The discrete version of Guass's law operator is $$G^a(\mathbf{n}) = \sum_i\left[E_i^a(\mathbf{n}) - E_i^a(\mathbf{n}-\hat{i})\right] + g\psi^\dagger(\mathbf{n})T^a\psi(\mathbf{n})$$

Physical Hilbert space states must satisfy $G^a(\mathbf{n})|\Psi\rangle = 0$

The fermion doubling problem

Consider $H_F = H_K + H_M$ for the free theory (i.e. no gauge interactions) $U_i(\mathbf{n}) = 1$

Fourier transforming $\psi(\mathbf{n}) = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^d p}{(2\pi)^d} e^{i\mathbf{p}\cdot\mathbf{n}a} \tilde{\psi}(\mathbf{p})$, inserting into H_K and massaging the equation gives

$$H_K = \int \frac{d^d p}{(2\pi)^d} \tilde{\psi}^\dagger(\mathbf{p}) \left[\frac{2i\alpha^i}{a} \sin(ap_i) \right] \tilde{\psi}(\mathbf{p}) = \int \frac{d^d p}{(2\pi)^d} \tilde{\psi}^\dagger(\mathbf{p}) \; (\alpha \cdot \mathbf{K}) \; \tilde{\psi}(\mathbf{p})$$

where $\mathbf{K} = \frac{2}{a}(\sin(ap_1), \sin(ap_2), \sin(ap_3))$

-> the eigenvalues are given by $E(\mathbf{p}) = \pm |\mathbf{K}| = \pm \frac{2}{a} \sqrt{\sum_{i=1}^{d} \sin^2(ap_i)}$

the energy vanishes when $\sin(ap_i) = 0$, which occurs at $p_i = 0$ and $p_i = \frac{\pi}{a}$

Thus, there are 2^d points in the Brillouin zone where $E(\mathbf{p}) = 0$. In four dims (d=4) there are 16 such points, indicating 16 fermion species (including doublers)

Introducing staggered fermions

To mitigate the fermion doubling problem, we introduce staggered fermions, which involve:

- Replacing the multi-component Dirac spinor $\psi(\mathbf{n})$ with a single-component fermion field $\chi(\mathbf{n})$
- Redistributing the spinor components across neighbouring lattice sites using staggered phases $\eta_i(\mathbf{n}) = (-1)^{n_1+n_2+\ldots+n_{i-1}}$

The staggered fermion Hamiltonian (for $U_i(\mathbf{n}) = 1$ for simplicity) is

$$H_F = \frac{1}{2a}\sum_{\mathbf{n},i}\eta_i(\mathbf{n})\Big[\chi^\dagger(\mathbf{n})\chi(\mathbf{n}+\hat{i}) - \chi^\dagger(\mathbf{n}+\hat{i})\chi(\mathbf{n})\Big] + m\sum_{\mathbf{n}}\chi^\dagger(\mathbf{n})\chi(\mathbf{n})$$

After Fourier transform, one has

$$H_F = \int \frac{d^dk}{(2\pi)^d}\,\tilde{\chi}^\dagger(\mathbf{k})\left[\frac{2i}{a}\sum_i \sin(ak_i)\,\tilde{\eta}_i\right]\tilde{\chi}(\mathbf{k}) + m\int\frac{d^dk}{(2\pi)^d}\,\tilde{\chi}^\dagger(\mathbf{k})\tilde{\chi}(\mathbf{k})$$

By distributing the spinor components across different lattice sites and introducing the staggered phases, the number of fermion species is reduced

- in d dimensions, the number of species reduces from 2^d to $2^{d/2}$
- In four dimensions, from 16 to 4

While this doesn't completely eliminate the fermion doubling problem, it significantly reduces the number of unphysical doublers.

Assembling the Lattice Hamiltonian

The total Hamiltonian is $H = H_E + H_B + H_F$

Electric Energy Term $H_E = \frac{g^2}{2} \sum_{\mathbf{n},i,a} [E_i^a(\mathbf{n})]^2$

Magnetic Energy Term $H_B = \frac{1}{g^2} \sum_{\mathbf{n},i<j} [N_c - \mathrm{Re}\,\mathrm{Tr}\,(U_{ij}(\mathbf{n}))]$

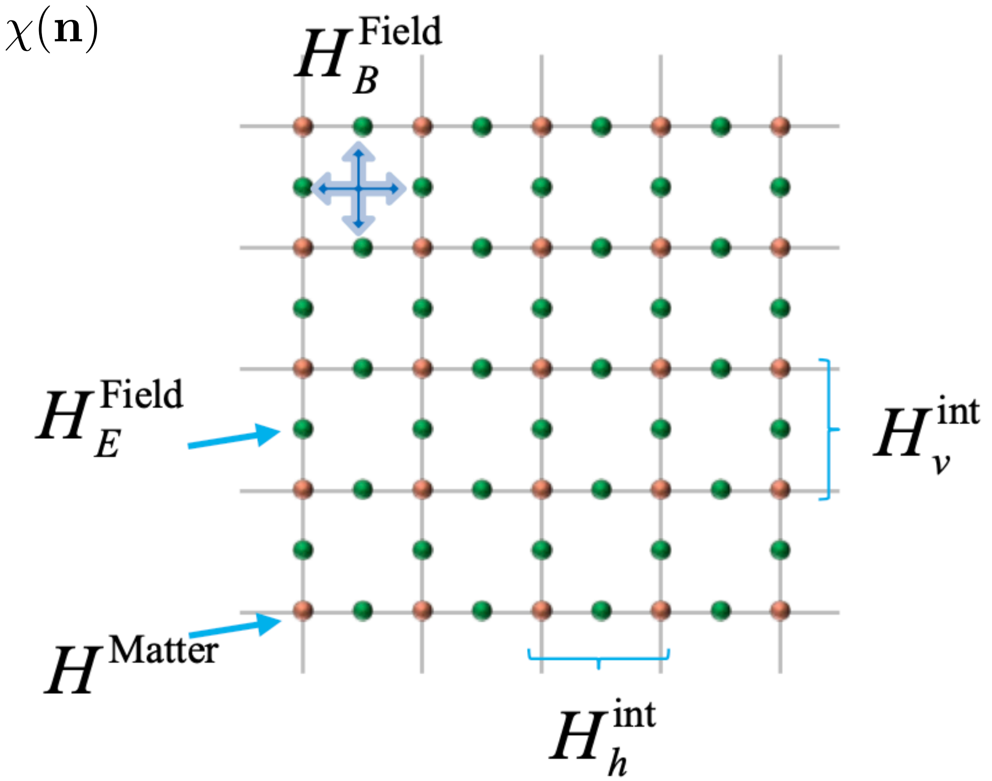
Fermion Energy Term

(Staggered Fermions)

$$H_F = \frac{1}{2a} \sum_{\mathbf{n},i} \eta_i(\mathbf{n}) \left[\chi^\dagger(\mathbf{n}) U_i(\mathbf{n}) \chi(\mathbf{n}+\hat{i}) - \chi^\dagger(\mathbf{n}+\hat{i}) U_i^\dagger(\mathbf{n}) \chi(\mathbf{n})\right] + m \sum_{\mathbf{n}} \chi^\dagger(\mathbf{n}) \chi(\mathbf{n})$$

Numerical methods for Hamiltonian simulation:

- Tensor Network Approches
- Quantum Simulations



Concrete example U(1) in 1-dimension

The U(1) gauge field is continuous $U(n) = e^{i\theta(n)}$ and has to be truncated

→ Assume 2 sites

→ Truncate the Electric Field $E(n)$ - assume $E(n) = -1, 0, +1$

→ Truncate the Link Variables $U(n)$ - e.g. assume $\theta(n) = 0, \frac{2\pi}{3}, \frac{4\pi}{3}$

→ Truncate fermions - assume single fermion mode per site, i.e. each site either 0 or 1 fermions

→ 3 states for electric field on each site, thus 3 links => $3 \times 3 = 9$

$|-1,\ -1\rangle, |-1,\ 0\rangle, |-1,\ +1\rangle, |0,\ -1\rangle, |0,\ 0\rangle, |0,\ +1\rangle, |+1,\ -1\rangle, |+1,\ 0\rangle, |+1,\ +1\rangle$

→ each site 0 or 1 fermions x 2 sites => fermion Hilber space $2^2 = 4$

$|0,0\rangle, |0,1\rangle, |1,0\rangle, |1,1\rangle$

} Hamiltonian 36 x 36

Thus, 36 basis states are labeled as $|E_0, E_1; n_0, n_1\rangle$

Calculate elements $H_{ij} = \langle E_0', E_1'; n_0', n_1' | H | E_0, E_1; n_0, n_1\rangle$

with $H = H_E + H_K + H_M$ (H_B is absent in 1d)

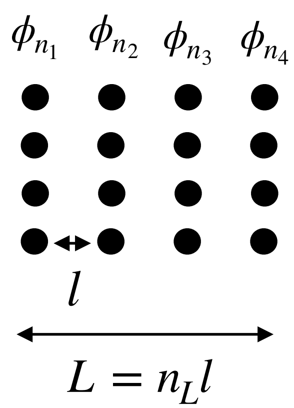
diagonal element $H_{ii} = \frac{1}{2}(E_0^2 + E_1^2)$

off-diagonal element $H_{ij} = -\frac{i}{2}\eta(0)U(E_0)\ \delta_{E_0', E_0-1}\ \delta_{n_0', n_0-1}\ \delta_{n_1', n_1+1}$

$$H = \begin{pmatrix} H_{1,1} & 0 & 0 & 0 & \dots & H_{1,6} & 0 & \dots & 0 \\ 0 & H_{2,2} & 0 & 0 & \dots & 0 & H_{2,7} & \dots & 0 \\ 0 & 0 & H_{3,3} & 0 & \dots & 0 & 0 & \dots & H_{3,9} \\ 0 & 0 & 0 & H_{4,4} & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ H_{6,1} & 0 & 0 & 0 & \dots & H_{6,6} & 0 & \dots & H_{6,9} \\ 0 & H_{7,2} & 0 & 0 & \dots & 0 & H_{7,7} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & H_{9,3} & 0 & \dots & H_{9,6} & 0 & \dots & H_{9,9} \end{pmatrix}$$

Hamiltonian simulation - what resources do we need?

- Discretisation of field $\phi_n(x_k)$



Hilbert space has dimension $\dim H = (n_\phi)^{n_L^d}$

Energy range: $\frac{1}{n_L l} < E < \frac{1}{l}$

n_ϕ : # of digitised field values

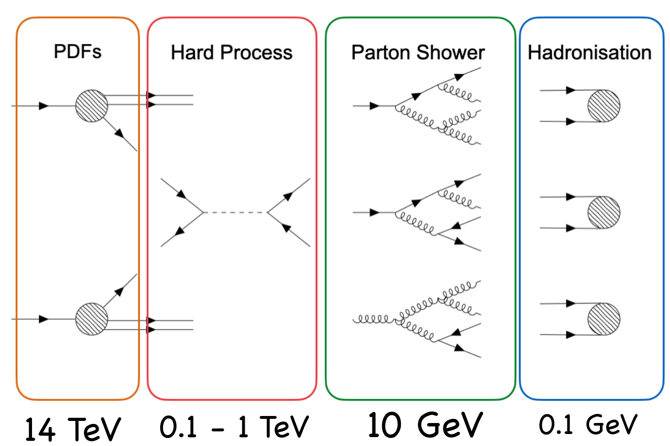
n_L : # of lattice points per dim

d : # of dimensions

[Jordan, Lee, Preskill '12]

- On quantum devices algorithms require exp less resources $\ln_2[\dim H]$

➡



➡

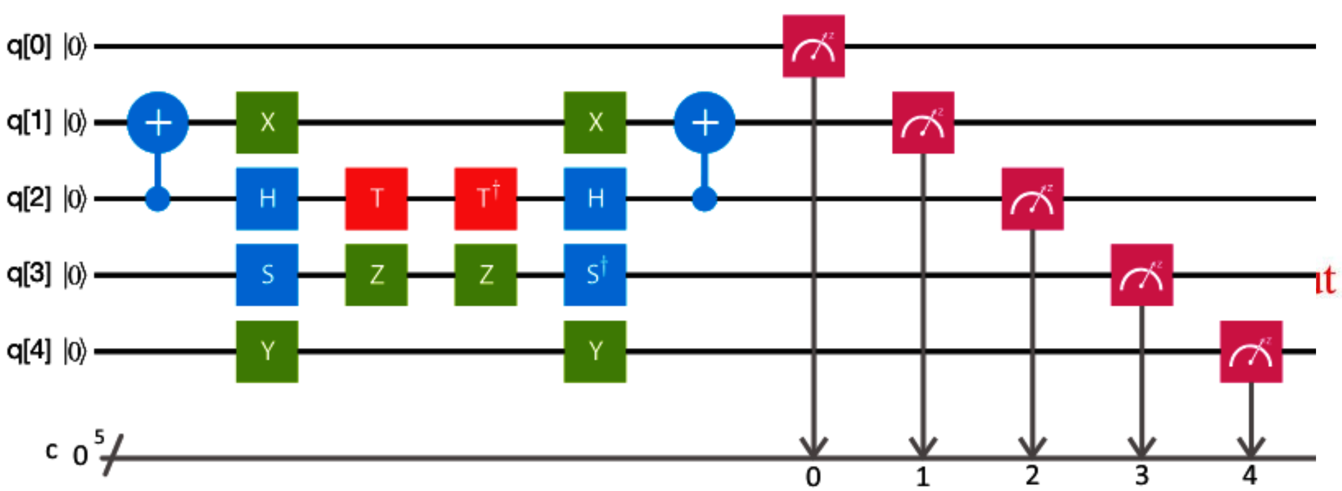
Lattice sites	field digitisation
$n_L^d \simeq 100^3$	$n_\phi = 2^5$

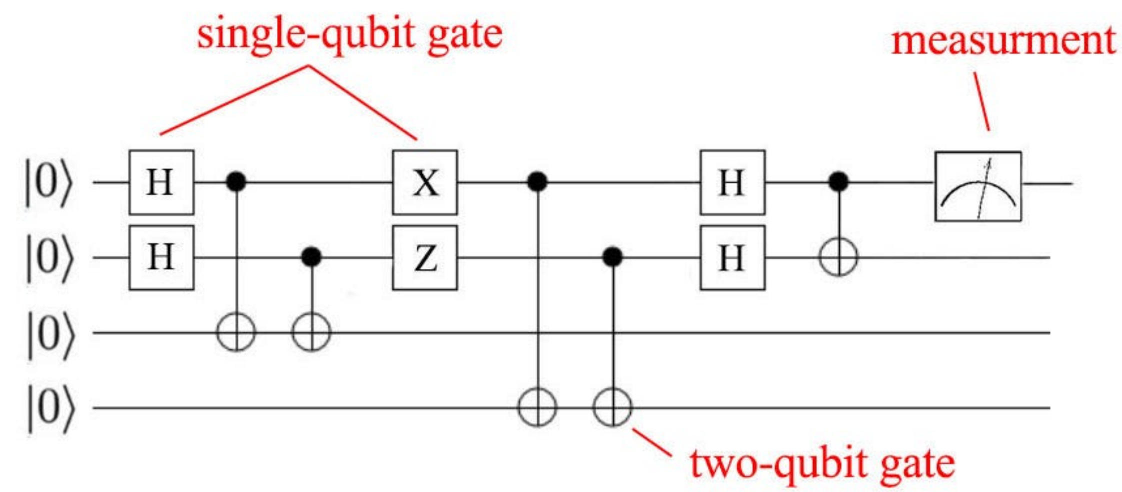
➡

Classical	Quantum
$32^{10^6} \simeq \infty$	$5 \cdot 10^6$

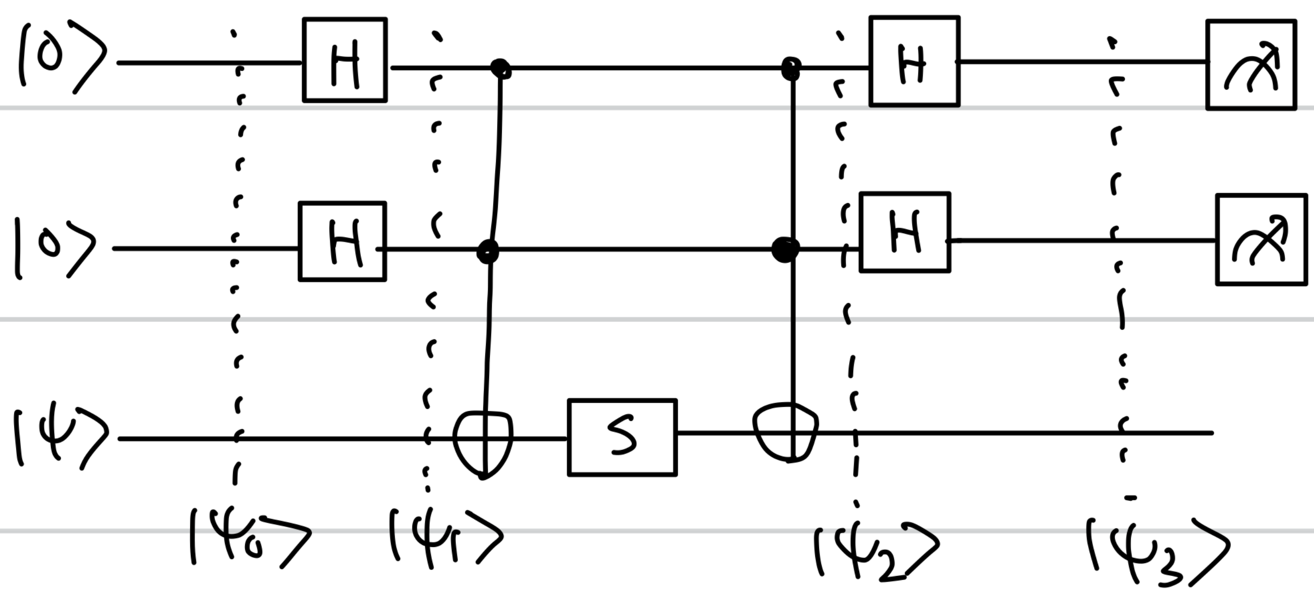
Quantum computing not optional for Hamiltonian simulation

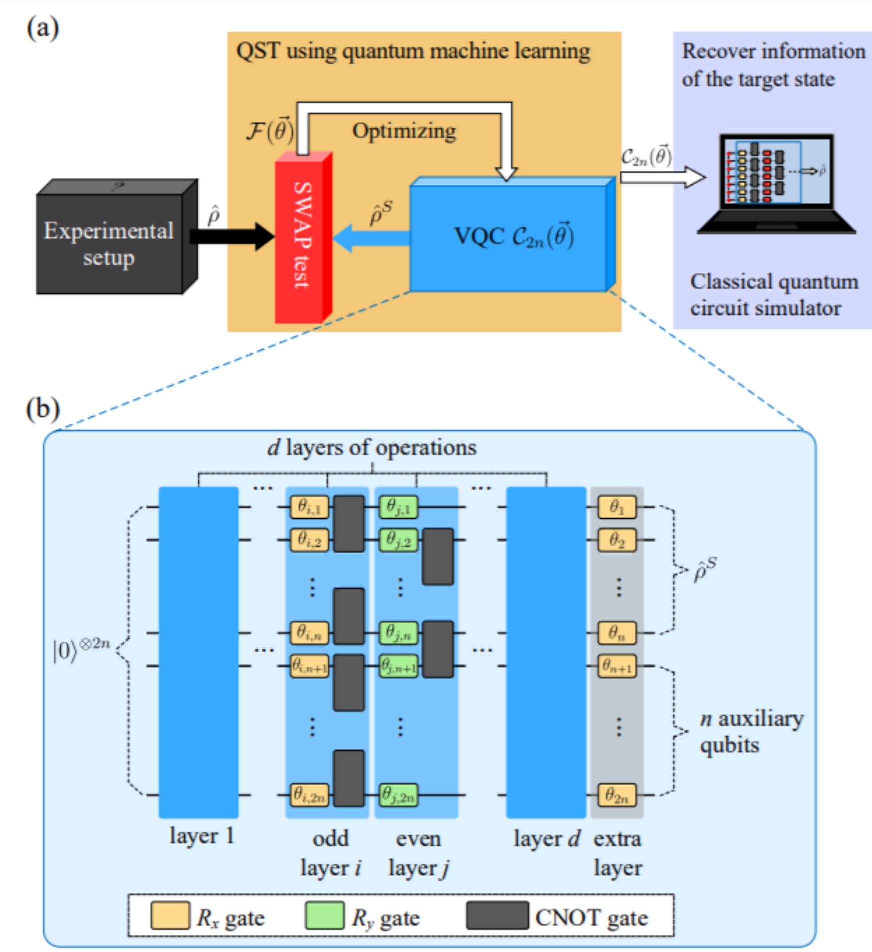
Effective Field Theories can ameliorate problem





Quantum Circuits

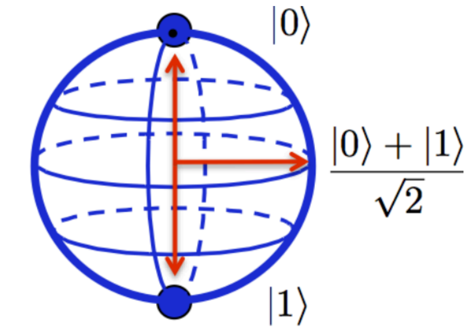




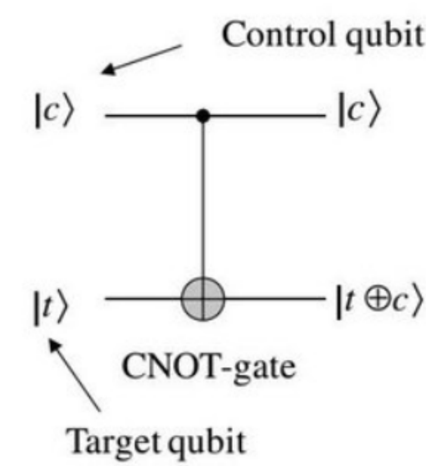
Need transition form classical to quantum:

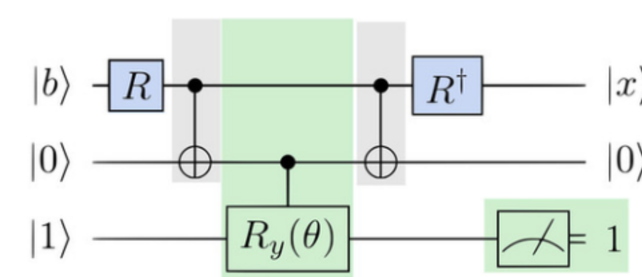
Classical Bit

Classical		Quantum
bits	⟷	qubits
gates	⟷	quantum gates
algorithms	⟷	quantum algorithms



Qubit





Single-Qubit Quantum Gates

Illustrative to write single-qubit operation as matrices

X-Gate: Quantum equivalent to classical NOT gate

$$|0\rangle \mapsto |1\rangle$$

$$|1\rangle \mapsto |0\rangle$$

⟶ Flips |0> to |1> and vice versa (hopping)

Represented by matrix $\mathbf{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

concretely $$\mathbf{X}|0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle$$

It is unitary $\mathbf{X}\mathbf{X}^\dagger = \mathbf{X}\mathbf{X}^{-1} = \mathbb{1}$

Z-Gate: Represented by matrix $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Action
$$|0\rangle \mapsto |0\rangle$$
$$|1\rangle \mapsto -|1\rangle$$

⟶ Eigenvalues +- 1

Note, the X, Y and Z gates are represented by the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad [\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$$

$$\det \sigma_j = -1$$
$$\operatorname{tr} \sigma_j = 0.$$

$$\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = -i\,\sigma_1\sigma_2\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$

Hadamard gate: Matrix representation $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

Action:

$$|0\rangle \mapsto \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \longleftrightarrow |+\rangle := \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

$$|1\rangle \mapsto \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \longleftrightarrow |-\rangle := \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

Phase gate: Matrix representation $P_\phi := \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$

With special phase values

$$S := P_{\pi/2} \qquad T := P_{\pi/4} \qquad R := P_{-\pi/4}$$

Summary of fixed 1-qubit gates:

Gate	Circuit representation	Matrix representation	Dirac representation
X	$-\boxed{X}-$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\|1\rangle\langle 0\| + \|0\rangle\langle 1\|$
Y	$-\boxed{Y}-$	$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$	$i\|1\rangle\langle 0\| - i\|0\rangle\langle 1\|$
Z	$-\boxed{Z}-$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\|1\rangle\langle 0\| - \|0\rangle\langle 1\|$
H	$-\boxed{H}-$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$	$\frac{1}{\sqrt{2}}(\|0\rangle + \|1\rangle)\langle 0\| + \frac{1}{\sqrt{2}}(\|0\rangle - \|1\rangle)\langle 1\|$
S	$-\boxed{S}-$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$	$\frac{1}{\sqrt{2}}\|0\rangle\langle 0\| + \frac{1}{\sqrt{2}}i\|1\rangle\langle 1\|$
T	$-\boxed{T}-$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & e^{(-i\pi/4)} \end{pmatrix}$	$\frac{1}{\sqrt{2}}\|0\rangle\langle 0\| + \frac{1}{\sqrt{2}}e^{(-i\pi/4)}\|1\rangle\langle 1\|$

Quantum gate can be parametrised

Pauli rotations:

$$R_x(\theta) = e^{-i\frac{\theta}{2}\sigma_x} = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -i\sin\left(\frac{\theta}{2}\right) \\ -i\sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}X$$

$$R_y(\theta) = e^{-i\frac{\theta}{2}\sigma_y} = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}Y$$

$$R_z(\theta) = e^{-i\frac{\theta}{2}\sigma_z} = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}Z$$

generalised form via $R(\theta_1, \theta_2, \theta_3) = R_z(\theta_1)R_y(\theta_2)R_z(\theta_3)$

$$R(\theta_1, \theta_2, \theta_3) = \begin{pmatrix} e^{i(-\frac{\theta_1}{2}-\frac{\theta_3}{2})}\cos(\frac{\theta_2}{2}) & -e^{i(-\frac{\theta_1}{2}+\frac{\theta_3}{2})}\sin(\frac{\theta_2}{2}) \\ e^{i(\frac{\theta_1}{2}-\frac{\theta_3}{2})}\sin(\frac{\theta_2}{2}) & e^{i(\frac{\theta_1}{2}+\frac{\theta_3}{2})}\cos(\frac{\theta_2}{2}) \end{pmatrix}$$

Measurement process

Measurement process of a generic (normalised) qubit state $|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle$

represented by projection onto eigenstates $P_0 = |0\rangle\langle 0|$ and $P_1 = |1\rangle\langle 1|$

Prob of measurement outcome 0 is then $p(0) = \mathrm{tr}(P_0|\psi\rangle\langle\psi|) = \langle\psi|P_0|\psi\rangle = |\alpha_0|^2$

and $p(1) = |\alpha_1|^2$

After measurement qubit is in state $|\psi\rangle \leftarrow \frac{P_0|\psi\rangle}{\sqrt{\langle\psi|P_0|\psi\rangle}} = |0\rangle$

The observable corresponding to a computational basis measurement is Pauli-Z observable

$$\sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|$$

(we know eigenvalues +1 for |0> and -1 for |1>)

The expectation value $\langle \sigma_z \rangle$ in a value in [-1, 1]. Its error can be estimated as sampling from a Bernoulli distribution.

Wald interval gives

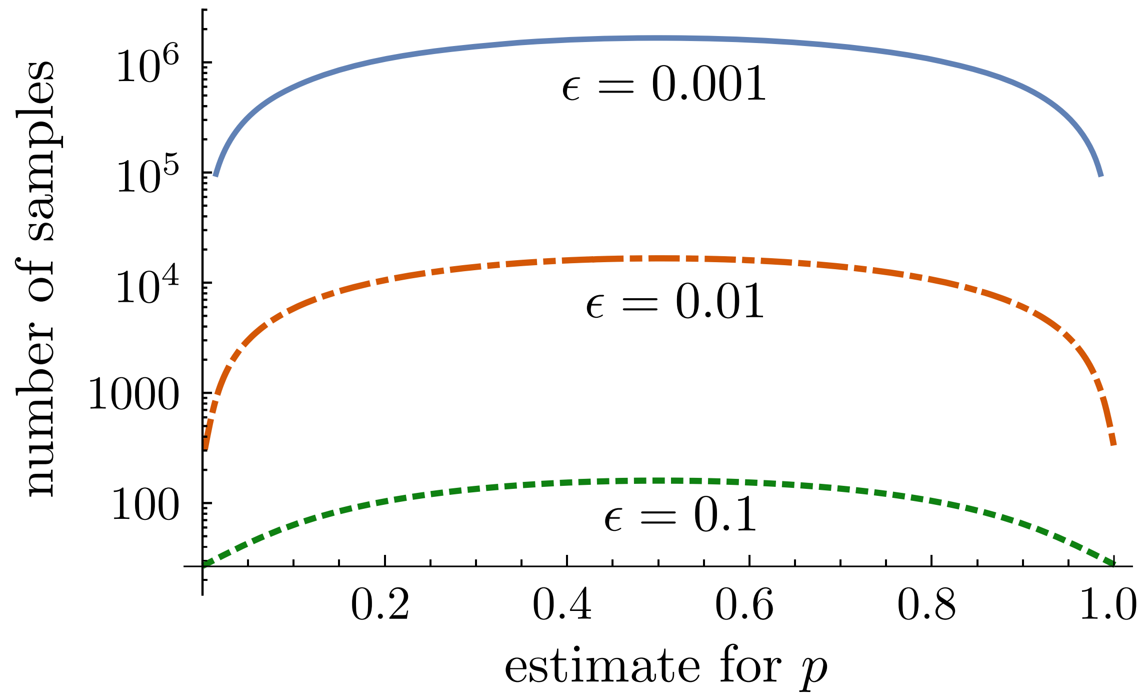
(suited for large s and p~0.5)

$$\epsilon = z\sqrt{\frac{\hat{p}(1-\hat{p})}{S}}$$

share of sample in state 1

shots

stat. z-value



→ For $\epsilon = 0.1$ and conf level 99% one needs 167 samples

For $\epsilon = 0.01$ and conf level 99% one needs $17{,}000$ samples

→ Overall might need a large number of shots on quantum computer

This needs to be taken into account when comparing quantum and classical computers in terms of speedups and quantum advantage

The Bloch Sphere

Since $|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$ with $|\alpha|^2 + |\beta|^2 = 1$

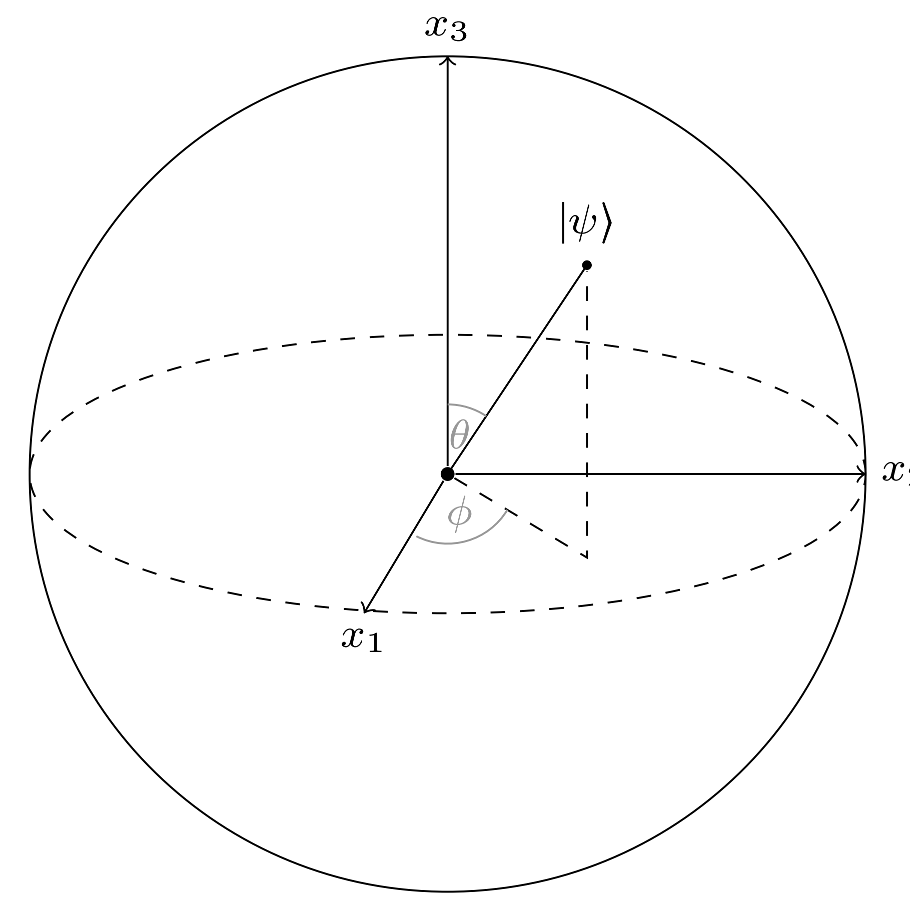
one can find angles such that

$$\alpha = e^{i\gamma}\cos\frac{\theta}{2} \qquad \beta = e^{i\delta}\sin\frac{\theta}{2}$$

Thus, with $\phi = \delta - \gamma$ single qubit can be parametrised as

$$|\psi\rangle = e^{(i\gamma)}\left(\cos\frac{\theta}{2}|0\rangle + e^{(i\phi)}\sin\frac{\theta}{2}|1\rangle\right)$$

where a global imaginary phase has no measurable effect and can be omitted.



$(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\phi)$

2-qubit states

Are built by tensor products, each qubit can be in state |0> or in state |1>

So, for two qubits we have four possibilities:

$$|0\rangle \otimes |0\rangle \,, |0\rangle \otimes |1\rangle \,, |1\rangle \otimes |0\rangle \,, |1\rangle \otimes |1\rangle$$

that we denote

$$|0\rangle \, |0\rangle \,, |0\rangle \, |1\rangle \,, |1\rangle \, |0\rangle \,, |1\rangle \, |1\rangle$$

or

$$|00\rangle \,, |01\rangle \,, |10\rangle \,, |11\rangle$$

We can have superposition as a generic state

$$|\psi\rangle = \alpha_{00} \, |00\rangle + \alpha_{01} \, |01\rangle + \alpha_{10} \, |10\rangle + \alpha_{11} \, |11\rangle$$

with complex coefficients such that $\sum_{x,y=0}^{1} |\alpha_{xy}|^2 = 1$

2-qubit states

Furthermore, we can express the state as a vector

$$\begin{pmatrix} \alpha_{00} \\ \alpha_{01} \\ \alpha_{10} \\ \alpha_{11} \end{pmatrix}$$

For which we find the inner products

$$\langle 00|00\rangle = \langle 01|01\rangle = \langle 10|10\rangle = \langle 11|11\rangle = 1$$

$$\langle 00|01\rangle = \langle 00|10\rangle = \langle 00|11\rangle = \cdots = \langle 11|00\rangle = 0$$

A 2-qubit quantum gate is a unitary matrix U of size 4 x 4

2-qubit gates

CNOT gate:

unitary matrix representation

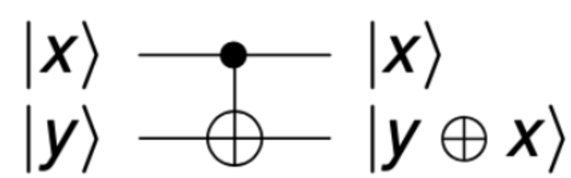
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

In words: if the first qubit is |0> nothing changes. If it is |1> we flip the second bit (and first stays the same)

Action: $|00\rangle \rightarrow |00\rangle \quad |01\rangle \rightarrow |01\rangle$

$|10\rangle \rightarrow |11\rangle \quad |11\rangle \rightarrow |10\rangle$

As a gate: $x, y \in \{0, 1\} \longrightarrow$



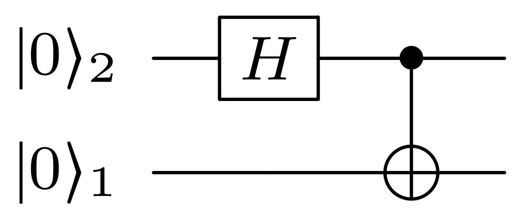
- A set of gates that can approximate any quantum operation
  -> Universal quantum computer

e.g. Rotation gates $R_x(\theta), R_y(\theta), R_z(\theta)$ + phase shift gate $P(\varphi)$ + CNOT

The CNOT gate is an extremely important gate

- It realises conditional probabilities

- It creates entanglement



read circuit from left to right

$$\mathrm{CNOT}((H_2 \otimes \mathbb{1}_1)(|0\rangle_2 \otimes |0\rangle_1))$$

$$\mathrm{CNOT}(\frac{1}{\sqrt{2}}|0\rangle_2 \otimes |0\rangle_1 + \frac{1}{\sqrt{2}}|1\rangle_2 \otimes |0\rangle_1) \;=\; \frac{1}{\sqrt{2}}(|0\rangle_2 \otimes |0\rangle_1 + |1\rangle_2 \otimes |1\rangle_1)$$

Bell state (fully entangled)

- It can copy classical information, because

$$|00\rangle \rightarrow |00\rangle$$

$$|10\rangle \rightarrow |11\rangle$$

- Constructs other control gates

N-qubit states

When we have n qubits, each of them can be in state |0> or |1>

Thus for n qubit states we have 2^n possibilities:

$$|00\ldots0\rangle, |00\ldots1\rangle, \ldots, |11\ldots1\rangle$$

or simply

$$|0\rangle, |1\rangle, \ldots, |2^n - 1\rangle$$

A generic state of the system will be

$$|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle + \ldots + \alpha_{2^n-1} |2^n - 1\rangle$$

With complex coefficients, such that $\sum_{i=0}^{2^n-1} |\alpha_i|^2 = 1$

Suppose we have the N qubit state

$$|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle + \ldots + \alpha_{2^n-1} |2^n - 1\rangle$$

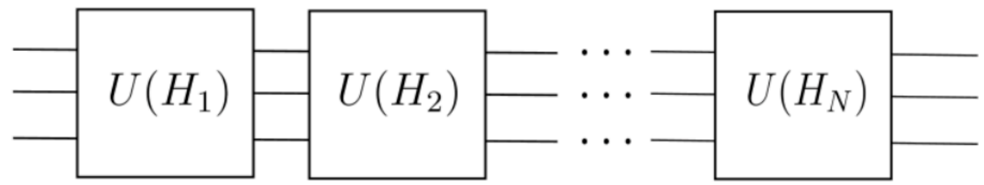
If we measure all its qubits, we obtain:

- 0 with probability $|\alpha_0|^2$ and the new state will be $|0\ldots 00\rangle$
- 1 with probability $|\alpha_1|^2$ and the new state will be $|0\ldots 01\rangle$
- ...
- $2^n - 1$ with probability $|\alpha_{2^n-1}|^2$ and the new state is $|1\ldots 11\rangle$

Completely analogous to 1 and 2 qubit situation but now with 2^n possibilities

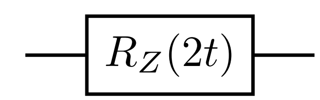
Example: Turning a Hamiltonian term into a gate

Recall $H = H_1 + H_2 + \cdots + H_N$



Assume, universal gate operations on device are $\{H, R_Z, CX\}$

Example 1 Assume $H_1 = Z \longrightarrow U = e^{-iZt} \longrightarrow$

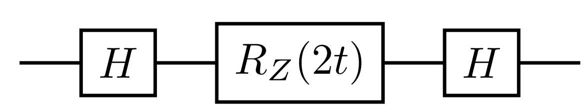


$R_Z(\theta) = e^{-i\frac{\theta}{2}Z}$

Example 2 Assume $H_2 = X \longrightarrow$ Since $HXH = Z \Rightarrow X = HZH$

$\longrightarrow U = He^{-iZt}H$ (proof via CBH Formula)

$\longrightarrow$



Example 3 $H = Z \otimes Z$ note $e^{-Z\otimes Zt} \neq e^{-iZt} \otimes e^{-iZt}$

with $(Z \otimes Z)^2 = \mathbb{I}$ one finds $e^{i(Z\otimes Z)t} = \cos(t)\mathbb{I} - i\sin(t) Z \otimes Z$

for the action on states we find

$$e^{i(Z\otimes Z)t}\,|00\rangle = (\cos(t)\mathbb{I} - i\sin(t) Z \otimes Z)\,|00\rangle = (\cos(t) - i\sin(t))\,|00\rangle$$

$$e^{i(Z\otimes Z)t}\,|11\rangle = (\cos(t)\mathbb{I} - i\sin(t) Z \otimes Z)\,|11\rangle = (\cos(t) - i\sin(t))\,|11\rangle$$

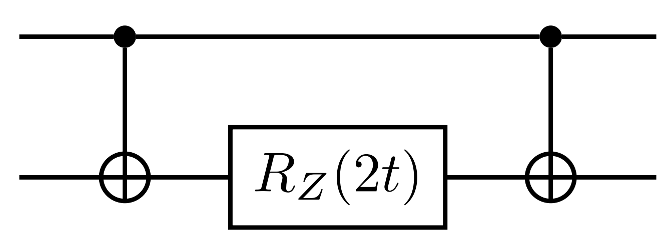
$$e^{i(Z\otimes Z)t}\,|01\rangle = \cos(t)\,|01\rangle - i\sin(t) Z\,|0\rangle \otimes Z\,|1\rangle = (\cos(t) + i\sin(t))\,|01\rangle$$

which can be written in matrix form as

$$e^{i(Z\otimes Z)t} = \begin{bmatrix} e^{-it} & 0 & 0 & 0 \\ 0 & e^{it} & 0 & 0 \\ 0 & 0 & e^{it} & 0 \\ 0 & 0 & 0 & e^{-it} \end{bmatrix} \begin{matrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{matrix}$$

if # of 1 is even one gets -
if #of 1 is odd one gets + (parity of state)

circuit that implements that



with $R_Z(2t) = \begin{bmatrix} e^{-it} & 0 \\ 0 & e^{it} \end{bmatrix}$

The Ising Model

- The Ising model is a fundamental mathematical model in statistical mechanics used to understand phase transitions and critical phenomena, particularly in ferromagnetic materials.
- Originally proposed by Wilhelm Lenz 1920, extensively studied by his student Ernst Ising 1925
- The model considers a lattice of spins in one of two states: up (+1) or down (–1). These spins represent magnetic dipole moments of atomic spins in material and interact with their nearest neighbours. -> Ferromagnetism, critical phenomena and phase transitions
- Exact solutions in 1-D and 2-D (Onsager's solution 1944) - no exact solution in 3-D (NP-hard)

interaction strength J   magnetisation

Classical Ising Model: $$H = -\sum_{\langle i,j \rangle} J_{i,j}\, \sigma_i \sigma_j - \mu \sum_i h_i\, \sigma_i$$

sum over neighbouring spins

transverse field

Quantum Mechanical Ising Model: $$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^z - \Gamma \sum_i \sigma_i^x$$

single trotter step

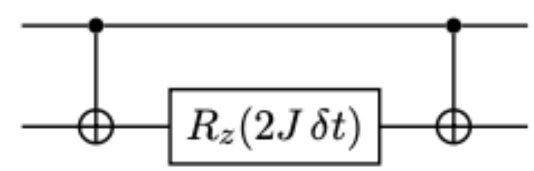
Real-time evolution $U(t) = e^{-iHt}$ with $H = -J \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z - \Gamma \sum_{i=1}^{N} \sigma_i^x$ → $e^{iJ\delta t\, \sigma_i^z \sigma_{i+1}^z}\, e^{i\Gamma \delta t\, \sigma_i^x}$

Now that the model has been constructed and Trotterised, we are ready to implement the real-time evolution on a quantum device:

Assume system with 2 sites:

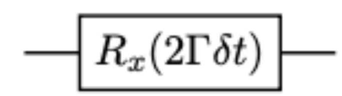
$e^{-iJ\sigma_Z^i\sigma_Z^{i+1}}$ = controlled Z

For the term $-J\sum_i \sigma_i^z\sigma_{i+1}^z$ $\longrightarrow$



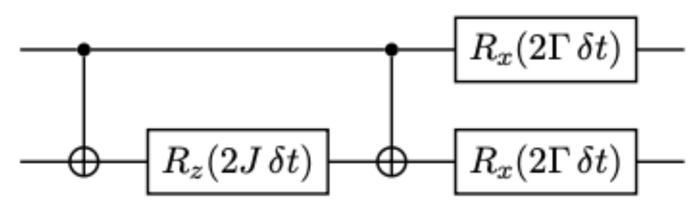
simple R_x rotation

For the term $-\Gamma\sum_i \sigma_i^x$ $\longrightarrow$

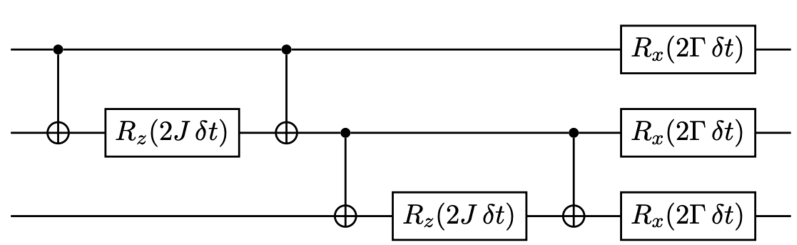


combined

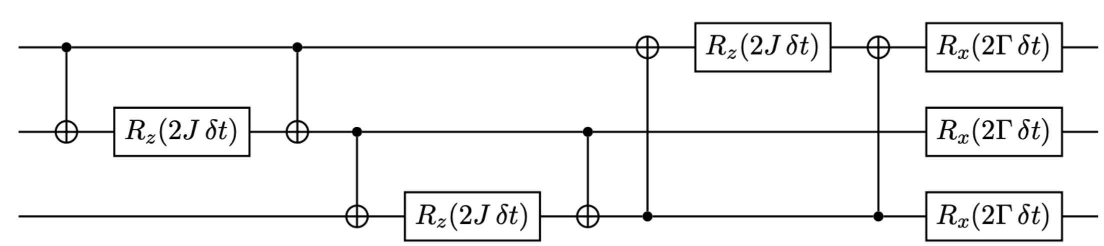
2-site Ising model - one trotter step:



3-site Ising model - one trotter step:



open boundary conditions



periodic boundary conditions

See hands-on session

https://github.com/simon-j-williams/QCIsingModel_KIT/tree/main

Examples of HEP usecases for Hamiltonian simulation

- Real-time evolution in QFTs: scattering processes, quark-gluon plasma formation, out-of-equilibrium dynamics

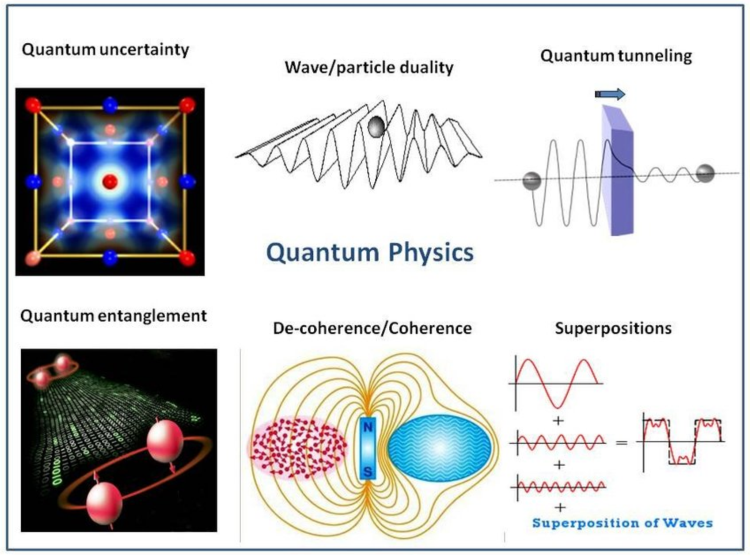
- Sign-problem in finite density QCD: QCD phase diagram at finite baryon density or nuclear matter in neutron stars

- Simulating Early Universe Physics: Phase transitions, reheating

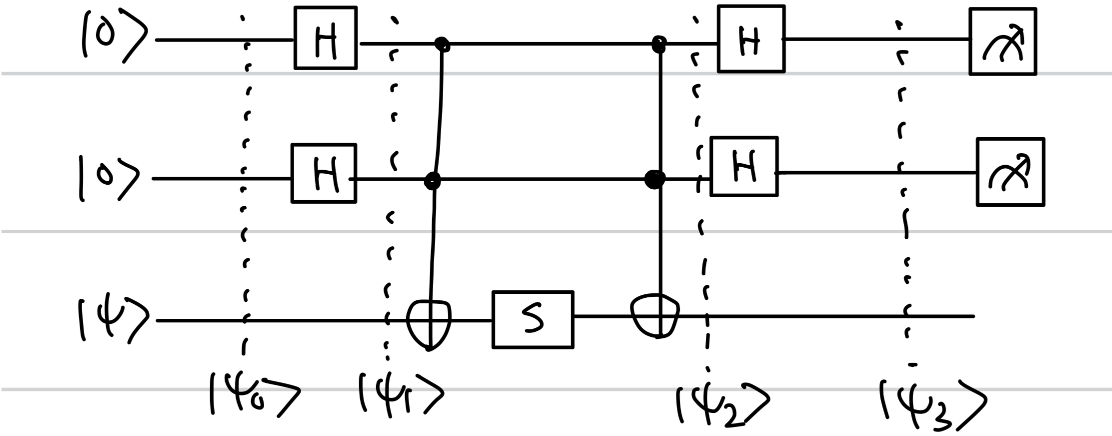
- Neutrino Oscillations in Dense Media: Neutrino osciallations in supenovae, neutron stars or early universe environments

- Gauge theories in higher dimensions: Classically expensive. Extra dim models

- Topological QFTs: Chern-Simons theory and Chern-Simons-like terms in SM



Summary



- Quantum computing is a new computational paradigm with a high potential for computational improvements in many science areas

- Hamiltonian simulation is an active research area ideally suited to be executed on quantum devices

- It might be key to avoiding the so-called 'sign problem' and to obtain a quantum advantage in computations for fundamental physics

- Hands-on session:

  https://github.com/simon-j-williams/QCIsingModel_KIT/tree/main