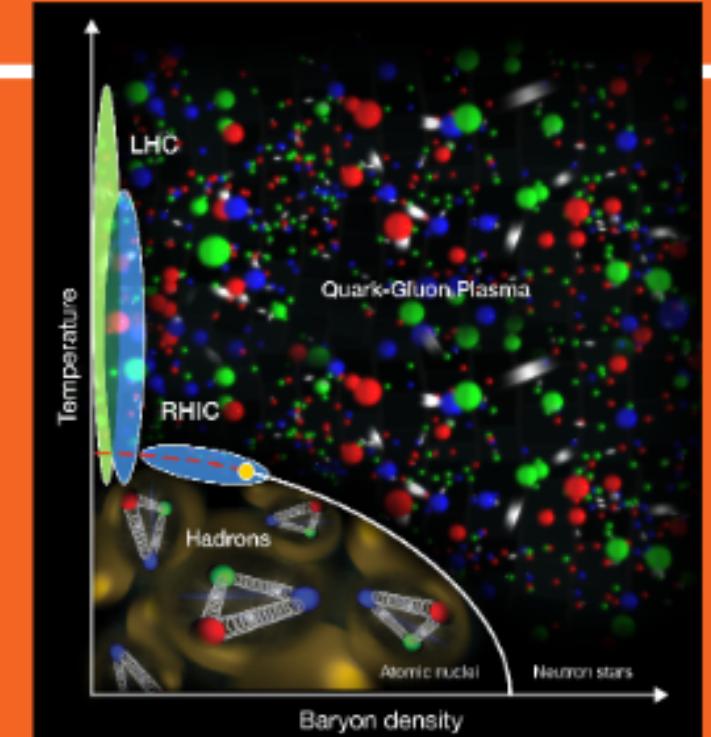


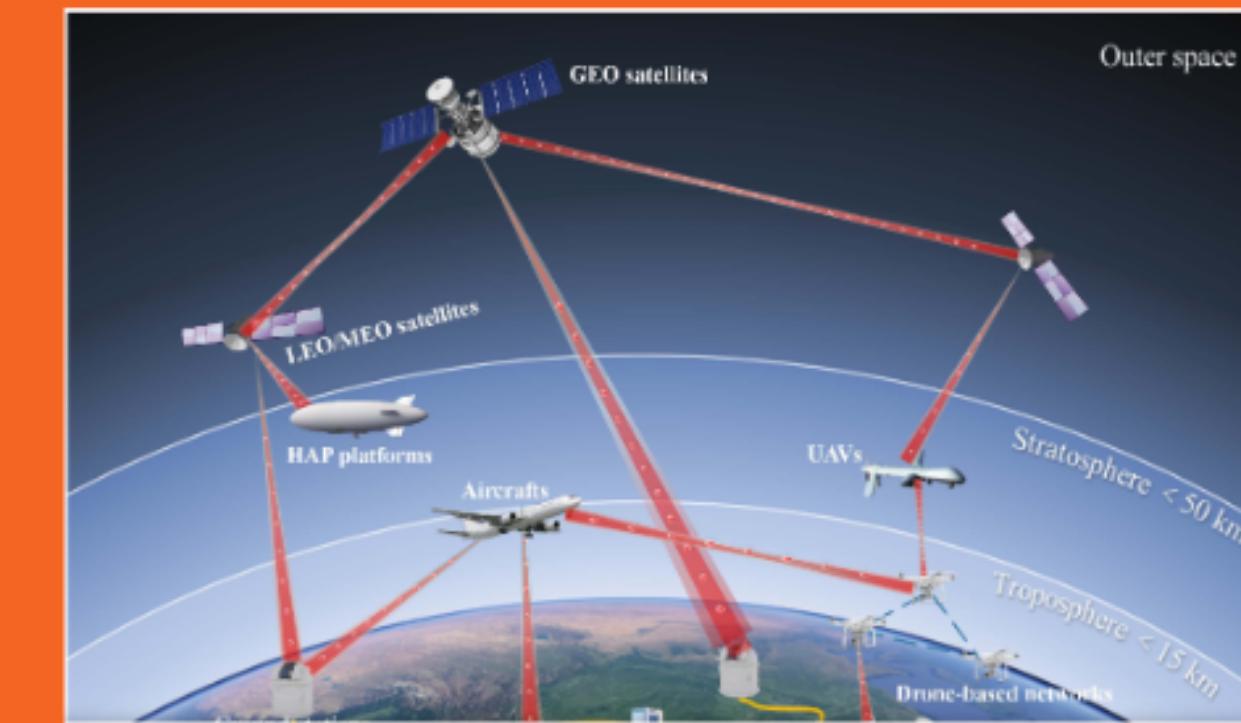
My Current Research:

- High Energy Physics (Theory/Phenomenology)
- With Prof Michael Strickland



My newly explored interest:

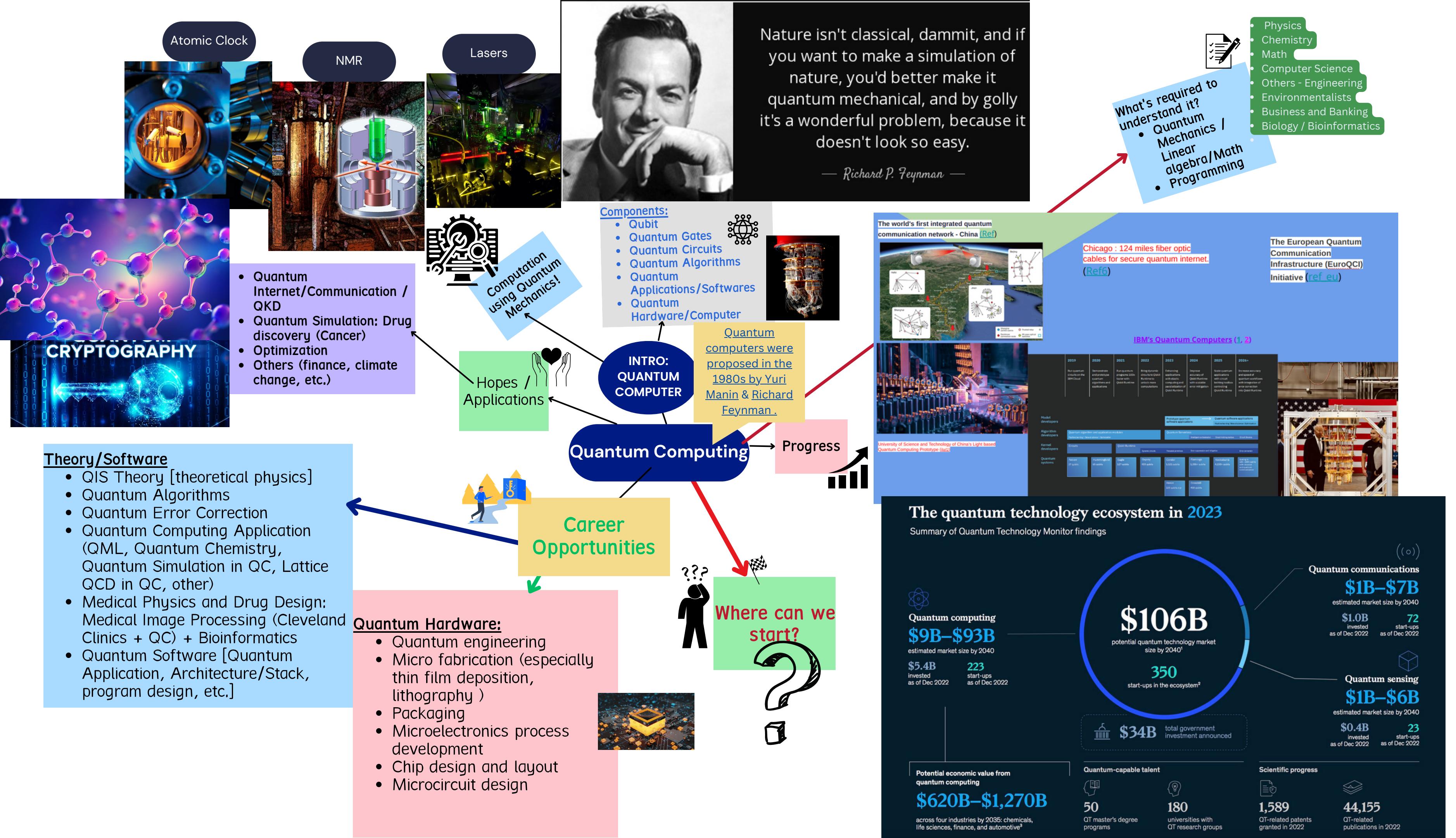
- Quantum Computing



A Presentation by Sabin Thapa, PhD Physics Candidate, Kent State University, Kent, Ohio, USA



[Ref: [1](#), [2](#), [3](#), [4](#)]



Quantum Operators

For instance, our fundamental law that any state can be made up from a linear combination of base states is written as

$$| \psi \rangle = \sum_i C_i | i \rangle, \quad (20.1)$$

where the C_i are a set of ordinary (complex) numbers—the amplitudes $C_i = \langle i | \psi \rangle$ —while $| 1 \rangle, | 2 \rangle, | 3 \rangle$, and so on, stand for the base states in some base, or *representation*.

If you take some physical state and do something to it—like rotating it, or like waiting for the time Δt —you get a different state. We say, “performing an operation on a state produces a new state.” We can express the same idea by an equation:

$$| \phi \rangle = \hat{A} | \psi \rangle. \quad (20.2)$$

An operation on a state produces another state. The *operator* \hat{A} stands for some particular operation. When this operation is performed on any state, say $| \psi \rangle$, it produces some other state $| \phi \rangle$.

Hermitian Matrix (Self-adjoint):

A is a complex square matrix that is equal to its own conjugate transpose.

Hermitian Operators

An operator is Hermitian if and only if it has real eigenvalues: $A^\dagger = A \Leftrightarrow a_j \in \mathbb{R}$.

$$A = A^H$$

i Hermitian adjoint operator

- Real Main Diagonals (Eigenvalues)
- Symmetric & Normal

We can introduce another operator related to \hat{A} and written as \hat{A}^\dagger which has the following defining property

$$\hat{A}|\psi\rangle = |\phi\rangle \text{ then } \langle\psi|\hat{A}^\dagger = \langle\phi|$$

The operator \hat{A}^\dagger is known as the *Hermitian adjoint* of \hat{A} .

What is then the action of this Hermitian adjoint operator on a ket vector? We can consider the following product

$$\langle\rho|\hat{A}|\psi\rangle = \langle\rho|(\hat{A}|\psi\rangle) = \langle\rho|\phi\rangle$$

using that $\hat{A}|\psi\rangle = |\phi\rangle$. The complex conjugate of the previous expression yields:

$$\langle\rho|\hat{A}|\psi\rangle^* = \langle\rho|\phi\rangle^* = \langle\phi|\rho\rangle$$

and if $\langle\psi|\hat{A}^\dagger = \langle\phi|$, then

$$\langle\rho|\hat{A}|\psi\rangle^* = \langle\phi|\rho\rangle = (\langle\psi|\hat{A}^\dagger)|\rho\rangle = \langle\psi|\hat{A}^\dagger|\rho\rangle.$$

$$A \text{ Hermitian} \iff a_{ij} = \overline{a_{ji}}$$

or in matrix form:

$$A \text{ Hermitian} \iff A = \overline{A^T}.$$

Unitary Operators

Transformations that preserve the length / norm / inner-product (keep the dot product invariant):

$$\langle \phi' | \psi' \rangle = \langle \phi' | \hat{U}^\dagger \hat{U} \psi \rangle = \langle \phi | \psi \rangle$$

Theorem 1.3. Given two sets of base kets, both satisfying orthonormality and completeness, there exists a unitary operator U such that

$$|b^{(1)}\rangle = U|a^{(1)}\rangle, |b^{(2)}\rangle = U|a^{(2)}\rangle, \dots, |b^{(N)}\rangle = U|a^{(N)}\rangle. \quad (1.5.1)$$

By a **unitary operator** we mean an operator fulfilling the conditions

$$U^\dagger U = 1 \quad (1.5.2)$$

and

$$UU^\dagger = 1. \quad (1.5.3)$$

Proof. We prove this theorem by explicit construction. We assert that the operator

$$U = \sum_k |b^{(k)}\rangle \langle a^{(k)}| \quad (1.5.4)$$

will do the job, and we apply this U to $|a^{(l)}\rangle$. Clearly,

$$U|a^{(l)}\rangle = |b^{(l)}\rangle \quad (1.5.5)$$

is guaranteed by the orthonormality of $\{|a'\rangle\}$. Furthermore, U is unitary:

$$U^\dagger U = \sum_k \sum_l |a^{(l)}\rangle \langle b^{(l)}| |b^{(k)}\rangle \langle a^{(k)}| = \sum_k |a^{(k)}\rangle \langle a^{(k)}| = 1, \quad (1.5.6)$$

where we have used the orthonormality of $\{|b'\rangle\}$ and the completeness of $\{|a'\rangle\}$. We obtain relation (1.5.3) in an analogous manner.

Reviewing Quantum Mechanics

Postulate 1. The state of a quantum mechanical system is completely specified by a function $\Psi(\mathbf{r}, t)$ that depends on the coordinates of the particle(s) and on time. This function, called the wave function or state function, has the important property that $\Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)d\tau$ is the probability that the particle lies in the volume element $d\tau$ located at \mathbf{r} at time t .

The wavefunction must satisfy certain mathematical conditions because of this probabilistic interpretation. For the case of a single particle, the probability of finding it *somewhere* is 1, so that we have the normalization condition

$$\int_{-\infty}^{\infty} \Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)d\tau = 1 \quad (110)$$

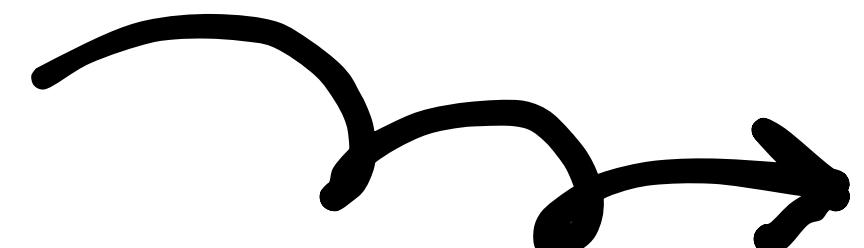
It is customary to also normalize many-particle wavefunctions to 1.² The wavefunction must also be single-valued, continuous, and finite.

Postulate 2. To every observable in classical mechanics there corresponds a linear, Hermitian operator in quantum mechanics.

Postulate 3. In any measurement of the observable associated with \hat{A} , the only values that will ever be observed are the eigenvalues a , which satisfy the eigenvalue equation

$$\hat{A}\Psi = a\Psi$$

Schrodinger's Equation



Postulate 4. If a system is in a state described by a normalized wave function Ψ , then the average value of the observable corresponding to \hat{A} is given by

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi d\tau$$

Postulate 5. The wavefunction or state function of a system evolves in time according to the time-dependent Schrödinger equation

$$\hat{H}\Psi(\mathbf{r}, t) = i\hbar \frac{\partial \Psi}{\partial t}$$



$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle$$

Postulate 6. The total wavefunction must be antisymmetric with respect to the interchange of all coordinates of one fermion with those of another. Electronic spin must be included in this set of coordinates.

The Nobel Prize in Physics 1933



Photo from the Nobel Foundation archive.

Erwin Schrödinger

Prize share: 1/2

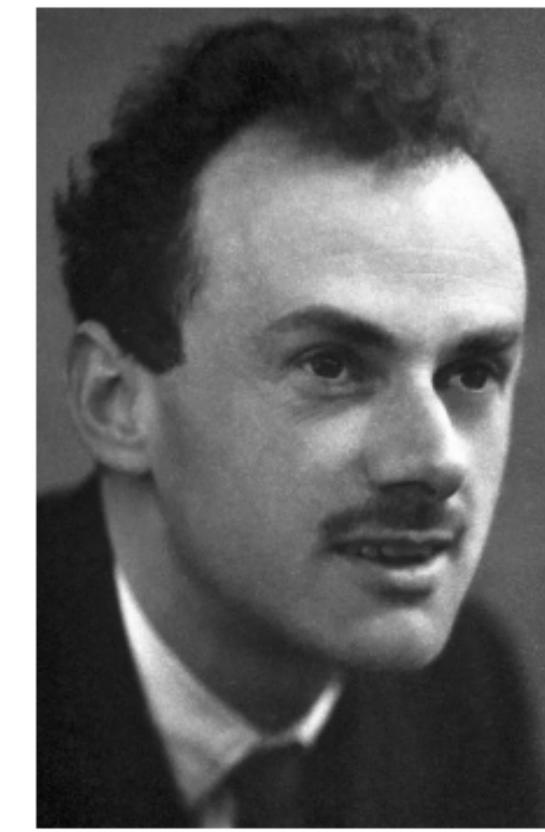


Photo from the Nobel Foundation archive.

Paul Adrien Maurice Dirac

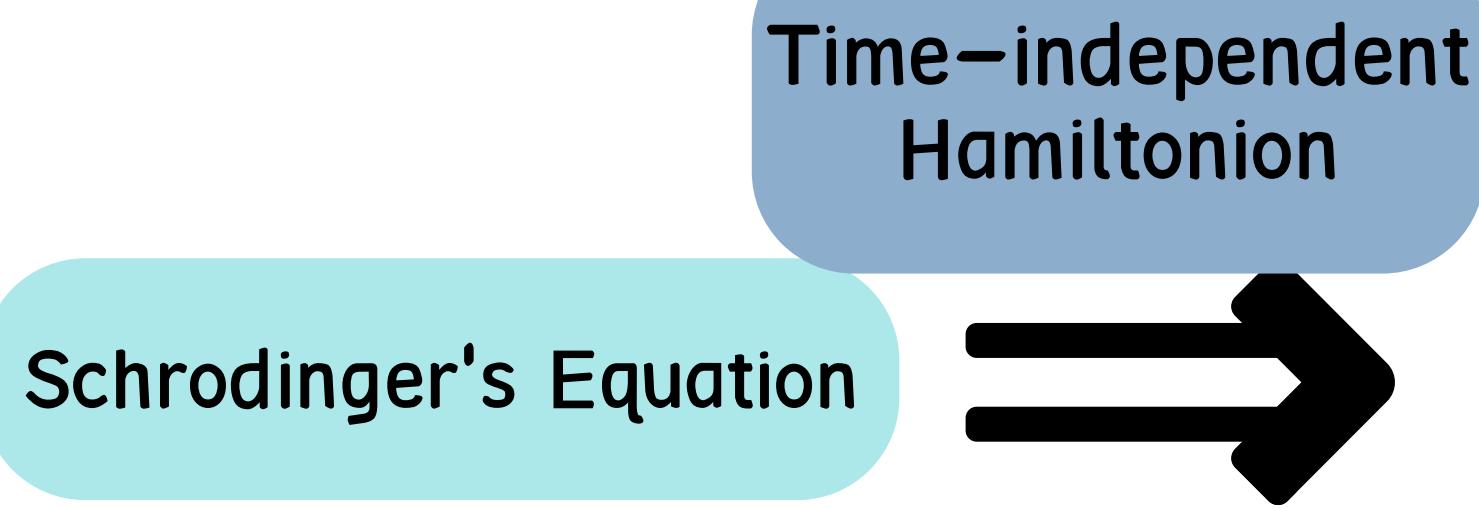
Prize share: 1/2

The Nobel Prize in Physics 1933 was awarded jointly to Erwin Schrödinger and Paul Adrien Maurice Dirac "for the discovery of new productive forms of atomic theory"

Quantum Simulation

Quantum simulation means that we simulate the behavior of one quantum system with another quantum system. In other words, if there is one quantum system, which may be complicated to prepare or certain things happen there on a microscopic scale, if I can create another quantum system where on a whole different scale the same equations apply, then the same equations have the same solution. That means, this system behaves like the other system and I can study the first system by deeply analyzing the second one. This is meant by quantum simulation – creating a quantum system with the same properties as the system you are interested in, but which is easier to manipulate and study.

Quantum Simulation: Dynamics of a Quantum System over Time!



$$|\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle$$

e^{-iHt} is a unitary operator because H is a Hermitian operator, hence e^{-iHt} it can be implemented with quantum gates.

Quantum Simulation in Quantum Computers

$|\psi(t)\rangle$

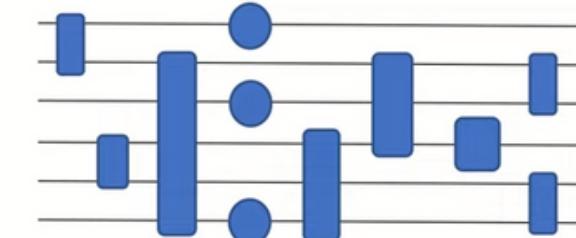
$$\hat{U} = e^{-i\hat{H}t}$$

large matrix

$$\hat{H} = \sum_{l=1}^L \hat{H}_l$$

Hermitian
 $\hat{H}_l = \hat{H}_l^\dagger$

$$e^{-i\hat{H}_l t} =$$



$$e^{-i\hat{H}t} = e^{-i\hat{H}_1 t} e^{-i\hat{H}_2 t} \dots e^{-i\hat{H}_L t}$$

if only $[\hat{H}_i, \hat{H}_j] = \hat{H}_i \hat{H}_j - \hat{H}_j \hat{H}_i = 0$

Sophus Lie (1875)
Hale Trotter (1959)
Masuo Suzuki (1976)

Lie product formula

Product formula

Trotter's formula

Trotter product formula

Lie-Trotter formula

Trotter-Suzuki

decomposition

Suzuki-Trotter expansion

Splitting method

$$e^{\hat{A}+\hat{B}} = \lim_{n \rightarrow \infty} \left(e^{\frac{\hat{A}}{n}} e^{\frac{\hat{B}}{n}} \right)^n$$

$$e^{-i \sum_{l=1}^L \hat{H}_l t} = \lim_{n \rightarrow \infty} \left(\prod_{l=1}^L e^{-i \frac{\hat{H}_l t}{n}} \right)^n$$

$$e^{-i \sum_{l=1}^L \hat{H}_l t} \simeq \left(\prod_{l=1}^L e^{-i \frac{\hat{H}_l t}{n}} \right)^n$$

$$\|\hat{U} - e^{-i \hat{H}t}\| \leq \varepsilon$$

for $\forall n$:

$$\hat{U}(t) = e^{-i \sum_{l=1}^L \hat{H}_l t} = \left(\prod_{l=1}^L e^{-i \frac{\hat{H}_l t}{n}} \right)^n + \mathcal{O}\left(\frac{t^2}{n}\right)$$

Trotter error

The heart of quantum simulation algorithms is the following asymptotic approximation theorem:

Theorem 4.3: (Trotter formula) Let A and B be Hermitian operators. Then for any real t ,

$$\lim_{n \rightarrow \infty} (e^{iAt/n} e^{iBt/n})^n = e^{i(A+B)t}. \quad (4.98)$$

Note that (4.98) is true even if A and B do not commute. Even more interestingly, perhaps, it can be generalized to hold for A and B which are generators of certain kinds of semigroups, which correspond to general quantum operations; we shall describe such generators (the ‘Lindblad form’) in Section 8.4.1 of Chapter 8. For now, we only consider the case of A and B being Hermitian matrices.

Proof

By definition,

$$e^{iAt/n} = I + \frac{1}{n} iAt + O\left(\frac{1}{n^2}\right), \quad (4.99)$$

and thus

$$e^{iAt/n} e^{iBt/n} = I + \frac{1}{n} i(A + B)t + O\left(\frac{1}{n^2}\right). \quad (4.100)$$

Taking products of these gives us

$$(e^{iAt/n} e^{iBt/n})^n = I + \sum_{k=1}^n \binom{n}{k} \frac{1}{n^k} [i(A + B)t]^k + O\left(\frac{1}{n}\right), \quad (4.101)$$

and since $\binom{n}{k} \frac{1}{n^k} = \left(1 + O\left(\frac{1}{n}\right)\right)/k!$, this gives

$$\lim_{n \rightarrow \infty} (e^{iAt/n} e^{iBt/n})^n = \lim_{n \rightarrow \infty} \sum_{k=0}^n \frac{(i(A + B)t)^k}{k!} \left(1 + O\left(\frac{1}{n}\right)\right) + O\left(\frac{1}{n}\right) = e^{i(A+B)t}. \quad (4.102)$$

Trotter's Formula

$$\lim_{n \rightarrow \infty} \left(e^{i\hat{A}\frac{t}{n}} e^{i\hat{B}\frac{t}{n}} \right)^n = e^{i(\hat{A} + \hat{B})t}$$

1st order approximation

$$e^{\hat{A} + \hat{B}} = \lim_{n \rightarrow \infty} \left(e^{\frac{\hat{A}}{n}} e^{\frac{\hat{B}}{n}} \right)^n$$

2nd order approximation

$$e^{\hat{A} + \hat{B}} = \lim_{n \rightarrow \infty} \left(e^{\frac{\hat{A}}{2n}} e^{\frac{\hat{B}}{n}} e^{\frac{\hat{A}}{2n}} \right)^n$$

pth order approximation

$$\hat{U}(t) = \left(\prod_{l=1}^L \text{some expression here} \right)^n$$

Trotter error

$$\mathcal{O}(t^2)$$

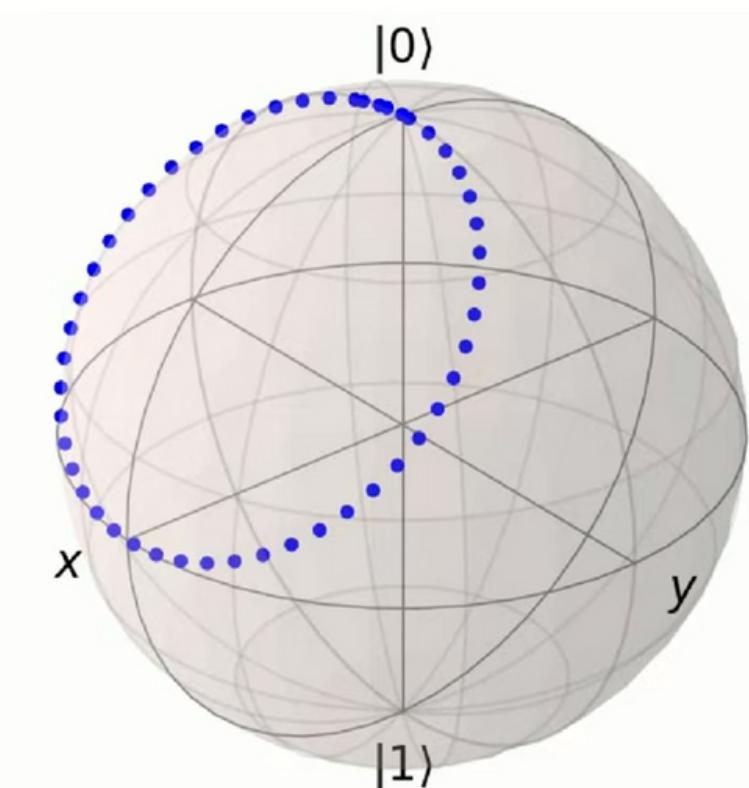
$$\mathcal{O}(t^3)$$

$$\mathcal{O}(t^{p-1})$$

Trotterization example

$$\hat{H} = \hat{X} + \hat{Z}$$

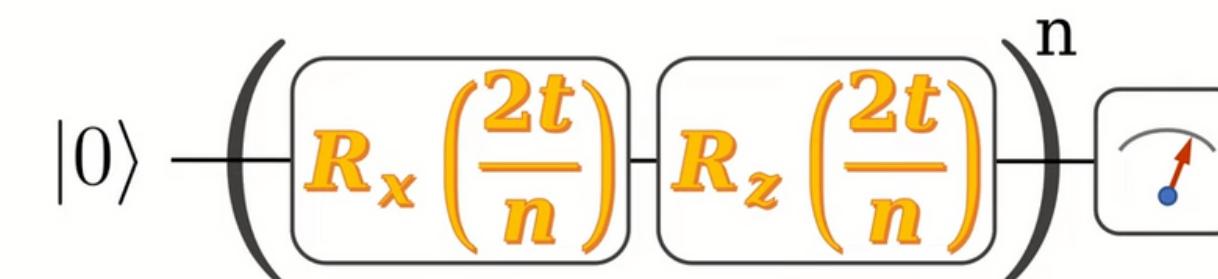
$$e^{-i\hat{H}t} \neq e^{-i\hat{X}t}e^{-i\hat{Z}t} \quad [\hat{\sigma}_z, \hat{\sigma}_x] = 2i\hat{\sigma}_y$$



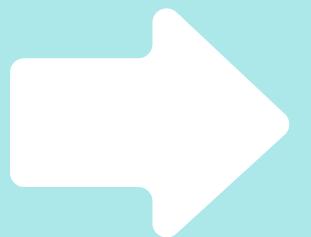
$$e^{-i\hat{H}t} = \left(e^{-i\hat{X}\frac{t}{n}} e^{-i\hat{Z}\frac{t}{n}} \right)^n$$

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

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

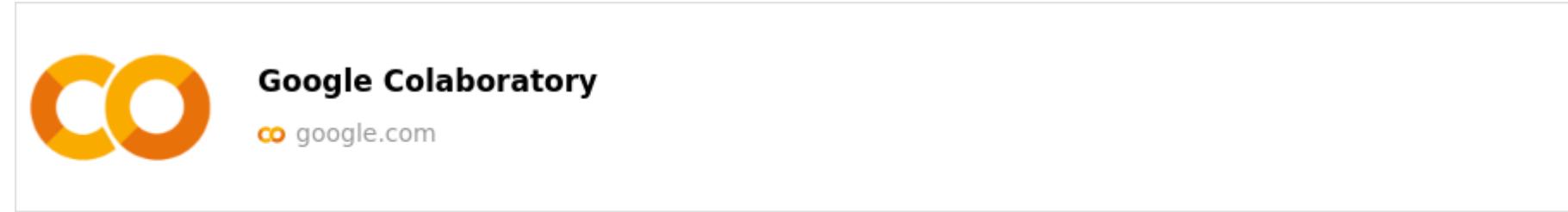


NEXT



QUANTUM PARTY: SATURDAY

HANDS-ON TUTORIAL: QUANTUM COMPUTING SERIES WITH QISKit



https://colab.research.google.com/drive/1gMObKXbpG0mls7xH5G_zhj84gYIOtBm1?usp=sharing

ANY QUESTIONS?

THANK YOU!