Introduction to Quantum Information and Qiskit

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Objectives

- Understand what quantum mechanical behaviour is important in quantum information theory.
- Understand the mathematical background used in quantum information theory(Dirac notation, Bloch Sphere,...).
- Study attempts to interpret how quantum mechanics is consistent with our experienced reality.
- Introduce quantum gates and circuits.
- Look at various applications of quantum information and computation.
- Study quantum simulation in Qiskit.
  - Introduce time evolution in quantum mechanics and the Trotter decomposition.
  - Simulate the time evolution of a simple quantum system in Qiskit using quantum circuits.

Definition (Quantum Information Theory)

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Key Quantum Properties:

Quantum Superposition: Quantum objects(such as qubits) can exist in a linear superposition of states until they are measured.

Quantum Entanglement: The phenomena whereby the individual states of a pair of particles are indefinite until one of the particles is measured. The state of the other particle is then determined from this measurement.

Mathematical Toolbox

A common way to study quantum systems is through its wavefunction, denoted $\Psi(\vec{x}, t)$. This is a function representation of a quantum state due to its dependence on a continuous variable such as position $\vec{x}$, or momentum $\vec{p}$.
If a discrete basis is used instead of a continuous basis the quantum state can then be represented in Dirac notation as a statevector.

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$$|\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}, \langle\alpha| = |\alpha\rangle^\dagger = (a_1^*, a_2^*, \ldots, a_n^*) \tag{1}$$

$|\alpha\rangle = \sum_{i=1}^{n} a_i|i\rangle$, a_i are called the probability amplitudes of each basis state $|i\rangle$.

The usual vector operations can be performed on quantum statevectors.

$$\langle\alpha|\beta\rangle = a_1^* b_1 + \cdots + a_n^* b_n = \sum_{i=1}^{n} a_i^* b_i \tag{2}$$

$$\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^* \tag{3}$$

$$|\alpha\rangle \otimes |\beta\rangle = \begin{pmatrix} a_1 \begin{pmatrix} b_1 \\ \vdots \\ b_m \end{pmatrix} \\ \vdots \\ a_n \begin{pmatrix} b_1 \\ \vdots \\ b_m \end{pmatrix} \end{pmatrix} = \begin{pmatrix} a_1 b_1 \\ \vdots \\ a_1 b_m \\ \vdots \\ a_n b_1 \\ \vdots \\ a_n b_m \end{pmatrix} \tag{4}$$

Note: The dimension of our new vector is $n \times m$.

Definition (Hilbert Space)

Def: All quantum states $|\psi\rangle$ exist in a linear vector space over the field $\mathbb{C}$ possessing an inner product which induces a norm and is complete with respect to this norm. This vector space is called a Hilbert space, $\mathcal{H}$, and has dimension $d = 2^n$ with n being the number of qubits.

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$\mathcal{H}$ satisfies the usual vector space properties of being **closed under vector addition and scalar multiplication**.

Properties satisfied by $|u\rangle, |v\rangle, |w\rangle \in \mathcal{H}$ are

$$\langle u|(c_1|v\rangle + c_2|w\rangle) = c_1\langle u|v\rangle + c_2\langle u|w\rangle \tag{5}$$

$$\langle v|v\rangle \geq 0 \tag{6}$$

$$\langle v|v\rangle = 0 \iff |v\rangle = 0 \tag{7}$$

A set of orthonormal vectors $|e_k\rangle$ is **complete** if

$$\sum |e_k\rangle\langle e_k| = \mathbb{I} \iff |v\rangle = \sum \langle e_k|v\rangle |e_k\rangle \tag{8}$$

In quantum mechanics there are also particular types of matrices which are important.

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These matrices are called **hermitian** and **unitary** matrices.

Hermitian matrices satisfy $H^\dagger = H$.

Unitary matrices satisfy $U^\dagger = U^{-1} \iff U^\dagger U = UU^\dagger = \mathbb{I}$.

Note: Matrices can be both hermitian and unitary.

Properties of the hermitian conjugate,

$$(AB)^\dagger = B^\dagger A^\dagger \tag{9}$$

$$(A|v\rangle)^\dagger = \langle v|A^\dagger \tag{10}$$

($\dagger$ is the hermitian conjugate = transpose and complex conjugate)

Recall eigenvalues and eigenvectors of a matrix.

$$A|v_j\rangle = \lambda_j|v_j\rangle \tag{11}$$

λ_j form the set of eigenvalues of A which is called the **spectrum**. $|v_j\rangle$ form the set of eigenvectors of A.

A can then be represented as $A = \sum_j \lambda_j|v_j\rangle\langle v_j|$.

Note: $\sum_j |v_j\rangle\langle v_j|$ can be considered as the projection operator P, which projects a quantum system onto the subspace created by the set of eigenvectors.

Properties of Hermitian Matrices:

(1). Hermitian matrices have real eigenvalues.

$$A|v\rangle = \lambda|v\rangle \implies \langle v|A|v\rangle = \lambda$$

$$\lambda^* = (\langle v|A|v\rangle)^* = \langle v|A^\dagger|v\rangle = \langle v|A|v\rangle = \lambda$$

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(2). Two eigenvectors of a hermitian matrix are orthogonal if their eigenvalues are unequal.

$A|v\rangle = \lambda|v\rangle$, $A|w\rangle = \mu|w\rangle$

$0 = \langle v|A|w\rangle - \langle v|A^\dagger|w\rangle = \mu\langle v|w\rangle - \lambda\langle v|w\rangle = (\mu - \lambda)\langle v|w\rangle \iff \langle v|w\rangle = 0$

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(3). The eigenvalues of a Hermitian matrix span the space.

Fundamentals of Quantum Mechanics

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Given a quantum state $|\psi\rangle$ which is normalised($\langle\psi|\psi\rangle = 1$), we can perform a measurement on it to obtain a resultant state $|\alpha\rangle$ with probability $|\langle\alpha|\psi\rangle|^2$.

A measurement can be considered as the projection operator $P = |\alpha\rangle\langle\alpha|$.

The resulting post measurement quantum state is given by $|\psi'\rangle = \frac{P|\psi\rangle}{\sqrt{\langle\psi|P|\psi\rangle}}$.

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Given the probabilistic nature of quantum mechanics we are not guaranteed to end up with the same eigenstate after every measurement of the same quantum state.

For N copies of a physical system allowing us to perform N measurements we obtain the eigenvalue a an amount of times $N|\langle\alpha|\psi\rangle|^2$ which gives the exact amount of times we should measure it in the limit $N \to \infty$.

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Another important quantity in measurement is the **expectation value**.
$\langle\psi|A|\psi\rangle = \sum_k a_k \langle\psi|\alpha_k\rangle\langle\alpha_k|\psi\rangle = \sum_k a_k p_k$
Note: If $|\psi\rangle$ is already an eigenstate then the expectation value will just be a because that is what we constantly measure when observing our physical system.

Quantum Entanglement

When studying a larger quantum system which is composed of n individual quantum systems the quantum state of the larger system is given by taking the tensor product of the states of the n individual systems

$$|\Psi\rangle = |\psi_1\rangle \otimes \cdots \otimes |\psi_n\rangle \tag{12}$$

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If we have a product state $|\psi\rangle \otimes |\phi\rangle$ of states from subsystems A and B, we therefore know the individual states of subsystems A and B. What if we can't deduce the states of the subsystems from the state of the larger system?

Any quantum state $|\Psi\rangle$ which cannot be decomposed as a tensor product of states is said to be **entangled**.

Therefore, if two quantum systems are entangled, we cannot know the states of the individual systems.

Quantum Entanglement

If we have an entangled quantum state we can actually measure its **degree of entanglement**. This can be done using several measures, with the most common being the Von Neumann entanglement entropy

$$S(\rho_A) = -\mathrm{tr}(\rho_A \ln \rho_A) = S(\rho_B) \tag{13}$$

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To see what this means physically, let's consider some examples

$$|\Psi\rangle = \frac{1}{\sqrt{5}}|00\rangle + \sqrt{\frac{2}{5}}|01\rangle - \frac{1}{\sqrt{5}}|10\rangle + \frac{1}{\sqrt{5}}|11\rangle \tag{14}$$

We see that we measure subsystem A to be in the state $|0\rangle$, we are more likely to find subsystem B to be in the state $|1\rangle$. So a measurement on one subsystem gives us some information as to the state of the other subsystem.

Quantum Entanglement

Now consider the following quantum state

$$|\Psi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \tag{15}$$

This state is known as a **Bell state** and is **maximally entangled**. This means a measurement on one of the subsystems tells us the state of the other subsystem with **absolute certainty**.

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There are 4 Bell states which form a set of basis states for a two-qubit system

$$|\Phi^+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}, |\Phi^-\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}}, |\Psi^+\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}, |\Psi^-\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}} \tag{16}$$

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In quantum information, for a single qubit we work in the 2-dimensional computational basis $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.
We describe our single qubit quantum state in the form $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$.

To obtain the correct probabilities when measuring our qubit we have the condition $|\alpha|^2 + |\beta|^2 = 1$. $\alpha, \beta \in \mathbb{C}$

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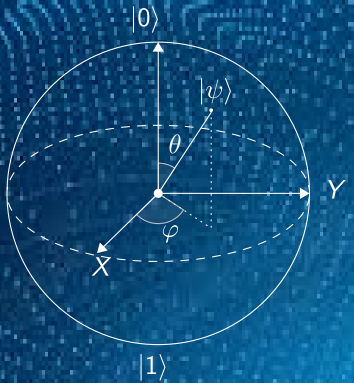
We typically measure in the computational basis(Z-basis). There are alternate bases in which we can perform measurements such as the X-basis($|+\rangle, |-\rangle$) or Y-basis($|+i\rangle, |-i\rangle$).

Visualizing Quantum States

Quantum states are pictured on the **Bloch Sphere**.



Note: $|0\rangle, |1\rangle$ are orthogonal because they are basis vectors. However, on the Bloch Sphere any angle between vectors is doubled. In terms of Bloch Sphere coordinates we can write the quantum state of a qubit as $|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$. The surface of the Bloch Sphere is a valid Hilbert Space. Any unitary transformation causes rotations of the quantum state around the Bloch Sphere.

How Do We Interpret Quantum Mechanics?

We have introduced the theory of how measurements are performed on quantum systems in experiments. In these experiments the quantum state collapses to some eigenstate and we measure the corresponding eigenvalue.

But what fundamentally happens to a quantum system during a measurement process? What behaviour does a quantum system exhibit that cannot be measured or observed?

In order to merge what we understand about quantum mechanics with how we experience reality, many physicists have put forward ideas on what this non-observable behaviour is. An interpretation of quantum mechanics with growing popularity favoured by many physicists such as information theorists and cosmologists is the Many-Worlds Interpretation.

First Interpretations

- Many introductions to quantum mechanics are taught using the Copenhagen Interpretation put forward by Niels Bohr and Werner Heisenberg.
- In the Copenhagen Interpretation each quantum system is described by a wavefunction $\psi(\vec{x}, t)$ and has a probability density given by the Born Rule, $|\psi(\vec{x}, t)|^2$.
- The interpretation is then that quantum mechanics is indeterministic. This is due to the act of measurement collapsing the wavefunction to a particular value and the rest of the information on the quantum system being lost.

Many-Worlds Quantum Mechanics

In 1957 American physicist Hugh Everitt proposed a Many-Worlds interpretation of quantum mechanics to avoid dealing with the collapse of the wavefunction.

- This interpretation originated from the fact that none of the equations of quantum mechanics imply that the wavefunction should collapse.
- Instead, the universe evolves until the of measurement is taken, at which point it splits into a number of other universes depending on the number of possible measurement outcomes.
- An alternative view of this process is that there are an infinite number of universes corresponding to all possible solutions to the wavefunction, and many of these universes evolve identically until the measurement is taken. After the measurement is performed each measurement outcome is observed in these different universes and their evolution is now no longer identical.

The Universal Wavefunction

- The development of Many-Worlds Quantum Mechanics included introducing a universal wavefunction, which includes observers and everything else.
- The universal wavefunction describes the position of every particle in the universe at a particular moment in time. But it also describes every possible location of those particles at that instant. And it also describes every possible location of every particle at any other instant of time.
- Simply put, a single wavefunction describes all possible universes at all possible times, as long as these universes obey the laws of physics.
- This universal wavefunction is of great interest to cosmologists, given that a single, uncollapsed wavefunction allows them to describe the entire univers quantum mechanically while not being entirely incompatible with general relativity.

Summary of Interpretations

- Quantum mechanics was originally interpreted as an indeterministic theory in which the wavefunction collapses once a measurement is taken.
- The Many-Worlds Interpretation states that each possible measurement outcome is realised in different universes, thus the "Many-Worlds" name.
- A single, uncollapsed wavefunction describes the behaviour of all possible universes at each instance of time.
    - There is no description of how one state changes into another, i.e a flow of time.
    - Each universe is described at a particular time step, but not a continuous collection of time steps.

Introduction to Quantum Circuits

We will now study how to perform operations on quantum states through the use of quantum circuits.

A quantum circuit with no operations takes the form

$$\begin{array}{l} |0\rangle \text{ ———————} \\ |0\rangle \text{ ———————} \\ \quad\vdots \\ |0\rangle \text{ ———————} \end{array}$$

All qubits are initialised in the state $|0\rangle$(the ground state) and the state of the composite system is denoted as

$|0\rangle^{\otimes n} = |0\rangle \otimes |0\rangle \otimes \cdots \otimes |0\rangle = |00\ldots0\rangle$

This composite state exists inside the Hilbert space

$\mathcal{H} = \mathcal{H}^0 \otimes \mathcal{H}^1 \otimes \cdots \otimes \mathcal{H}^{n-1}$

Single Qubit Quantum Gates

The simplest gates which are performed in quantum circuits are the X, Y and Z gates.

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = |0\rangle\langle 1| + |1\rangle\langle 0| \tag{17}$$

$$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = -i|0\rangle\langle 1| + i|1\rangle\langle 0| \tag{18}$$

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = |0\rangle\langle 0| - |1\rangle\langle 1| \tag{19}$$

These matrices are also the Pauli matrices σ_X, σ_Y and σ_Z which are hermitian and unitary.

Single Qubit Gates

The Pauli gates act on the computational basis state in the following way.

$X|0\rangle = |0\rangle\langle 1|0\rangle + |1\rangle\langle 0|0\rangle = |1\rangle$
$X|1\rangle = |0\rangle\langle 1|1\rangle + |1\rangle\langle 0|1\rangle = |0\rangle$
The X-gate is a bit flip gate.

$Y|0\rangle = -i|0\rangle\langle 1|0\rangle + i|1\rangle\langle 0|0\rangle = i|1\rangle$
$Y|1\rangle = -i|0\rangle\langle 1|1\rangle + i|1\rangle\langle 0|1\rangle = -i|0\rangle$
The Y-gate results in a bit flip along with a change in phase.

$Z|0\rangle = |0\rangle\langle 0|0\rangle - |1\rangle\langle 1|0\rangle = |0\rangle$
$Z|1\rangle = |0\rangle\langle 0|1\rangle - |1\rangle\langle 1|1\rangle = -|1\rangle$
The Z-gate results in a phase flip for $|1\rangle$.

Single Qubit Gates

There are other more complex single qubit gates.

Let's look at the Hadamard gate.

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1|) \tag{20}$$

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle\langle 0|0\rangle + |0\rangle\langle 1|0\rangle + |1\rangle\langle 0|0\rangle - |1\rangle\langle 1|0\rangle) = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle$$

$$H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle\langle 0|1\rangle + |0\rangle\langle 1|1\rangle + |1\rangle\langle 0|1\rangle - |1\rangle\langle 1|1\rangle) = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = |-\rangle$$

Note that the $|+\rangle$ and $|-\rangle$ differ by a **relative** phase and thus describe different physics.

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Note that the $|+\rangle$ and $|-\rangle$ differ by a **relative** phase and thus describe different physics. Other generalised single qubit gates such as

$R_X(\phi), R_Y(\phi), R_Z(\phi)$ are also possible which correspond to rotations of an angle ϕ around the corresponding axis on the Bloch Sphere.

Two Qubit Gates

We now turn our attention to two-qubit gates which are mainly used to perform entangling operations between two qubits.

The most common of these gates is the CNOT gate.

$$\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{21}$$

This is a conditional operation where the resulting state of the second(target) qubit depends on the state of the first(control) qubit. If the control qubit is in the state $|0\rangle$ then nothing happens to the target qubit. If the control qubit is in the state $|1\rangle$ then a bit-flip(X-gate) is performed on the target qubit.

Two Qubit Gates

The CNOT-gate could also be called the CX-gate because X is the conditional operation which is performed.

This means there are also the less common CY- and CZ-gates which operate in the same way as CX but instead perform the Y and Z operations.

Theoretically, in a quantum circuit a controlled gate which will perform some arbitrary unitary gate can be constructed.

Two Qubit Gates

Other two-qubit operations not related specifically to entangling operations can also be performed.

One such gate is the SWAP-gate which swaps the state of two qubits.

$$\mathrm{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{22}$$

This gate is particularly useful when looking at real quantum processors. If we want to entangle two qubits which are not very closely connected on the quantum chip several SWAP gates can be performed which will improve the connectivity.

Two Qubit Gates

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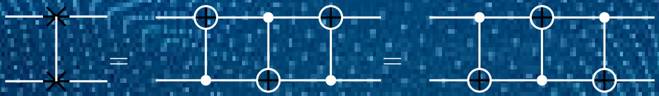
In quantum hardware systems there is a set of basis gates.
These basis gates typically consist of gates such as the I, X, R_Z, S_X and CNOT gates.

The SWAP gate is not in this set of basis gates, so how is it performed?

Gates such as the SWAP gate which are not a part of the basis gates are implemented using a composition of basis gates.

Two Qubit Gates

The SWAP gate can be decomposed in the following way using CNOT-gates.



The gates are composed in this way in order to remove the conditional behaviour of the CNOT-gates.

It is done in this way so that any initial state goes through a sequence of bit-flips in such a way that the states of the two qubits are swapped.

Applications of Quantum Information

We have seen a lot about quantum information, but what can it actually do?
Here are some applications of quantum information associated with quantum computing.

- Quantum Simulation
  - The nearest-term application with uses in quantum chemistry, drug development and material design.
- Quantum Cryptography
  - Using quantum mechanical ideas to encrypt data so it cannot be hacked or studying how quantum decryption algorithms can be used to hack classical encryption methods.
- Quantum Machine Learning
  - The incorporation of quantum algorithms into machine learning along with aiming for a quantum advantage in the training of the algorithms.
- Quantum Finance
  - Finding difficult to see patterns in complex financial data, studying the probabilistic fluctuations in financial markets.

Quantum Simulation

We will focus on the application of quantum simulation.

Definition (Quantum Simulation)

Def: For a particular model of a quantum system its simulation consists of the ability to emulate how the state of the system changes in time.

The simulation of the time evolution(dynamics) of a quantum system can be performed in different ways.

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Definition (Analog Quantum Simulation)

Def: Experimentally emulating one quantum system using another.

Definition (Digital Quantum Simulation)

Def: The encoding of a target quantum system within qubits and implementing its evolution using quantum gates.

Quantum Simulation

Quantum simulation is an important application of quantum computing due to its ability to overcome the resource bottleneck encountered by classical computers when trying to simulate quantum systems.

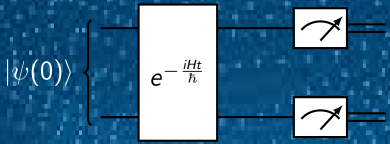
The Hilbert space of a quantum system scales exponentially with the system size, 2^N, where N is the number of qubits. If we want to simulate a system of around 256 qubits, our Hilbert space would be of size 2^{256}, which is roughly the number of atoms in the universe.

To simulate a Hilbert space of this size on a classical computer without approximations would require the algorithm to explore all 2^{256} states of the system.

The ability to simulate large quantum systems of interest opens up the possibility of advancements in areas such as material design and drug discovery.

Quantum Simulation Methods

The goal of any quantum simulation method is to initialise a qubit register in some initial state $|\psi(0)\rangle$ and the evolve it to a quantum state $|\psi(t)\rangle$ by implementing the time evolution operator, $e^{-\frac{iHt}{\hbar}}$, as a set of quantum gates.



The exact operator, and therefore the exact gates we want to add to the circuit will depend on the Hamiltonian, H, meaning one quantum simulation circuit architecture will not work in all cases.

Quantum Simulation Methods

In an ideal world we would be able find a collection of gates which implements $e^{-\frac{iHt}{\hbar}}$ exactly. However, Hamiltonians of interest can be very large and even exactly knowing the operator we want implement can be difficult.

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To overcome this difficulty the Hamiltonian is decomposed into a sum of non-commuting terms

$$H = \sum_{k=1}^{L} H_k, \; [H_i, H_j] \neq 0 \text{ for } i \neq j \tag{23}$$

The time evolution operator is then approximated as

$$e^{-\frac{iHt}{\hbar}} \approx \lim_{N_{Tr} \to \infty} \left(\prod_{k=1}^{L} e^{-\frac{iH_k t}{N_{Tr} \hbar}} \right)^{N_{Tr}} \tag{24}$$

Introduction to Qiskit

Qiskit is a Python based quantum software development kit from IBM.

It is capable of creating and executing quantum circuits and algorithms on both the local classical device and IBM's quantum hardware.

Like any software, Qiskit contains various modules and packages.

Qiskit contains individual application modules which are Qiskit Nature, Qiskit Finance, Qiskit Optimization and Qiskit Machine Learning. This makes performing the applications easier and also allows each module to be updated without affecting the others.

Other quantum softwares are available. Some options are OpenQasm(IBM), Cirq(Google), Q#(Microsoft) and Braket(Amazon).

Introduction to Qiskit

Let's now look at some important commands to construct quantum circuits and algorithms in Qiskit.

- qc = QuantumCircuit(no. of qubits, no. of bits)
- qc.*quantumgate*(qubit) (e.g qc.x(), qc.h(), qc.rx(angle,))
- qc.cx(control qubit, target qubit)
- qc.measure(qubit, bit)
- qc.draw('mpl')
- backend = Aer.get_backend('qasm_simulator')
- results = execute(qc, backend, shots=).result()
- counts = results.get_counts()

Resources

Quantum Mechanics

Introduction to Quantum Mechanics - David J. Griffiths

Modern Quantum Mechanics - J. J. Sakurai

Quantum Information

Quantum Computation and Quantum Information - I. Chuang and M. Nielsen

Simulating Physics With Computers - Feynman(1982)

Universal Quantum Simulators - Lloyd(1996)

Qiskit

Qiskit textbook - `https://qiskit.org/learn`

Qiskit Youtube Channel - `https://www.youtube.com/c/qiskit`

Qiskit Slack - `https://join.slack.com/t/qiskit/shared_invite/zt-1dancl0jq-iR3zqEmEQa7pRsMN_Bmz1g`

Qiskit Github - `https://github.com/Qiskit`