An Introduction to Quantum Mechanics for Quantum Computing

Practical Quantum Computing using Qiskit and IBMQ

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Outline

What is the use of Quantum Mechanics?

- Quantum Mechanics (also referred to as Quantum Physics or Quantum theory) is a physical framework that was originally developed to explain atomic and subatomic and related phenomena. It was formally developed almost a hundred years ago and was very successful in its initial objective.
- In addition to the aforementioned phenomena, quantum mechanics was successful in explaining the following phenomena:
  - Electrical Conductivity (metals, insulators and semiconductors)
  - Magnetism
  - The structure of stars (Chandrashekhar's mass limit)
  - Nuclear radiation and related phenomena[1]
  - Laser (proposed theoretically and then constructed)
  - Antimatter (first predicted theoretically and then observed)
- In addition to the above quantum physics is now accepted as an essential ingredient for describing the physical reality of this universe.

[1] Some phenomena were predicted before observation.

Of Springs and Masses: the classical approach

- Consider the spring and mass system shown below. For simplicity, gravity is not being considered and the spring is taken to be massless.

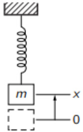

Figure 1: The Spring-Mass system, [Source: The Feynman Lectures on Physics, https://www.feynmanlectures.caltech.edu]

- The complete behaviour of this system can be described using the following quantity:

$$H(p, x) = \frac{p^2}{2m} + \frac{1}{2}kx^2 \tag{1}$$

where x is the displacement of the mass from the mean position "0", k is the spring constant and $p = mv = m\frac{\mathrm{d}x}{\mathrm{d}t}$, is the momentum of the mass.

Hamilton's way

- The first part of $H(p, x)$ defined in (1) is called the kinetic energy of the mass and the second part is referred to as the potential energy.
- The quantity $H(p, x)$ is therefore the total energy of the spring-mass system. It is possible to use this quantity and define the values x and p for all time if their values is known at only one point in time.
- This approach was introduced in the 1830's by the Irish mathematician, William Rowan Hamilton. This approach is known as Hamiltonian mechanics.
- The quantity $H(p, x)$ is formally referred to as the "Hamiltonian" of the spring-mass system. x is referred to as a coordinate and p is known as the momentum conjugate to x.
- The value of (x, p) at any point of time specifies the state of the system
- The Hamiltonian approach to solving problems can be generalized and used for studying such as electrical circuits, heat engines and even the stock market!

The Interference of Waves

- It is a known fact that waves of water interfere with each other. Light was also shown to possess this same property by Thomas Young in 1801 through his double-slit experiment.

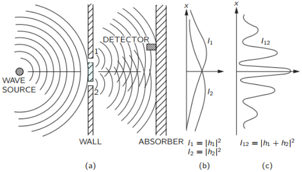

Figure 2: The interference of waves, [Source: The Feynman Lectures on Physics, https://www.feynmanlectures.caltech.edu]

- the resultant intensity at the absorber is equal to the square sum of the amplitudes of the waves arriving from both the slits at the point on the absorber.
- As shown is the above figure, as the detector is moved along the the absorber, an interference pattern is observed.

Playing with Bullets

- Particles unlike waves do not show any interference behaviour. Young's experiment when performed with particles (bullets from a gun) shows the following result.

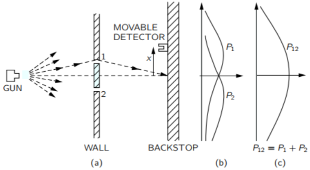

Figure 3: The absence of interference with particle, [Source: The Feynman Lectures on Physics, `https://www.feynmanlectures.caltech.edu`]

- The probability of a bullet hitting a point on the backstop (absorber) is equal to the sum of the probabilities of the bullet hitting the point after having passed through either one of the slits.
- This was one of the chief distinguishing factors between waves and particles.

Particle Interference?

- In 1927, Davison and Germer showed that electrons can show interference behaviour too.

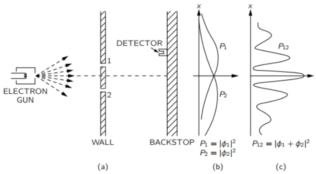

Figure 4: The interference of electrons, [Source: The Feynman Lectures on Physics, `https://www.feynmanlectures.caltech.edu`]

- This would imply that electrons, which were understood to be particle up until that point had wave-like properties too.
- This led to the concept of Wave-Particle duality and it was accepted that all particles have wave nature and vice versa.
- The waves associated with particles like electrons were referred to as matter waves as opposed to conventional waves that carried energy through a medium (or vacuum).

Observing Matter Waves

- Any attempt to observe the matter waves of electrons seemed to destroy the interference patterns implying that the matter waves themselves were being destroyed.

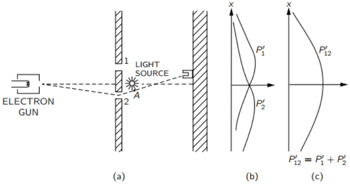

Figure 5: The interference of electrons, [Source: The Feynman Lectures on Physics, `https://www.feynmanlectures.caltech.edu`]

- This behaviour of matter waves was a very curious one and it was impossible to describe it using any previously available classical theory.
- Quantum Mechanics allowed for an interpretation of this phenomena.

The Quantum picture

- Classically, waves interfere due to the fact that the same wave passed through both the slits and interferes at the absorber.
- Similarly, the same matter wave passes through both the slits in the case of electrons and interfere at the absorber.
- This means that the same electron is travelling through both the slits simultaneously and this leads to the interference pattern.
- The probability of an electron reaching a point on the screen was the square of the sum of the amplitude of the waves from the individual slits.
- Any attempt to observe this simultaneous passage of electrons actually destroys the matter wave and the electron passes through only one of the slits, like the bullets.
- The matter wave is thus considered to have collapsed.

Observables and states

- In case of the classical spring-mass system shown in figure [1] it is possible to measure the values of x and p at any time. The state is said to be deterministically known.
- As seen before, preforming measurements on a quantum particle seems to be destroy the matter wave associated with it.
- A different approach was therefore required to represent the state of quantum particles.
- In quantum mechanics, quantities such as x and p that can be measured in a classical situation are referred to as observables and are represented by operators.
- Operators corresponding to observables are denoted by adding a hat ($\hat{}$) to the variable.
- The position (coordinate) operator is therefore represented as $\hat{x}$ and the momentum operator is given by $\hat{p}$

States and Observable values

- The state of the quantum particle is represented by a vector $|\psi\rangle$ in a *Hilbert space*, and the value of the observable $\hat{x}$ can be mathematically calculated as

$$\hat{x}\,|\psi\rangle = x\,|\psi\rangle$$

  In mathematics this expression is referred to as an eigenvalue expression.
- Therefore an operator of this form can be used to represent the position of the electron in the interference experiment shown in figure [4].
- However as seen before, the electron passes through both slits simultaneously, this means the above equation will not have a unique value.
- In such cases, one can no longer meaningfully talk about the precise value of x but only the average (expectation) value of the observable that is given by:

$$\langle x\rangle = \langle\psi|\hat{x}|\psi\rangle$$

Hermitian operators and the Hamiltonian

- The expectation values of the observable has to be a real value, this condition implies that the operator corresponding to an observable is self-adjoint or Hermitian. An operator $\hat{A}$ is hermitian if:

$$\hat{A} = \hat{A}^{\dagger}$$

- The Hamiltonian for a classical system sometimes was its energy and is therefore a measurable quantity. Therefore, it is possible to define is a quantum operator also called the Hamiltonian ($\hat{H}$).
- The quantum Hamiltonian can be used to specify the state of a quantum particle for all time provided the state is known at one instant of time.
- It is to be noted that even if the state is precisely known, the value of an observable may still not have a precise value.
- Mathematically, the fact that an observable can simultaneously have different values is represented by linear combinations of the quantum state.

Linear superposition

- Let $|x_1\rangle$ and $|x_2\rangle$ represent that state of the electron passing through slits 1 and 2 in figure [4]. The state of the electron passing through the two slits is given by.

$$|\psi\rangle = a\,|x_1\rangle + b\,|x_2\rangle$$

  The superposition coefficients are referred to as the amplitudes and are in general complex numbers.

- This state vector needs to be *normalized* for meaningfully obtaining expectation values.
- The square of the absolute value of the amplitude gives the probability of the electron to be seen passing through each slit in an experiment similar to figure [5].
- Therefore a state where the probability of observing the electron at each slit is equal is given by:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\,|x_1\rangle + \frac{1}{\sqrt{2}}\,|x_2\rangle$$

Hamilton's way: The Quantum version

- As mentioned before, the Hamiltonian can be used to specify the state of a particle/system at any point in time.
- There are many ways of representing this property of $\hat{H}$, the most famous version is the Schrödinger equation.

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi\rangle = \hat{H} |\psi\rangle \tag{2}$$

- This equation is exactly equivalent to the wave equation of the associated matter wave. Therefore the above equation is also referred to as Schrödinger wave equation.
- The matter wave is now mathematically represented by the wave function which is case of one dimensional single particle systems can be defined as $\psi(x) \equiv \langle x|\psi\rangle$

Unitary operators

- Solving the Schrödinger equation will show that the time evolution of the state $|\psi\rangle$ is also given by an operator

$$|\psi(t)\rangle = \hat{U}(t; t_0)\,|\psi(t_0)\rangle \tag{3}$$

  here, t_0 is usually taken as the initial instant of time.
- This operator is a unitary operator:

$$\hat{U}^\dagger \hat{U} = I$$

  where I is the identity operator.
- While the Hermitian operators corresponding to observables were mathematical representation of physical quantities, the unitary operators corresponding to time evolution denote a physical transformation of the state.
- Any change in the state of a quantum system is given by a unitary transformation. This includes quantum gates too.

Quantum reality: The Measurement Postulate

- Any state that is a superposition of the basis states when measured with respect to that basis will result in an outcome that is one of the basis states.
- The occurrence of the each of the basis states is totally random and is dependent on the amplitudes. Therefore for a normalized state given by:

$$|\psi\rangle = a|x_1\rangle + b|x_2\rangle$$

- Therefore, a position measurement will give the outcomes x_1 with probability $|a|^2$ and x_2 with probability $|b|^2$ and:

$$|a|^2 + |b|^2 = 1$$

the expectation value of the position measurement will be given by $\langle x\rangle = |a|^2 x_1 + |b|^2 x_2$

Measurement errors in Quantum Mechanics

- If a particle is in a quantum state $|\psi\rangle = \sum_i a_i |x_i\rangle$, normalization condition dictates that,

$$\sum_i |a_i|^2 = 1$$

this state describes that the particle if its position is measured, maybe found in any one of the position coordinates x_i with probability $|a_i|^2$.

- The outcome of a position measurement may be treated as a random variable. It is therefore possible to define the variance of this distribution as

$$\Delta x^2 \equiv \left\langle x^2 \right\rangle - \langle x \rangle^2 = \sum_i |a_i|^2 {x_i}^2 - \left(\sum_i |a_i|^2 x_i \right)^2$$

the the standard deviation, which is the square root of the above quantity is known as the error or uncertainty in the position of the particle Δx.

The Uncertainty Principle

- The uncertainty in the momentum of a particle is also defined as Δp.
- Heisenberg established that in quantum mechanics, the product of the uncertainties in position and momentum are related to each other as,

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

  the above relation is known as the Uncertainty principle and is the a direct consequence of the quantum behaviour of particles.
- Since the uncertainties are treated as measurement errors in a quantity, the principle is said to imply that the values of position and momentum of the a particle cannot be simultaneously measured with precision (zero error).

The physicality of $|x\rangle$ and $|p\rangle$

- As per the previous definitions, a particle in the state $|x\rangle$ implies that the particle is at position x. The uncertainty in position of this particle 0.
- This implies that for such a particle, the uncertainty in momentum Δp is infinitely large. This is a physically meaningless outcome for a measurement.
- Due to this consequence of the uncertainty principle, a quantum particle is never in a precisely defined quantum state, either $|x\rangle$ or $|p\rangle$.
- The inherent variations in the state of a quantum system is referred to as quantum fluctuation and is a fundamental trait of all quantum systems.
- These fluctuations are the source of randomness in quantum mechanics.
- Despite being physically unrealistic, the position states nonetheless form a basis that can describe any physical system.