THE EVOLUTION OF QUANTUM MECHANICS: HEISENBERG, SCHRODINGER & DIRAC

We all are familiar with the contribution of Neils Bohr in quantum theory of atomic structure (or see https://arxiv.org/ftp/arxiv/papers/1603/1603.00353.pdf). At the age of 20, working for Ph.D, Heisenberg rose to make objection of Bohr's lectures to which Bohr replied hesitantly. They went for a walk through the Hainberg mountain, and during the conversation Heisenberg found that one of the founders of quantum mechanics is deeply worried about its difficulties. Bohr had immense insight. He could sense a relationship intuitively rather than to derive it formally.

Heisenberg hated the imaginary electron orbits of Bohr. They could never be observed. What good it is to speak about invisible electron paths inside invisible atoms?

HEISENBERG PICTURE

His picture was not to treat atom as a solar system but like a simple virtual oscillator which could produce all frequencies. In classical theory P times x is equal to x times P. But in quantum theory this is not the case. He guessed $(xP-Px) \neq 0$ but is equal to $i\hbar$. That night at 3' o clock he was able to show that the energy states were quantised and time independent ie; they were stationary as in Bohr's theory. In the morning he sent the results to Pauli, whom he was friends with. Pauli's reaction was favourable. Pauli submitted the paper before Max Born and Born identified these strange multiplication with matrix calculus. Thus matrix mechanics was "Born". Working with talented student Pascal Jordan-an expert in matrix methods- Born transposed Heisenberg theory into systematic matrix language. This theory came with no visual aids- purely mathematical, difficult to use and impossible to visualise. It simply gave right answers. Here the energy levels were represented by numbers.

SCHRODINGER PICTURE

Heisenberg picture was not well received because it cannot be visualised. Schrodinger despised Heisenberg's theory. He set out to develop another version starting from de Broglie's concept of matter waves (https://qudev.phys.ethz.ch/phys4/PHYS4_lecture02v1_2page.pdf). He thought that his approach is more acceptable and marks a return to continuous world of classical mechanics.

Schrodinger was right at first part but wrong at the second part. Schrodinger's equation was appeared in January 1926. He was considering the wave equation based on Fourier technique called the method of eigen values. 'Eigen' in German means certain. The trick was to find the correct functions and the amplitudes of each that added together by superposition to get the desired solution. In the solution of the Schrodinger equation the wave function of the system was replaced with an infinite series, consisting of wave functions of individual states, which are natural harmonics of each other. What Schrodinger did was to reduce the problem of energy states in an atom to the problem of finding the natural overtones of its vibrating system using Fourier analysis.

Schrodinger's remarkable discovery was that the replacement waves described the individual states of the quantum system and their amplitudes gave relative importance of that particular state to the whole system. The integers called quantum numbers by Bohr, Sommerfield and Heisenberg were now related in a natural way to the number of nodes in a vibrating system.

Schrodinger's equation was successful in explaining spectra, deriving Balmer formula, Zeeman and Stark effects. Schrodinger was able to observe that integers (no. of nodes) derived from 3 dimensional wave equation precisely correspond to three quantum numbers n, k and m respectively from old quantum theory.

Frequencies of bright line spectrum may be visualised as beats between the vibration frequencies of two quantum states (without the need of postulate of quantum jumps). Quantum transition results in energy exchanges continuously from one vibration pattern to another rather than undesirable electron jumps. He was proposing classical theory of matter waves that have same relationships to mechanics as Maxwell's electromagnetic theory had to optics.

Schrodinger began to doubt the existence of particles. The image point or particle of a mechanical system can be represented by a wave group with small dimension in every direction. This is called a wave packet. The image point or particle moves with the velocity of the wave packet. This behaves like a particle but it is really a superposition of thousands of waves as de Broglie described. Schrodinger wanted to describe all particles as the superposition of waves.

But classical physicist, Henrik Lorentz brought him to his senses by brutal criticism of his physical interpretation:

1. Wave packets will spread with time and the idea of representing particles completely in terms of the superposition of waves is invalid.
2. Beat frequencies will not produce spectral lines.
3. New discoveries cannot fit at all into a classical framework.

It was soon shown that Lorentz was right. From the summer of 1926, Schrodinger's thought of importance of wave motion as the source of all physical reality began to waver. Then what is the relationship between particle's wave function and particle itself?

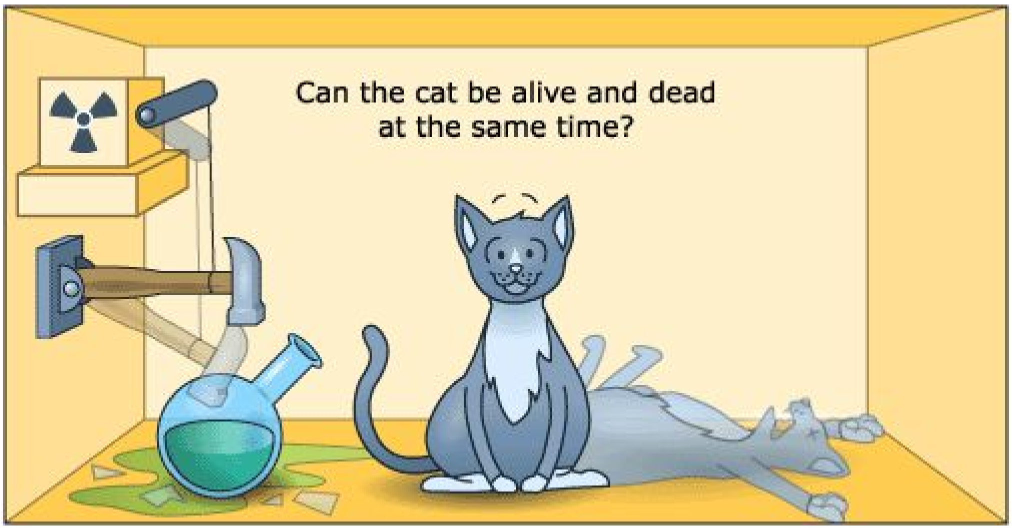
Later, Schrodinger found that a relationship exists between Heisenberg's model and his model. One was based on a clear conceptual wave model of atomic structure and the other claimed that such a model is meaningless. But both give same results!!

In July 1926, Schrodinger gave a lecture in Munich where Heisenberg shot a question, " can you explain Photoelectric effect and Blackbody radiation, two quantised processes based on your model?" Heisenberg was right. Schrodinger decided to represent ψ as a 'shadow' wave that somehow indicated the position of electron. Then he changed it as 'density of electron charge'. Truthfully he was confused.

In 1926, Max Born considered ψ as quantum mechanical probability. It is the probability amplitude for an electron in state n to scatter into a direction m ie; it is in its own intensity wave. One month later Max Born stated that existence of the state is given by square of normalized amplitude of individual wave function ie; the probability that a certain quantum state exists. In atomic theory all we get are probabilities. Born had found a way to reconcile particles and waves by introducing the concept of probability. The wave ψ determines the likelihood that the electron will be in a particular position. Unlike electromagnetic field, ψ has no physical reality.

About 10 years after the notion of probability, superposition of quantum states was generally accepted. Schrodinger was distressed that his own equation was being misused, created a thought experiment to establish the absurdity of this concept.

Live cat placed in a box with radioactive source and a G.M counter, a hammer and a poisonous fume container. Our act of observation collapses the superposition of two wave functions to a single one making the cat definitely dead or alive.



In 1925, Heisenberg gave a talk at Cambridge where he handed over a version of his unpublished work to Ralph Fowler, which he handed over to a young graduate student PAM Dirac. Dirac realised that the non-commuting property is the essence of new approach. Within two months he sent a 30 page paper to Heisenberg in which he accepted his ideas.

After Dirac's work the dual nature of light as a wave and as a particle has been free of paradox for those who can follow the mathematics.

Schrodinger was not able to explain successfully the magnetic property of electron, the spin. He was also not able to incorporate Einstein's relativity theory into his wave equation. Dirac did it for him in breath taking style, using mainly aesthetic arguments. He put forward the idea of antimatter. Positron- anti particle of electron was discovered by Carl Anderson in 1932. In 1933 Nobel prize was given to Dirac together with Schrodinger. His work was carried forward by Richard Feynman, Freeman Vyson, Julian Schwinger ..(QED). It describes the interaction of light and matter with remarkable accuracy.

KEY CONCEPTS IN QUANTUM MECHANICS:

The Copenhagen Interpretation

The description of a state of an atomic system before measurement is undefined having only potentiality of certain values with certain probabilities. In 1927 at Italy Neil Bohr gave his lecture on complementarity- Einstein could not come to Fascist Italy.(*Einstein was against the concept of uncertainty*)

Suppose one set of experimental evidence can only be interpreted on the basis of wave properties and other by particle properties. These sets are not contradictory. They are obtained under different experimental conditions, cannot be combined in a single picture and is regarded as complementary.

Einstein wanted a theory to explain the thing itself and not the probability of its occurrence. Three years later at Solvay conference Einstein's thought problem of **box of light** was announced. He described a box full of light and energy and time emitted via photon can be precisely determined.

STERN – GERLACH EXPERIMENT

You can watch the experiment (https://vimeo.com/204167284)

OR

Stern –Gerlach simulation: A simulation of the Stern –Gerlach experiment from the PHET group at the University of Colorado (https://phet.colorado.edu/sims/stern-gerlach/stern-gerlach_en.html)

Through the Stern –Gerlach experiment we have learned several key concepts about quantum mechanics

- Quantum mechanics is probabilistic. We cannot predict the results of experiments precisely. We can predict only the probability that a certain result is obtained in a measurement.
- Spin measurements are quantized. The possible results of a spin component measurement are quantized. Only these discrete values are measured.
- Quantum measurements disturb the system. Measuring one physical observable can "destroy" information about other observables.

POSTULATES

The postulates of quantum mechanics dictate how to treat a quantum mechanical system mathematically and how to interpret the mathematics to learn about the physical system in question. These postulates cannot be proven, but they have been successfully tested by many experiments, and so we accept them as an accurate way to describe quantum mechanical systems.

POSTULATES OF QUANTUM MECHANICS

1. The state of a quantum mechanical system, including all the information you can know about it, is represented by a normalized ket $|\psi\rangle$. These kets are abstract entities that obey many of the rules you know about ordinary spatial vectors. Hence they are called **quantum state vectors**. These vectors must employ complex numbers in order to properly describe quantum mechanical systems. Quantum state vectors are part of a vector space called **Hilbert space**. The dimensionality of the Hilbert space is determined by the physics of the system at hand. Can you guess the dimensions of the vector space in Stern-Gerlach experiment? The analog to the complex conjugated vector of classical physics is called a **bra** in the dirac notation of quantum mechanics, written as $\langle\psi|$.

If a general ket $|\psi\rangle = a|+\rangle + b|-\rangle$ then bra $\langle\psi| = a^*\langle+| + b^*\langle-|$

$\langle+|+\rangle = 1$ $\quad \langle-|-\rangle = 1$ normalization

$\langle+|-\rangle = 0$ $\quad \langle-|+\rangle = 0$ orthogonality

$|\psi\rangle = a|+\rangle + b|-\rangle$ completeness

2. A physical observable is represented mathematically by an operator A that acts on kets

3. The only possible result of a measurement of an observable is one of the eigenvalues a_n of the corresponding operator A.
4. The probability of obtaining the eigenvalue a_n in a measurement of the observable A on the system in the state $|\psi>$ is

$$\mathbf{P}(a_n) = |< a_n|\psi>|^2 \ ,$$

where $|a_n>$ is the normalized eigenvector of A corresponding to the eigen value a_n

5. After a measurement of A that yields the result a_n, the quantum system is in a new state that is the normalized projection of the original system ket onto the ket corresponding to the result of the measurement:

$$|\psi'> \ = \frac{P_n|\psi>}{\sqrt{<\psi|P_n|\psi>}}$$

6. The time evolution of a quantum system is determined by the Hamiltonian or total energy operator H(t) through the Schrodinger equation

$$i\hbar \frac{d}{dt}|\psi(t)> \ = H(t)|\psi(t)>$$

OBSERVABLES AND OPERATORS

OBSERVABLES AND THEIR QUANTUM MECHANICAL OPERATORS

Observable	Operator	Symbol for Operator
Momentum $\mathbf{p} = m\dot{\mathbf{r}}$	$-i\hbar\frac{\partial}{\partial x}$	$\hat{p}_x$
Kinetic energy $T = \frac{1}{2}m\dot{\mathbf{r}}^2 = \mathbf{p}\cdot\mathbf{p}/2m$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$	$\hat{E}_{kinetic} = \frac{1}{2m}(\hat{p}_x)\hat{p}_x$
Position	x	$\hat{x}$
Potential energy	$V(x)$	$\hat{E}_{potential}$
Total energy $H(\mathbf{r},\mathbf{p}) = T(\mathbf{p}) + V(\mathbf{r})$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$	$\hat{H}$
Angular momentum	$-i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$	$\hat{l}_x$
	$-i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$	$\hat{l}_y$
	$-i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$	$\hat{l}_z$

For detailed information Postulates and operators read...(http://web.mit.edu/8.05/handouts/jaffe1.pdf)