ELEC4705 – Fall 2009

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LECTURE 3
Fundamentals of Quantum Theory

Contents

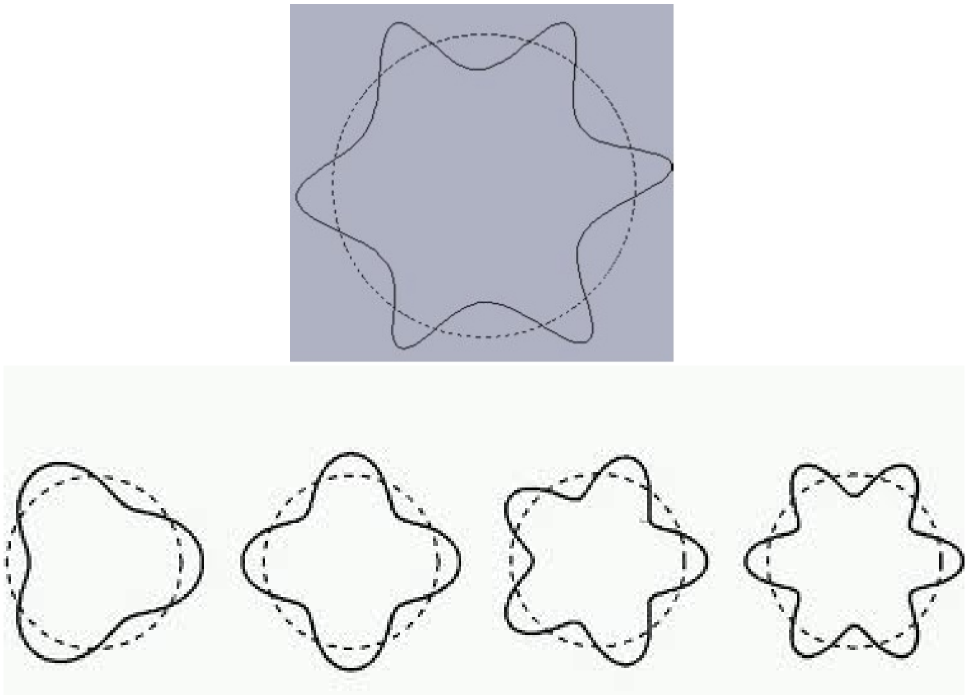

Figure 1. Electron model

3.1. History of Quantum/Wave Mechanics

In 1924 De Broglie proposed that wave-particle duality did not belong to light only and matter (particles) could also exhibit wave-particle duality. The famous de Broglie's wavelength relation is as below:

$$\lambda = h/p = h/mv \tag{3.1}$$

where

- h is Planck's constant
- p is the momentum
- m is the mass
- v is the velocity of the particle

In his work De Broglie was inspired by Einstein's theory in photoelectric effect i.e. $E = hf$. He described an electron as a standing wave around the circumference of an atomic orbit see figure 1 such that,

$$n\lambda = 2\pi r \tag{3.2}$$

Also at that time, Bohr was working on a planetary model for an atom in which electron-orbits could only have certain discrete quantized energies.

Bohr's second postulate states:

> *Instead of the infinity of orbits which would be possible in classical mechanics, it is only possible for an electron to move in an orbit for which its orbital angular momentum is and integral multiple of $\hbar$.*

from which we obtain:

$$m\,v\,r = n\hbar \tag{3.3}$$

However, using an assumption of electronic standing waves around a nucleus and wavelength relationship we have by combining 3.2 with 3.1:

$$2\pi r = n\frac{h}{mv} \tag{3.4}$$

$$mvr = n\frac{h}{2\pi} \tag{3.5}$$

which is also the Bohr postulate. This shows that the wave interpretation of a particle supports Bohr's theory which had experimental verification.

Example 1. Calculate the de Broglie wavelength of an electron which has a kinetic energy of 4 eV.

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} = 6.13A$$

Note: The wavelength has the dimensions of interatomic spacing.

Example 2. Whats the de Broglie wavelength of a tennis ball having a mass of $50g$ and traveling with a velocity of $200\,km/h$?

With the same calculations as example 1 we have:

$$p = mv = 0.05 \times \frac{200000}{60} = 166.67$$

$$\lambda = \frac{h}{p} = \frac{6.625 \times 10^{-34}}{166.67} = 3.97 \times 10^{-26}A$$

Does this explain why tennis balls don't diffract?

3.2. Wave-like Behavior of Electrons

If particles have wavelengths we should expect that they should have wave-like behavior. Diffraction is an easily observed and entirely wave-like effect. Consider Figure 2, in left picture we see a wave impinging on a screen with a small opening. This wave is said to be diffracted, and diffraction is observed when a wave is distorted by an obstacle which has dimensions comparable to the wavelength of the wave. The effect is due to interference of the waves.

In right hand side picture in figure 2 we see a stream of electrons (assuming electrons as particles) seeing a small opening. The wave like behavior of electrons was experimentally confirmed by Davisson and Germer. The experiment determined that the reflected electrons had the same diffraction patterns that Bragg's law predicts for X-Rays see figure 3. Bragg's law allows us to calculate the wavelength and therefore the energy of the incident x-ray beams (EM waves). Also it was observed that the same diffraction pattern was produced by electrons with the same de Broglie wavelength $\lambda = h/p$. So we have

$$n\lambda = 2d\sin\theta = n\frac{h}{p} \tag{3.6}$$

which holds for other particles including photons, neutral atoms, protons, positive ions, etc.

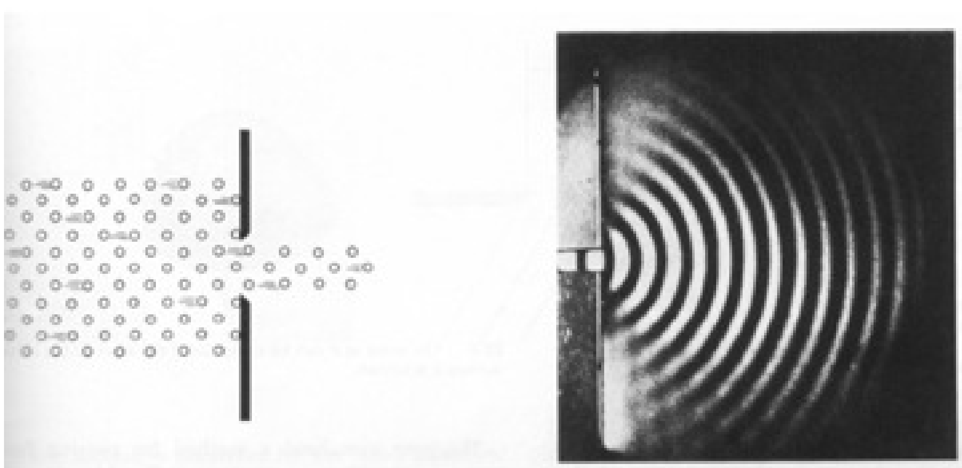

Figure 2. Wave or particle like behavior of electrons diffraction through a slit

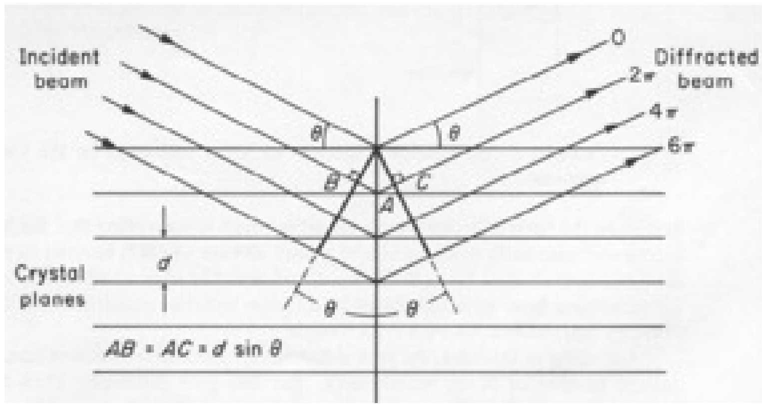

Figure 3. Wave like behavior of electrons. Thin film diffraction.

3.3. Quantum Mechanics - the wave function Ψ

Quantum mechanics is based on Planck's quantum theory $E = \hbar\omega$ and De Broglie's wave-particle duality. It is a revision of the "laws of mechanics" designed to extend the subject into the realm of atomic and nuclear phenomena.

A big question was "what is waving?". For water waves the water is moving (waving). We have pressure waves (sound) where there is pressure wave (atoms moving). What is the wavelength "**of**" in QM? Well the function that waves is called the wavefunction and is denoted Ψ – what it "is" is difficult.

Born showed that the wave amplitude is related to the **probability** of finding a particle in a given region of space or state, this was identified as the concept behind the wave function Ψ. The wavefunction of the system, Ψ gives us all the information about the system such as momentum and energy of the particles as well as probability of finding the particles. The latter which is the most useful information is given by $\Psi\,\Psi^*\,dxdydz$ for a particle in space between $(x\,,\,x+dx)$ and $(y\,,\,y+dy)$ and $(z\,,\,z+dz)$.

Since the probability of finding a particle in the entire domain is unity, the wavefunction must satisfy the normalization condition as below

$$\int_{-\infty}^{+\infty} \Psi\,\Psi^*\;dxdydz \;=\; 1 \tag{3.7}$$

This makes it clear that in quantum mechanics probability statements are obtained telling us what the system might do and with what chance.

Another important concept in QM which arises from the wavefunction is Heisenberg's Uncertainty Principle which states *it is impossible* *to precisely measure the position and momentum as well as the energy and time of a particle at the same time.*

QM is therefore not deterministic. Whereas in classical mechanics the location of a particle can be determined exactly and its subsequent motion precisely predicted.

3.3.1. Schrodinger equation (SCE

An equation was need to solve for Ψ and Schrodinger's equation is the fundamental equation of quantum mechanics, which is equivalent to Newton's laws of motion in classical mechanics. It predicts the wave behavior of matter and governs the microscopic world. The solution of the Schrodinger equation is the wave function Ψ. This equation is a hypothesis and must be confirmed my experimental measurements.

Schrodinger's equation has two basic forms, time-dependent and time-independent Schrodinger equation. The solution of the time-dependent form demonstrates how the system changes with time, and the time-independent Schrodinger equation gives us the energy eigenstates (values) of the system for individual wave states. We will use the time independent equation for all of our work.

Although the SCE is a hypothesis it can be postulated by using some physical insight.

As the electron exhibits wave-like behaviour we would expect a form of the wave equation for the SCE. According to Bohr's theory of atomic model, an electron wave "orbiting" the atom is in a standing wave or "stationary state" with an energy E has the frequency $f = E/h$.

In this case the wavefunction $\Phi(r,t)$ can be written as a standard wave solution;

$$\Psi(r,t) = \psi(r)\exp(-j\frac{E}{\hbar}t) = \psi(r)\exp(-jwt) \tag{3.8}$$

where $r = (x,y,z)$. In this equation the complex exponential $\exp(-jwt)$ represents an oscillatory sinusoidal function and can often be a simple sin or cosine.

Schrodinger used classical ideas of energy conservation to obtain a likely SCE. From classical mechanics a function known as the Hamiltonian had been derived which represented the total energy of a system. For QM he postulated that "*the quantum Hamiltonian H is the observable corresponding to the total energy of the system.*" The Hamiltonian H is a function that relates the energy of a system to its coordinates and momentum. If r is the position vector and p is the momentum vector of the particle then the Hamiltonian H is given by:

$$E = H(r,p) = P^2/2m + V(r) \tag{3.9}$$

where

- P is the momentum operator given as for QM as $P = -j\hbar\nabla$
- m is the mass of the particle
- V is the potential energy.

Considering the above notes and applying H on the wavefunction we well have:

$$E\,\psi = (\frac{1}{2m}(-j\hbar\nabla)^2 + V(r))\psi$$

$$\frac{-\hbar^2}{2m}\nabla^2\psi(r) + V(r)\Psi(r) = E\,\psi(r) \tag{3.10}$$

which is the time-independent Schrodinger equation. The first term can be associated with the kinetic energy and the second with the potential energy.

3.3.2. Solution of the Schrodinger equation for Free Space

In free space we have no forces and the potential energy can be defined as $V(r) = 0$. For simplicity we assume the 1D case.

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\,\psi(x) \Longrightarrow \psi(x) = Ce^{jkx} \tag{3.11}$$

$$k = \frac{\sqrt{2mE}}{\hbar} \Longrightarrow \Psi(x,t) = Ce^{jkx}e^{-jwt} = Ce^{j(kx-wt)} \tag{3.12}$$

which is the equation of a traveling wave.

Consider Figure 4, the phase velocity is the speed at which the profile moves and is defined as:

$$v_{ph} = \frac{\Delta x}{\Delta t} = \frac{\omega}{k} = \frac{E}{\hbar}.\frac{\hbar}{\sqrt{2mE}} = \sqrt{\frac{E}{2m}} \tag{3.13}$$

Which is the velocity of a particle with a kinetic energy of E. Makes some sense!

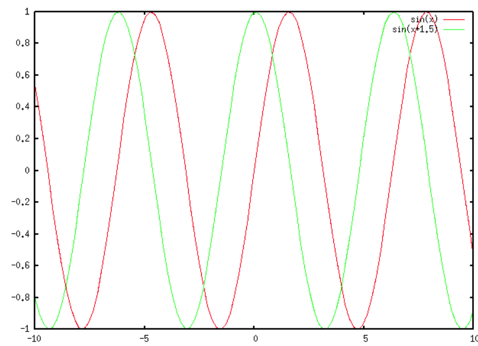

Figure 4. A wave moving through space plotted at two times. The phase velocity is how fast the wave moves from one point to the other.

3.3.3. 3D Plane Waves

Now for harmonic plane waves moving through a 3D space consider figure 6.

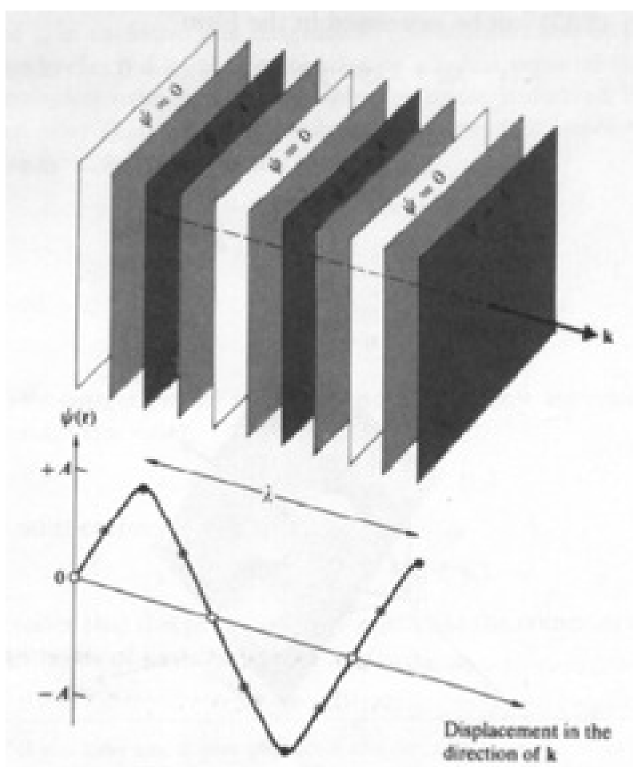

Figure 5. Plane waves moving in the direction $\vec{k}$.

Harmonic waves should repeat themselves in space after a displacement of λ in the direction of propagation ($\vec{K}$). If k is the magnitude of $\vec{K}$ and $\vec{K}/k$ is the unit vector parallel to it, then we will have:

$$\psi(r) = \psi(r + \frac{\lambda\vec{K}}{k}) \tag{3.14}$$

$$Ae^{j\vec{K}\cdot\vec{r}} = Ae^{j\vec{K}\cdot(\vec{r}+\frac{\lambda\vec{K}}{k})} = Ae^{j\vec{k}\cdot\vec{r}}e^{j\lambda k} \tag{3.15}$$

$$e^{j\lambda k} = 1 = e^{je\pi} \tag{3.16}$$

$$\lambda = \frac{2\pi}{k} \tag{3.17}$$

In 3D free particle case we will have the solution to the Schrodinger equation as

$$\psi(r) = Ce^{j\vec{K}\cdot\vec{r}} \tag{3.18}$$

where k is the wave vector such that

$$\mid k \mid = \frac{2\pi}{\lambda} \tag{3.19}$$

and we have a sinusoidal wave propagating in the direction prescribed by $\vec{K}$ with a wavelength given by the normal wave equation.

3.4. Interpretation of the Wavefunction*

The physical interpretation of the wavefunction has been problematic since the development of QM. The difficulties stem from:

(a) The interpretation of probabilistic nature of the results. The wavefunction only tells you the probability of what a system might do not what it does.
(b) The uncertainty relationship – the indeterminacy of reality.
(c) The apparent contradiction of macroscopic (our) reality and the QM description
(d) Entanglement – action at a distance.

3.4.1. Quantum Randomness

The SCE provides a solution for Ψ which is used to predict the probability of outcomes. For example an electron is scattered off an atom; it has a probability X of going to the right and Y to left. QM can calculate X and Y but does (and can not) say which it does. Very disturbing to classical physicists.

3.4.2. Measurements – "the line between QM and classical"

We can, however, watch an electron scatter using experimental measurements. What we see is an electron go either to the right or left. This seems to mean that wavefunction "collapses" to a probability of one and is in a particular state after a system is measured, however, QM has fundamentally no explanation for this phenomena. This is known as the measurement problem.

3.4.3. Uncertainty Relation

QM also shows that certain variables, for example position and momentum, are coupled in way that if you try to measure one you disturb the other and this leads to limit to our knowledge of system ie an uncertainty in position and momentum.

3.4.4. Entanglement

In a QM system of two objects if the objects interact their Ψ functions become coupled and inseparable. Quantum entanglement (non-local connection) is when the quantum states of the constituting objects are linked together so that one object can no longer be described without knowing the state of the other object – even if the individual objects are spatially separated. For example two electrons in close proximity can be coupled so one must be spin *up* and the other spin *down* (spin is a quality of an electron). If the two electrons are then separate and drift apart the net spin must still be zero. However, QM does not tell you which electron is *up* and which is *down* it can only calculate the probability of each electron being spin *up* or *down*. Fundamentally, each electron is both spin *up* and *down* at the same time (in a "mixed" state). When we measure one of the electron's spin and find *up* we now know that the other must be *down* as the net spin is zero. However, the electrons could be separated by light years of distance! By measuring one electron we forced the other to be the complementary spin – action at a distance. Not Good! Very strange. Einstein very unhappy.

3.4.5. Schrodinger's Cat

A thought experiment was developed in attempt to show the ludicrous nature of QM (by this time Einstein and Schrodinger were beginning to regret the whole idea).

Schrdinger wrote:

> *One can even set up quite ridiculous cases. A cat is penned up in a steel chamber, along with the following*

device (which must be secured against direct interference by the cat): in a Geiger counter, there is a tiny bit of radioactive substance, so small that perhaps in the course of the hour, one of the atoms decays, but also, with equal probability, perhaps none; if it happens, the counter tube discharges, and through a relay releases a hammer that shatters a small flask of hydrocyanic acid. If one has left this entire system to itself for an hour, one would say that the cat still lives if meanwhile no atom has decayed. The psi-function of the entire system would express this by having in it the living and dead cat (pardon the expression) mixed or smeared out in equal parts.

It is typical of these cases that an indeterminacy originally restricted to the atomic domain becomes transformed into macroscopic indeterminacy, which can then be resolved by direct observation. That prevents us from so naively accepting as valid a "blurred model" for representing reality. In itself, it would not embody anything unclear or contradictory. There is a difference between a shaky or out-of-focus photograph and a snapshot of clouds and fog banks.

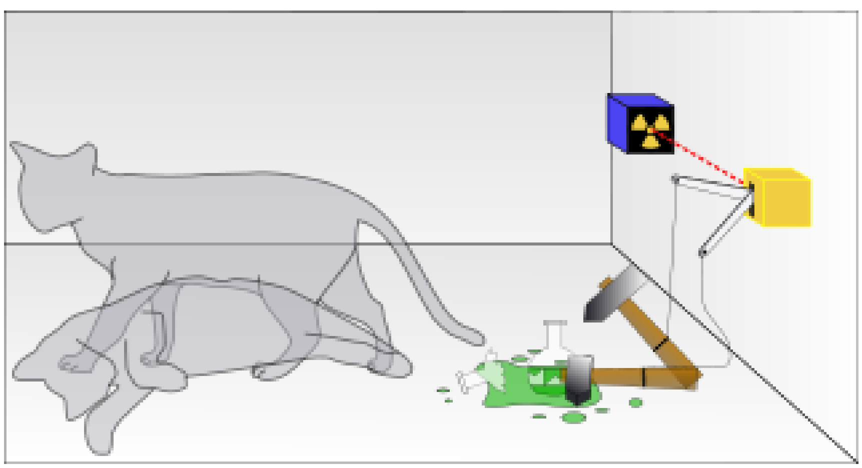

Figure 6. Schrodingers Cat experiment

3.4.6. Interpretations

There are various physical/philosophical interpretations of this sort of experiment and the meaning of the wavefunction:

Copenhagen – the classical and original one:
In the Copenhagen interpretation of quantum mechanics, a system stops being a superposition of states and becomes either one or the other when an observation takes place. This experiment makes apparent the fact that the nature of measurement, or observation, is not well-defined in this interpretation. Some interpret the experiment to mean that while the box is closed, the system simultaneously exists in a superposition of the states "decayed nucleus/dead cat" and "undecayed nucleus/living cat", and that only when the box is opened and an observation performed does the wave function collapse into one of the two states. More intuitively, some feel that the "observation" is taken when a particle from the nucleus hits the detector.

Problem defining observer and observing system – where to draw the line between macro and microscopic.

Many Worlds/Many minds – Collapse who needs it!:
In 1957, Hugh Everett formulated the many-worlds interpretation of quantum mechanics, which does not single out observation as a special process. In the many-worlds interpretation, both alive and dead states of the cat persist, but are independent of each other. In other words, when the box is opened, that part of the universe containing the observer and cat is split into two separate universes: one containing an observer looking at a box with a dead cat, and one containing an observer looking at a box with a live cat.

Since the dead and alive states are independent, there is no effective communication or interaction between them. When an observer opens the box, he becomes entangled with the cat, so "observer states" corresponding to the cat's being alive and dead are formed, and each can have no interaction with the other.

Another version has a splitting of the "mind of the observer" not the universe.

Consciousness causes collapse? – we are *SO* special:
Viewed by some as mysticism, Wheeler's Participatory Anthropic Principle is the speculative theory that observation by a conscious observer is responsible for the wavefunction collapse. It is an attempt to solve a similar experiment involving two observers by simply stating that collapse occurs at the first "conscious" observer. What is Is consciousness? Is the cat an

observer? Is a bacteria? What about the universe before life? God as an observer?

Many forms of these and others:

- Ensemble interpretation, or statistical interpretation
- The Copenhagen interpretation
- Participatory Anthropic Principle (PAP)
- Consistent histories
- Objective collapse theories
- Many worlds
- Many minds
- Stochastic mechanics
- The decoherence approach
- Quantum logic
- The Bohm interpretation
- Transactional interpretation
- Relational quantum mechanics
- Modal interpretations of quantum theory
- Incomplete measurements

3.4.7. Does it matter?

For engineers does it matter? Not really just use it. Calculate and move on. Nothing to see here. But it is really, **really** interesting.

*Partially from: http://en.wikipedia.org/wiki/Schrodingers_cat