UNDERSTANDING WAVE FUNCTIONS WITH REFERENCE TO QUANTUM MECHANICS

Aneesh Kumar Katkam (Grade XII)

1 Introduction

It is very important for us to grasp an understanding of particles, which play a huge role in the heart of quantum mechanics: the science of subatomic phenomena that defies common sense. Dealing with the behavior of matter and light on the atomic scale are often peculiar and the quantum theory are accordingly difficult to understand and believe. The quantum theory of gravity, still being assumed to use the Einstein's Theory of Relativity, exemplifies that there are still many opportunities to explore this regime. The fundamental aspect of classical physics is to determine relationships and create an outcome. The ideology of quantum physics, being the media to illustrate this statement, much deeply comes through the understanding of quantum fluctuations. On a cosmological scale, it is believed that quantum fluctuations play a crucial role in the formation of large-scale structures such as galaxies and cluster of galaxies. On the other hand, on the subatomic scale, quantum fluctuations can be observed in various phenomena such as vacuum polarization, Lamb Shift, and Casimir effect. The basis of understanding these differences comes when understanding the analogy of quantum mechanics, which is the main focus of this research paper.

2 Background information

2.1 Phillip Lenard's experiment

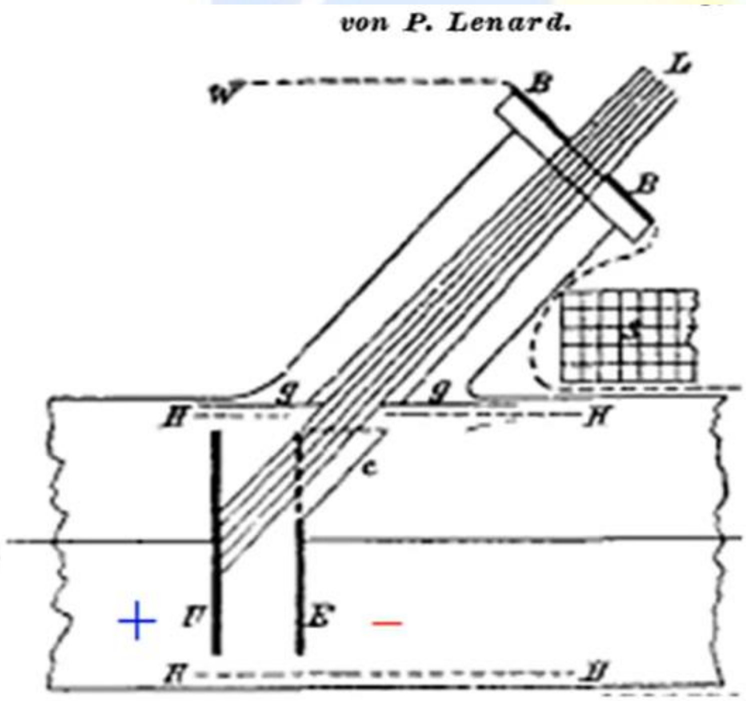

Figure 1: P. Lennard and Hertz Experiment

This experiment, also known as the photoelectric effect, was conducted in 1902 by Phillips Lenard with two metal plates connected via an electrical circuit. We observe from the diagram that light comes from an arbitrary source and illuminates the metal plate. The amount of light falling on the plate was initially believed to have provided the electrons with enough energy to overcome the potential difference between the plates which makes them move to the opposite plate. This eventually closes the circuit and results in measurable current. Hence, by adjusting the voltage across the plates, one can measure the energy of the emitted electrons.

If we analyze the older classical theory of light, which predicted that increasing the intensity of light should lead to more energetic photoelectrons, light of any frequency should be able to kick some electrons out of the metal plate.

However, from the experiment, Lenard observed the exact opposite. The resulting inferences of the photoelectric effect were as follows:

1) The energy of electrons did not depend on the intensity of light
2) No photoelectrons were produced if the frequency was smaller than a certain critical value.

2.2 Einstein's explanation of photons:

At the time of Phillips Lenard's research, we must take into note that Einstein was analyzing the properties of light at the time. In 1905, that is, three years after Lenard had published his paper, talking about his results, Einstein was able to resolve the mystery of the photoelectric effect. 1905 was, as we know, called the miracle year during the time because Einstein had published 4 outstanding papers, which make physics as it is today. One of the papers was called, "Concerning a Heuristic Point of View Toward the Emission and Transformation of Light." In this paper he introduced the notion of a photon which points to Lenard's pioneering paper.

He stated that the energy of a photon with wavelength, λ could be given as,

$$E = \frac{hc}{\lambda}$$

Where h is the Plank's constant which results to $6.626 \times 10^{-34} Js^{-1}$ and c is the speed of light which results to $3 \times 10^{8} ms^{-1}$.

This explanation, however, does not complete our blueprint on how we can pin point an exact inference from the photoelectric effect. More details could be seen from Davisson's and Germer's experiment verified by De Broglie in 1925.

2.3 Davisson and Germer Experiment:

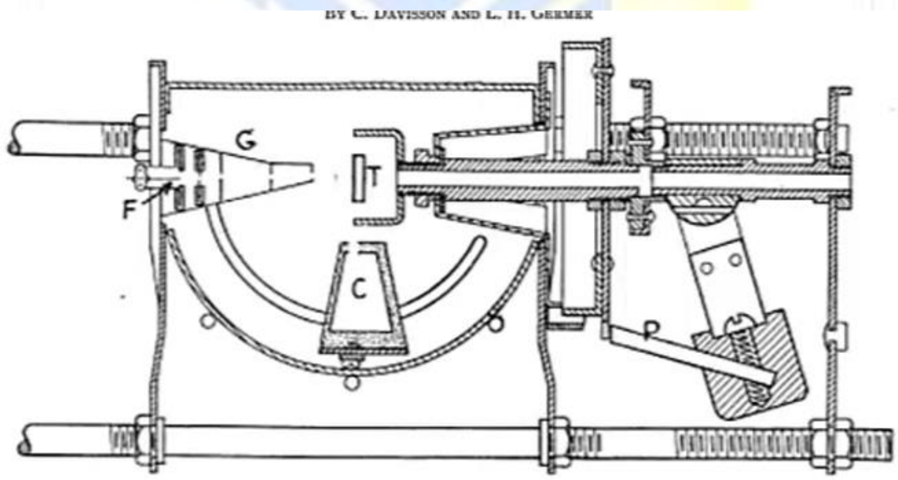

Figure 2: Apparatus used in Davisson and Germer Experiment

If we observe the diagram, G represents an 'electron gun' which shoots electrons onto a nickel target, T. Another part of the apparatus is a detector, C, which can detect the motion of electrons and determine its angular distribution. However, what this diagram does not show is the full history of the event. There was apparently some liquid air sitting nearby, which exploded from the heat produced by the nickel target. This resulted in the damaging of the apparatus, heavily oxidizing the nickel target. They heated the nickel target once again and conducted a second trial and noticeably observed something different from the first. The visualized clear indicators (beams) of electrons scattered at specific angles. These angles were strongly dependent on the energy coming from the incoming electrons.

When De Broglie verified this experiment, he indicated that there's some evidence that electrons (sometimes) behave as waves. This was proved by this equation:

$$\lambda = \frac{h}{mv}$$

Where m is the mass of the electron and v is its velocity. Personally, when I first researched about this, I was very much confused how this relation put its pin on Einstein's analysis. But once I understood wave equations, I was able to identify that although particles have a well-defined velocity and position at any given time, the characterization of its sinusoidal wave gives me greater insights of it. From that characterization, the learning was enhanced when examining the quantum wave equation.

3 Fourier Series And Fourier Transforms

The prominent idea about the Fourier series applies to an arbitrary function $f(x)$ which is periodic on some domain. One of the most interesting facts about the Fourier series is it applies to any type of wave and could be expressed as an infinite sum of sinusoids, that is higher harmonics of sines and cosines.

If we were to look deep into the basics of this, we could consider a function $f(x)$ of period 2π and expand it as a sum of sinusoids as seen below:

$$f(x) = a_0 + a_1 \cos(x) + a_2 \cos(2x) + \cdots a_n \cos(kx) + \cdots$$
$$b_1 \sin(x) + b_2 \sin(2x) + \cdots b_k \sin(kx) + \cdots$$

Given below are some proved equations using regular integration:

$$1) \int_0^{2\pi} sin(\lambda x)\, dx = 0, \lambda \in \mathbb{Z}$$

$$2) \int_0^{2\pi} \cos(\lambda x)\, dx = 0, \lambda \in \mathbb{Z}, [m \neq 0]$$

$$3) \int_0^{2\pi} \cos(\lambda x) \cos\, (\gamma x)\, dx = 0, where\ \lambda, \gamma \in \mathbb{Z}, [l \neq q]$$

$$4) \int_0^{2\pi} \sin(\lambda x) \cos(\gamma x)\, dx = 0, where\ \lambda, \gamma \in \mathbb{Z}$$

$$5) \int_0^{2\pi} \cos^2(\lambda x)\, dx = \pi, where\ \lambda \in \mathbb{Z}$$

By considering the above proofs we could implement each of them in equation $f(x)$ to process some eliminations to individually get our baseline constant and the other coefficients. Eventually we are left with the following three conjectures for each coefficient.

1) $a_0 = \frac{1}{2\pi} \int_0^{2\pi} f(x)\, dx$

2) $a_k = \frac{1}{\pi} \int_0^{2\pi} f(x) \cos\, (kx)\, dx$

3) $b_k = \frac{1}{\pi} \int_0^{2\pi} f(x) \sin(kx)\, dx$

We must keep in mind that $f(x)$ in these equations does not depend on time. What's causing the wave however to depend on time is remaining part of the equation, that is the sinusoidal element. The idea of the Fourier series leads us to Fourier Transforms. What if we consider a wave with period from negative infinity to positive infinity? Let us look into this exciting example by considering this equation for $f(x)$,

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} X(j\omega)e^{j\omega t}d\omega$$

Note that as not seen in the Fourier series we are expressing $f(x)$ using another function $X(j\omega)$. This is called a frequency domain function (a complex function) which depends on the frequency ω. Let's see what this means. Think about which component of the equation on the right-hand side depends on time. This is because 'time' is the main depicter of the period of the harmonic. As seen from the Fourier series it must not be $X(j\omega)$ but $e^{i\omega t}$.

Using complex methods $e^{i\omega t}$can be re-written as,

$$\cos(\omega t) + isin(\omega t) - (Z)$$

Therefore, we could easily identify $f(x)$ being a sum of sinusoids, in which we have both a real part and an imaginary part. All frequency changes in this equation take place due to ω therefore, if we were to add $X(j\omega)$ to equation (Z) by considering any frequency, we could actually get a one of the terms in $f(x)$. Hence, we increment ω by 1 as we add the terms thus constantly keep changing it. This changes the sinusoidal frequency for every term. Adding all terms from $-\infty$ to ∞, we receive a unique time-domain signal on a graphic calculator for the function $f(x)$.

What's different about the Fourier series is that it has limited applications. One good application of it is seen in the Gibbs Phenomenon when finding terms to represent a square wave. On the other hand, the Fourier transform represents a wave of an altering period. As we keep increasing the frequency, the wavelength just gets more microscopic and eventually falls into a domain of quantum wavelengths. We could see more applications of this in the next section when understanding quantum wave equations.

4 Quantum Wave Equation

Learning about the Quantum Wave Equation and the expansion of Quantum Wave Packets requires prior knowledge in the areas of Fourier Transforms and Gaussian Integral identities. From this section, we will be able to obtain a form of a Schrodinger Equation and utilize it understand the expansion of Quantum wave packets.

It is very important to note that we could define a sinusoidal wave as:

$$u(x,t) = A_0(kx - wt + \phi) - (1)$$

where x is the horizontal direction coordinate, t is the time, u is the vertical displacement as a function of x and t, and k is the wave vector which has a relation to λ as follows:

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

Over here, w is the frequency which has a relationship with k. In this case,

$$w = ck$$

We could also express an equation of a sinusoidal wave as an expression of an imaginary component,

$$u(x,t) = A_0 Im e^{i(kx - wt + \phi)} - (2)$$

The equations (1) and (2) are equivalent to each other and their equivalence is determined by the general expression of e^{ix} given as,

$$e^{ix} = cosx + isinx$$

Now, it's hard to represent a wave with particles, but I could decompose a localized particle into waves using Fourier Transforms:

$$f(x) = \int A_k e^{ikx} dk$$

Where A_k is the Amplitude/Harmonic of the wave and e^{ikx} corresponds to our expression in equation (2). Hence, we can essentially represent it as a linear combination of waves.

4.1 Deriving wave-equation from its solution

From the wave-equation we could resolve the dilemma presented by the experiments seen in the section 2 where the dilemma is how we want to describe our quantum mechanical objects as particles or waves. However, as seen from our conditions above, it is more appropriate to find a generic form to represent these objects as waves. Let's consider the equation below:

$$\psi(x,t) = Ce^{i(kx-wt)}$$

Where, $\psi(x,t)$ is the wave function of x and t and C is a random coefficient. Now De Broglie considered relations for w and k in terms of momentum and energy. The relations are as follows:

$$p = hk \ and \ E = hw$$

Where h is the Plank's constant in both cases. Hence, we could rewrite the above equation as:

$$\psi(x,t) = Ce^{\frac{i}{h}(px-Et)}$$

But we know that $p = mv$ and hence $E = \frac{p^2}{2m}$. Hence, there must be a further relationship. Before expanding the above equation let's first assume that the wave function holds true for a one-dimensional situation by using partial derivatives of x and t. This gives us:

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\psi = 0$$

Although this equation works for photons (quantum electromagnetic waves), it does not work for electrons because we can't have a linear relationship between E and w . We need another equation: But we do have the relationship between the partial derivative of the variable and its coefficient expressed as,

$$\frac{\partial}{\partial t}\psi = -\frac{i}{h}E\psi$$

And,

$$\frac{\partial}{\partial x}\psi = \frac{i}{h}p\psi$$

Now we could find an expression for E and p as:

$$E = ih\frac{\partial}{\partial t} \ and \ \hat{p} = -ih\frac{\partial}{\partial x}$$

This expression gives us the unit vector of momentum but we could also have a three-dimensional vector of momentum where $-ih$ acts on the gradient of our function ψ given by:

$$\hat{p} = -ih \vee$$

Where $\vee$ is the gradient.

Now as we know the relationship between energy and momentum, we could make the expression as follows,

$$E \rightarrow ih\frac{\partial}{\partial t}\psi = \frac{\hat{p}^2}{2m}\psi - (3)$$

$$\Rightarrow \left[ih\frac{\partial}{\partial t} + \frac{\hat{p}^2}{2m}\right]\psi(r,t) = 0, where\ r\ is\ the\ three\ dimensional\ position$$

This gives us a form of a Schrodinger Equation but we can't necessarily say we derived it because we could never derive a fundamental law of physics. So, we could say that this equation is a 'guess' but a very convenient guess because it gives us a generalization of a very important class of problems. Namely to the problems where electrons are not free electrons but move in the presence of a potential difference. Hence, to see how this happens let me identify the right-hand side of equation (3) which in quantum mechanics is called Hamiltonian given as,

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(r)$$

Where $V(r)$ is the potential energy as a function of the position. This could also be written as,

$$ih\frac{\partial}{\partial t}\psi = \hat{H}\psi, which\ is\ the\ fundamental\ equation\ of\ Quantum\ Physics$$

4.2 The Idea of Spreading a Quantum Wave-Packet

Assume we have a Gaussian wave packet at time, $t = 0$,

$$\psi(x,0) = Ae^{-\frac{x^2}{2d^2}}$$

Where x is the horizontal direction coordinate and d is the horizontal length of the amount of wave spread out. However, solving the Schrodinger equation with this initial condition shows it's unstable. Without going into technicalities, it actually shows a proportionality status of the wave function in relation to a quantum delocalization time scale:

$$|\psi(x,0)|^2\ \alpha\ exp\left[-\frac{x^2}{d^2\left(1+\frac{t^2}{\tau^2}\right)}\right] - (4)$$

Where τ is the time scale expressed as,

$$\tau = \frac{md^2}{h}; h \rightarrow Plank's\ constant$$

This tells us that the size of the wave-packet grows with time, the typical delocalization time, for example in the case of,

1) An electron $(m{\sim}10^{-27}g, h{\sim}10^{-27}cm^2gs^{-1}, d{\sim}10^{-8}cm)$
$$\Rightarrow \tau{\sim}10^{-16}sec$$
2) Typical Human $(m{\sim}50\ kg, d{\sim}1cm)$
$$\Rightarrow \tau{\sim}10^{30}sec$$

4.3 Fourier Transform and Uncertainty Relation of Gaussian Wave-Packet

We could decompose the Gaussian wave-packet into plane waves using Fourier Transforms:

$$\psi(x,0) = Ae^{-\frac{x^2}{2d^2}} = \int \frac{1}{2\pi h}\phi_p e^{\frac{i}{h}px}dp$$

Where ϕ_p is the Fourier Harmonic which provides further detail about the wave-function in the momentum space:

$$\phi_p = \int \psi(x,0)\, e^{-\frac{i}{h}px}\, \alpha\, e^{-\frac{p^2 d^2}{2h^2}}$$

This proportionality status of $e^{-\frac{p^2 d^2}{2h^2}}$ comes directly from the Gaussian Integral Identity:

$$\int_{-\infty}^{\infty} \left(e^{-ax^2} + \beta x\right) dx = \sqrt{\frac{\pi}{\alpha}}\, e^{\frac{\beta^2}{4a}}$$

In this case,

$$a = \frac{1}{2d^2}; \beta = -\frac{i}{h}p \ and \ hence \ \beta^2 = \frac{p^2}{h^2}$$

Now we have the Schrodinger Equation,

$$ih\partial t\psi(x,t) = \frac{p^2}{2m}\psi(x,t) - (5)$$

With the initial condition,

$$\psi(x,0)\ \alpha \int e^{\frac{p^2 d^2}{2h^2}}\, e^{\frac{i}{h}px}\, dp$$

If we observe that if $\psi_1(x,t), \psi_2(x,t), \dots$ are solutions to equation (5), their sum is also a solution, with initial condition

$$\psi(x,0) = \sum\nolimits_n \psi_n(x,0)$$

We must remember that the plane wave, $e^{\frac{i}{h}[px - \epsilon(p)t]}$ solves equation (5) where $\epsilon(p) = \frac{p^2}{2m}$. The reason I'm directly inheriting the solution here is because the need to go beyond abstraction isn't necessary when deriving equation (4).

When incorporating the above solution, the wave-packet time thus evolves as,

$$\psi(x,0)\ \alpha \int e^{\frac{p^2 d^2}{2h^2}}\, e^{\frac{i}{h}\left(px - \frac{p^2 t}{2m}\right)} dp$$

Recalling the Gaussian Integral identity, in this case,

$$a = \frac{d^2}{dh^2} + \frac{it}{2mh}; \beta = \frac{cx}{h}$$

Hence,

$$\psi(x,0)\ \alpha \int e^{\frac{p^2 d^2}{2h^2}}\, e^{\frac{i}{h}\left(px - \frac{p^2 t}{2m}\right)} dp\ \alpha\ \exp\left[-\frac{x^2}{2d^2}\left(1 + \frac{iht}{md^2}\right)^{-1}\right]$$

$$\Rightarrow |\psi|^2 = exp\left[-\frac{x^2}{d^2\left(1 + \frac{t^2}{\tau^2}\right)}\right] - (4)$$

This brings us back to equation (4) signifying that it holds true for all values of x and t. From these constructions we could describe the behaviour of waves in the quantum world. The spreading of wave-packets is due to the uncertainty principle, which states that we cannot know both the position momentum of the particle and its absolute uncertainty. To conclude, these wave-packets are a necessary conceptual physical tool to bring into consistency creation and annihilation of wave operators as seen in this section operating on plane wave solutions.

5 Bibliography

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