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Mathematics Behind the Heisenberg Uncertainty Principle

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Abstract: Most physics books do not reveal clearly how the Heisenberg uncertainty principle was derived. This uncertainty comes from the consequence of the wave-particle duality of matter giving statement that position and momentum cannot be measured in the same time. This article tries to reveal mathematics background behind the expression the Heisenberg uncertainty using supported mathematics background such as Fourier transform, Fourier transform integral, the probability of Gaussian distribution and it ends up with the expression of wave function which describe the localized particle giving relation Heisenberg uncertainty principle.

Keywords: Fourier series; Heisenberg uncertainty; Integral transform; Wave packet

Introduction

The theory of quantum physics (Ren et al., 2020) was developed in a series of guesses based on physical insight rather than in a logical way and it is considered as the most successful human mind in expressing theoretical physics. The birth of quantum physics theory was based the failure classical physics in explaining natural phenomena particularly in atomic model (Sujito et al., 2019). The classical physics could not explain the line spectra from emission or absorption spectrum (Atalay et al., 2023; Lyulin et al., 2023). Actually, Bohr's model of the hydrogen atom proposed quantization of angular momentum but he could not give physical reason why this happened. This quantization condition was able to explain the existence of line spectra of hydrogen atom related to any quantum level as designated by the quantum number n.

The dual nature of light as wave-particle should have implication to open new paradigm for looking phyics in the atomic world (Pawly et al., 2019; Ray, 2023; Zhu et al., 2020). By symetry, it is reasonable to suppose that particle as an electron can behave like waves. It was Louis de Broglie who proposed matter waves, particles having zero mass exhibit a wave-particle duality as had been established for light. He deduced a relation between momentum and wavelength of photon and applied the same relation for particle. He proposed the expression of the wavelength associated with particle.

$$\lambda = \frac{h}{p} \quad (1)$$

Where h is Planck's constant and p is momentum of the particle.

This was indeed a brilliant idea. The problem corresponds to quantization of angular momentum $L = n\hbar$ in Bohr's model for hydrogen atom can be explained. Electron orbits the nucleus associated with a wavelength λ. It relates to a whole number of waves fitting into circular orbit,

$$n\lambda = 2\pi r \quad (2)$$

Recalling the Broglie relation, $\lambda = h/p$ then gives $L = pr = n\hbar$ which is just Bohr's quantization condition (Carosso, 2022; Dolce, 2023).

The wave matter (Bercioux et al., 2020; Carnio et al., 2019) was confirmed first by Davisson and Germer when they fired a known energy of electron beam to a nickel crystal in which the crystal is functioned as an arranged slit. And what they got a such much surprise, the scattered of electrons formed an interference pattern. The existence of the pattern showed the evidence of wave properties of electrons that their wavelengths were consistent with de Broglie formula.

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The experimental evidence shows that the particle of microscopic particle system behaves as wave (Amico et al., 2020). Thus, the behavior of particle is represented by wave function that can be found by solving the Schrodinger equation and for one dimensional motion, the equation is defined as follows:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t) \quad (3)$$

Where $V(x,t)$ is potential energy and $\Psi(x,t)$ is wave function associated with the motion of particle of mass m and $\hbar = h/2\pi$. The time-independent Schrodinger equation gives the following form:

$$E\Psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x)}{\partial x^2} + V(x)\Psi(x) \quad (4)$$

The simplest case is for free particles where the motion particle does not influence of forces which are described by potential energy function. Solving the Schrodinger equation for $V(x) = 0$ and we get the wave function:

$$\Psi(x,t) = Ae^{ikx} \quad (5)$$

Where $k = \frac{\sqrt{2mE}}{\hbar}$ that can be connected with momentum of particle by relation $p = \hbar k$.
The coefficient A can be determined by normalization condition,

$$\int_{-\infty}^{\infty}\Psi^*(x)\,\Psi(x)dx = 1 \Longrightarrow A^*A\int_{-\infty}^{\infty}dx \quad (6)$$

The integral value does not finite so the particle is completely delocalized in space. The problem is how to define a free particle wavefunction that is more realistic. This requires mathematical concepts such as Fourier series and Fourier transform integral and this will end up with wave packet (Kaneyasu et al., 2021; Uhl et al., 2022) to describe the localized particle giving Heisenberg uncertainty principle.

Method

The method in this research is literature study through various references. Started to the question, how Heisenberg could derive the phenomenal equation called the Heisenberg Uncertainty Principle. Most references do not reveal directly the derivation of this equation. In fact, it needs mathematics background. Thus, study was started by showing a periodic function can be described using Fourier series. To give real representation of matter wave that localize in space, it needs integral transform that represent a single pulse in space and through Gaussian distribution as reference then it gets relation position and momentum known as Heisenberg Uncertainty Principle.

Result and Discussion

Let's discuss briefly the previous mathematic background behind the Fourier series to give important points. The periodicity wave function can be explained by Fourier series.

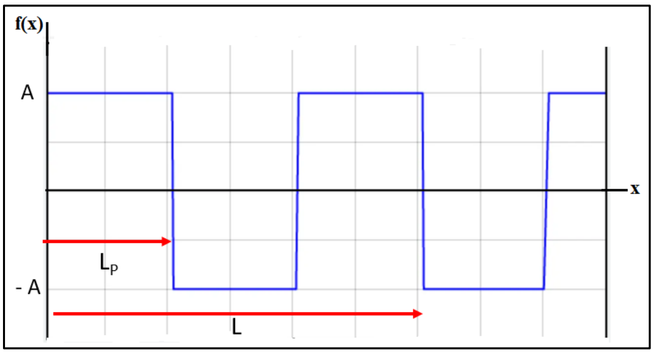

Figure 1. The simple periodic signal, square-wave function

The periodicity signal can be occurred in position along the x direction and also can occur in time along the time axis. The periodicity of signal is shown in distance capital L . This shape of periodic function can be represented as a closed as using an infinite series of periodic sines and cosines.

The repeating signals can be explained using trigonometric function such as $\sin x$, $\cos x$ or combination of these functions. The properties of these periodic functions are well understood such as the orthogonality. This orthogonality plays important roles in expressing Fourier series (Dani et al., 2021; Salim et al., 2022). Fourier theorem (Sutrisna et al., 2019) defined that arbitrary periodic function can be written as a sum of sines and cosines function.

$$f(x) = a_0 + \sum_{n=1}^{N}\left[a_n\cos\left(\frac{2\pi nx}{L}\right) + b_n\sin\left(\frac{2\pi nx}{L}\right)\right] \quad (7)$$

where a_0, a_n and b_n are coefficients that can be determined as below:

$$a_0 = \frac{1}{L}\int_0^L f(x)\,dx \quad (8a)$$

$$a_n = \frac{2}{L}\int_0^L f(x)\cos\left(\frac{2\pi nx}{L}\right)dx \quad (8b)$$

$$b_n = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{2\pi nx}{L}\right)dx \quad (8c)$$

The arguments of the sin and cos terms in the Fourier series (7) can be written in terms of wavenumbers (k) or wavelengths (λ) with the relation $k_L = \frac{2\pi}{L}$ and $\lambda_n = \frac{L}{n}$.

The Fourier series is an extremely important result for any sort of math, physics or engineering applications because no matter how complicated the periodic function $f(x)$, it can be represented as an infinite summation of sines and cosines. In following section, it will be revealed the basic concept how the periodic system can be expressed in the Fourier series.

For example, let's take the simple periodic function as shown in figure.1.

The periodic function which is comprised of a sequence of square pulses with distance L along the x-axis. The width of this pulse is L_P. To represent the periodic system in terms of Fourier series, it should know the coefficients a_0, a_n and b_n. To simplify take $L_P = L/2$, and Eqs. (8) become:

$$a_n = \frac{A\sin(n\pi)}{\pi n} = 0 \quad for\ all\ n \tag{9a}$$

$$b_n = \frac{A[1-\cos(n\pi)]}{\pi n} = \begin{cases} \frac{2A}{n\pi} & for\ n\ odd\ (1,3,5,\dots) \\ 0 & for\ n\ even\ (2,4,6,\dots) \end{cases} \tag{9b}$$

$$a_0 = \frac{1}{2}A \tag{9c}$$

Thus, the periodic function can be expressed as follows:

$$f(x) = \frac{1}{2}A + 0 + \frac{2A}{\pi}\sum_{n=1,3,5}^{N}\frac{1}{n}\sin\left(\frac{2\pi nx}{L}\right) \tag{10}$$

The b_n coefficients when $L_P = L/2$ and A=1 are represented with the following graph

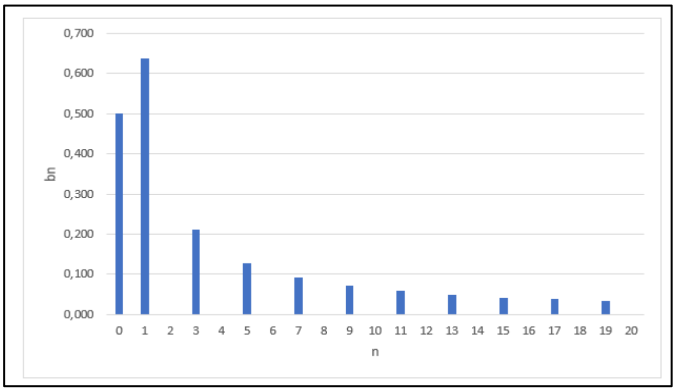

Figure 2. Square wave Fourier coefficients

The reconstruction periodic function can be built by evaluating each terms in the Fourier series and adding all terms. The original periodic system, $f(x)$ is shown in the blue color while the summation for $n = 1,2,\dots,20$ in the Fourier series is shown in the red color. It can be seen that just take n=20, it will get a shape that roughly approximates the square shape of $f(x)$ and it will be precisely match by adding infinite terms.

Figure 3. Square Wave function combined with Fourier series

It can be concluded that Fourier series contains an infinite number of sines and cosines to represent a periodic function $f(x)$ which is specified by the parameter L and the pulse width is designated by the parameter L_p. It will be analyzed what happens if the spacing of periodicity L go infinity meaning that only one pulse located at the origin of the coordinate system. The implications of this condition making the Fourier series need more and more terms sines and cosines progressively. The sines and cosines are represented by e^{ikx} and the mathematics to describe the coefficients multiplied the sines and cosines are now turn going to be a continuous function $g(k)$.

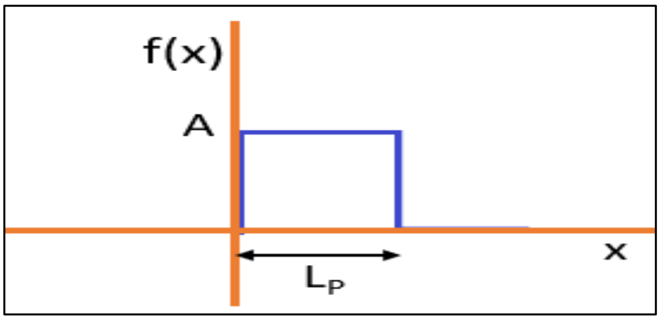

Figure 4. A single square pulse

The function $f(x)$ is now specified by function $g(k)$ and $f(x)$ no longer periodic. To reconstruct $f(x)$, it needs a continuous distribution of sines and cosines represented $g(k)e^{ikx}$ and the summation change into integral (Kusuma, 2020). The connection of function of $f(x)$ and $g(k)$ can be determined using the following formula:

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(k)\, e^{ikx}\, dk \tag{11a}$$

$$g(k') = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)\, e^{-ik'x}\, dx \tag{11b}$$

The function $g(k')$ can actually be determined by the known function $f(x)$integrated over all space times $e^{-ik'x}$ so in this case, k' which is a dummy variable. If the function g(k') put back into here and then got an identity, so it's very similar to a Fourier series but now the coefficients that multiply with sines and cosines are not discrete but a continuous function called $g(k')$. Now there are a number of things that can be recognized with this formula. In the case of $f(x)$ is described in fig. 4 which is consider as a single pulse with width L_p, thus the integral from minus infinity to infinity change into 0 to L_p, the $g(k')$ becomes:

$$g(k') = \frac{1}{\sqrt{2\pi}}\int_0^{L_p} A\, e^{-ik'x}\, dx = \frac{AL_p}{\sqrt{2\pi}} e^{-ik'L_p/2}\left[\frac{\sin(k'L_p/2)}{k'L_p/2}\right] \tag{12}$$

It means that $g(k')$ which is represent single function of $f(x)$. This result show important point that there is no restriction on k' that contrast with the case of periodic function. Due to k' is a dummy thus it can be changed with k and the magnitude of $g(k)$ is:

$$|g(k)|^2 = g^*(k)g(k) = \frac{A^2 {L_p}^2}{2\pi}\left[\frac{\sin(kL_p/2)}{kL_p/2}\right]^2 \quad (13)$$

The Fourier integral (Riyani et al., 2019) provide some insight into what it's actually doing the physical application of this Fourier integral. In fact, it represents wave function which are going to be localized in space. This localized wave function is used to represent free particles that are moving either to the left or to the right. Let's bring this consequence to explain the particle in microscopic world represented by wave function.

The free particle wave functions are completely delocalized in space because the probability to find these particles which are represented by the square of wave functions gives constant value meaning that the amplitude is constant throughout space implying the wave function cannot give information on the position of particle. To represent a physical particle, the amplitude of wave function should be nearly zero in throughout space except for one localized region, ideally a point. Thus, to construct the wave function that has this property, we consider to combine together an infinite large number of harmonic waves for $t = 0$, each with infinitesimally different wavelength number. The summation of this infinite harmonic waves turns into an integral called the Fourier integral or Fourier transform and this result can be plotted as a single beat. This single beat is usually referred to as a wave packet.

The localization of particle represented by a small region in space as an envelope function that can be brought to the concept of Gaussian distribution function (Rosdianto et al., 2017) that can be related with uncertainties in position and momentum.

$$P(x) = \frac{1}{\sqrt{2\pi {\sigma_x}^2}} e^{-\frac{(x-\bar{x})^2}{2{\sigma_x}^2}} \quad (14a)$$

$$P(k) = \frac{1}{\sqrt{2\pi {\sigma_k}^2}} e^{-\frac{(k-\bar{k})^2}{2{\sigma_k}^2}} \quad (14b)$$

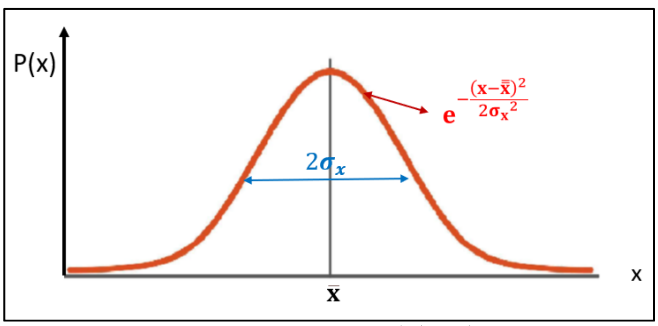

Figure 5. Gaussian normal distribution

The probability density associated with wavefunction is represented by Gaussian probability distribution factor. The expression of Gaussian distribution in real x space is also equivalent with expression in k space. There are two important parameters of this curve distribution. Firstly, the mean position of curve is represented by $\bar{x}$ and secondly, the width of the curve is designated by σ_x. These two parameters can identify the location of particle thus the integral of $P(x)$ over all x is equal to unity known as normalization.

If a particle which is represented as a wave has an uncertainty in position meaning that the particle is localized to some region in space which is corelated to uncertainty in the momentum of particle. This correlation is fundamental in physics to explain characteristic of quantum particle known as the Heisenberg uncertainty principle.

To represent localized particle, it can be conclude that the wave function of free particle in eq. (5) change into the form of integral transform defined as follows:

$$\Psi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \Phi(k) e^{ikx} dk \quad (15a)$$

where

$$\Phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \Psi(x) e^{-ikx} dx \quad (15b)$$

The wave function $\Psi(x)$ that produces a localized in space around $x = 0$ indicated by the following form:

$$\Psi(x) = \left(\frac{1}{2\pi\alpha}\right)^{1/4} e^{ik_0 x} e^{-x^2/4\alpha} \quad (16)$$

The first term of the above wave function (Eq.16) represents a normalization term to assure that the probability density of wave function identified as integral of $\Psi(x)\Psi(x)^*$ over dx is equal to unity. The second term identify free particle wave function (Eq.5) at wave vector k_0 and the last term invoked the envelope function which is a basically comes from the Gaussian distribution.

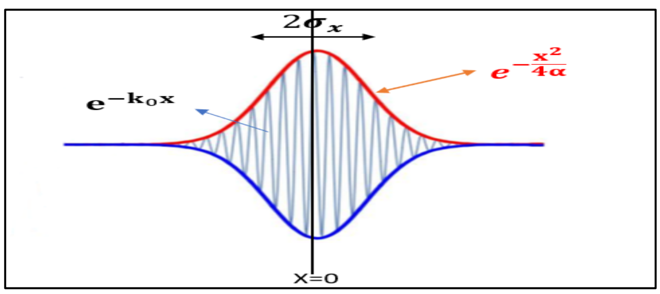

Figure 6. Wave packet in envelope

Substituting Eq. 16 to Eq. 15b, then it can be calculated $\Phi(k)$ giving the Fourier transform pair as below:

$$\Phi(k) = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-2\alpha(k-k_0)} \quad (17)$$

the magnitude of quantum mechanical probability as below:

$$\Phi(k)^{*}\Phi(k) = \left(\frac{2\alpha}{\pi}\right)^{1/2} e^{-2\alpha(k-k_0)^2} \quad (18)$$

Comparing this the quantum mechanical probability density to the standard form of probability of distribution Gaussian in Eq. (14) with $\bar{k} = k_0$ gives the following relation:

$$2\alpha = \frac{1}{2\sigma_k^2} \Rightarrow \sigma_k = \frac{1}{2\sqrt{\alpha}} \quad (19)$$

The obtained parameters give the following relation:

$$\sigma_x \sigma_k = \Delta x \Delta k = \sqrt{\alpha}\frac{1}{2\sqrt{\alpha}} = \frac{1}{2} \quad (20)$$

Using the relation $p = \hbar k \Rightarrow \Delta p = \hbar \Delta k$, then

$$\Delta x \Delta p = \frac{\hbar}{2} \quad (21)$$

The above equation known Eq. 21 as Heisenberg uncertainty principle. The equal sign comes out when it deals with Gaussian shape wave packets. In fact, if the wave packet does not the Gaussian shape, then the greater sign comes into play (Pebralia, 2020). It can be shown for case one-dimensional quantum harmonic oscillator giving $\Delta x \Delta p = \hbar\left(n+\frac{1}{2}\right) \geq \frac{\hbar}{2}$ and for case a particle in one-dimensional box of length L resulting $\Delta x \Delta p = \frac{\hbar}{2}\sqrt{\frac{\pi^2}{3}-2} \approx 0.568\hbar \geq \frac{\hbar}{2}$. The implication of Heisenberg uncertainty explain that it is impossible to measure both the position and the momentum of a particle at the same time. This principle is based on the wave-particle duality of matter. But for macroscopic world the uncertainties in the position and velocity of objects with relatively large masses can be ignored (Firman, 2019). This contrast to the quantum world, since atoms and subatomic particles have very small masses, the effect increasing of the accuracy of their positions will be accompanied by increasing uncertainty related with their velocities. It can be stated that one of fundamental principles in quantum physics is Heisenberg uncertainty since this principle reveal a fundamental aspect of the behavior of matter and energy at the quantum level (Dalimier et al., 2014), and it has important implications for our understanding of the fundamental nature of the universe. There are several applications of Heisenberg uncertainty that will discuss briefly in the following: (1) The uncertainty principle proves a limitation measurement on the precision with which certain physical quantities, such as position and momentum, also energy and time. This principle has important implications for the precision of measurements in physics and other fields, and it is a fundamental limitation on our ability to know and understand the world around us; (2) This principle describes the behavior of subatomic particles that explain the strange and counterintuitive behavior of particles at the quantum level; (3) The uncertainty principle is used in modern quantum mechanics theory such as quantum field theory and quantum electrodynamics to describe the behavior of particles and fields at the quantum level, and they are essential for understanding the fundamental forces of nature. (4) This principle has important implications for the development of new technologies, such as quantum computers and quantum cryptography. These technologies rely on the principles of quantum mechanics, and they use the uncertainty principle to achieve capabilities that are not possible with classical computers. It ends up that Heisenberg's uncertainty principle is a fundamental principle in quantum mechanics with many important applications in physics, technology, and other fields

Conclusion

The certain concept in mathematics is needed to derive Heisenberg uncertainty principle. The first step is an understanding of the Fourier series. This concept gives a way how the periodic function can be described in discrete parameters identified as a_n and b_n coefficients. In fact this Fourier series cannot described localized of wave function identified as single pulse called a beat which is an envelope function. The next step is how to describe this single beat. It needs the integral transform. This transform changes discrete parameters into continuous function identified with $g(k)$. By comparing the quantum mechanical probability density to the probability of distribution Gaussian gives relation of Heisenberg uncertainty principle. This result gives important point to explain microscopic world feature as consequence of the wave-particle duality of matter that explains both position and velocities cannot be measured accurately in the same time.

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