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Course Number: PHYS 300
Course Name : Mathematical Methods of Physics
Title of the paper : Mathematical Methods and Finite Difference method to solve a Quantum System
Date of submission : April 27^{th}, 2020

Abstract

In this paper, the principle of quantum mechanics and its underlying mathematics is discussed. This paper sheds light on how quantum objects are considered to be wave and how that will provide with different tools that allow for a better description of the object. This paper also touches on the relation between position-space and momentum-space and their conversion through the Fourier transformation. The simulation of a 1-D model which makes use of the finite difference method is illustrated. MATLAB is used to implement the finite difference method to simulate the time evolution of the wave in infinite-square-well.

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1 Introduction

Quantum mechanics is a physical science dealing with the behaviour of matter and energy on the scale of atoms and subatomic particles / waves. The concepts of quantum mechanics frequently conflict with common-sense notions derived from observations of the everyday world. There is no reason, however, why the behaviour of the atomic world should comply with that of the familiar, large-scale world. Quantum mechanics also fairly describes the non-relativistic classical behavior of object. However, the strange behavior, that subatomic objects show, is diminished in large objects. Nonetheless, it is the most accurate model for the atomic or sub-atomic level physics.

2 A Brief Overview of Quantum Mechanics

2.1 Wave-particle Duality

The concept of treating a quantum entity as both wave and particle is called wave-particle duality. Scientists throughout generations proved through a series of experiments that physical entity possesses both wave-like and particle-like characteristics. Albert Einstein, with his famous photo-electric effect, proved that that light, which had been thought to be a wave, behaves like a particle as well. The results of Compton's scattering could only be understood if light had wave-particle duality. De Broglie suggested that every physical object shows both wave-particle duality. He theorized that $\lambda = \frac{h}{p}$, where λ is de Broglie wavelength, h is the plank's constant, and p is momentum. Macroscopic objects have too small wavelengths to show wavelike characteristics. Later, multiple experiments showed wave-like behavior of electron, proton, and even bigger objects such as buckminsterfullerene (C_{60}).[1]

2.2 Wave Function

In quantum mechanics, a state of a quantum system such as electron is entirely described by a complex-valued wave function $\mathbf{\Psi}(\mathbf{r}, t)$.[2] The square of the norm of the function gives the probability density function. There are certain conditions:[3]

1. The wave function must satisfy Schrödinger's Equation given in equation 1

$$i\hbar\frac{\partial}{\partial t}\mathbf{\Psi}(\mathbf{r}, t) = -\frac{\hbar}{2m}\nabla^2\mathbf{\Psi}(\mathbf{r}, t) + V(\mathbf{r}, t)\mathbf{\Psi}(\mathbf{r}, t) \tag{1}$$

2. The wave function must be square-integrable or L^2 function.
   - $\int_{-\infty}^{\infty} \psi(x)^*\psi(x)dx < \infty$.
   - It resides in L^2 space which is a Hilbert Space
   - Since, $||\psi(x)||^2$ gives probability density, $\int_{-\infty}^{\infty} \psi(x)^*\psi(x)dx = 1$
3. The wave function and its first order derivative must be continuous everywhere

A solution of the equation 1 is $Ae^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$. Since the solution of this second-order differential equation follow linearity. Any linear combination of solutions is also a solution to the differential equation. For example $\mathbf{\Psi}(\mathbf{r},t) = 3e^{i(\mathbf{a}\cdot\mathbf{r}-4t)} + 2e^{i(\mathbf{b}\cdot\mathbf{r}+4t)}$ should also be a solution. This is what enables superposition of quantum stats.

3 Vector Space

Vector space is defined as set that is closed under vector addition and scalar multiplication. There are certain conditions that elements in the set should satisfy in order of that set to be the vector space that includes Commutativity and Associativity of vector, Additive identity Existence of Additive Inverse, Associativity of scalar multiplication, Distributivity of scalar sums, Distributivity of vector sums and Scalar multiplication identity.[4]

3.1 Hilbert Space

Hilbert Space is an abstract space which extends the methods of linear algebra and calculus from Euclidean space to infinite dimensions. An example of infinite dimension Hilbert space might include all functions $f : \mathbb{R} \to \mathbb{C}$. A continuous function can be represented as a vector, that resides in Hilbert Space, of infinite dimension.[5] For example $\psi_n : x \to Ae^{ik_n x}$ can be written as $|\psi_n\rangle$. Superposition of states can be represented as $\alpha_1 |\psi_1\rangle + \alpha_2 |\psi_2\rangle$.

3.1.1 Inner Product

Similar to vector, inner product for functions can be defined. The inner product between $|\psi_1\rangle$ and $|\psi_2\rangle$ is written as $\langle\psi_1|\psi_2\rangle$ and has following properties:[5]

- $\langle\psi_1|\psi_2\rangle = \int_{-\infty}^{\infty} \psi_1(x)^* \psi_2(x) dx$
- $\langle\psi_2|\psi_1\rangle = \langle\psi_1|\psi_2\rangle^*$
- If $\langle\psi_1|\psi_2\rangle = 0$, then the functions are orthogonal.
- If $\langle\psi_1|\psi_2\rangle = 0$ and $\langle\psi_i|\psi_i\rangle = 1, \forall i$, then the functions are orthonormal.

3.1.2 Basis of a Hilbert Space

In Euclidean space, any vector can be written as linear combination of basis vectors. For example, in $\mathbb{R}^3$, $|a\rangle = \sum_{i=1}^{3} a_i |i\rangle$ where $a_i = \langle i|a\rangle$ and $\langle i|j\rangle = \delta_{ij}$. Any set of orthonormal vectors that spans the vector space can form such basis. Given that, the vectors span the entire vector space, they should show completeness relation.

$$\sum_i |i\rangle \langle i| = \mathbb{I}$$

Similarly, basis of Hilbert Space can be used to create functions. For example, any vector can be written as continuous sum of orthonormal basis vectors. $|a\rangle = \int_{-\infty}^{\infty} a(i)\,|i\rangle\,di$, where $a(i) = \langle i|a\rangle$. Similarly, the basis vectors shows completeness.

$$\int_{-\infty}^{\infty} |i\rangle\,\langle i|\,di = \mathbb{I}$$

4 Operators

Every observable physical quantity such as position, momentum, energy of a quantum particle has an operator associated with it. Operators are linear transformations of the quantum state. The eigenvalues of the operator are the possible values for the observable and the state associated with the eigenvalue is the eigenstate. The eigenvalues are the only possible values that can be observed.[2]

4.1 Momentum operator

For example, an operator $\hat{p}$ can be applied to a quantum state to measure the momentum of the quantum system.[6] If the $|\psi_p\rangle$ is a quantum state with momentum 'p', then $\hat{p}\,|\psi_p\rangle = p\,|\psi_p\rangle$. A wave function with given momentum as a function of x can be written as follows.

$$\psi_p(x) = Ae^{i(kx-\omega t)}$$

Since p = $\hbar k$,

$$\psi_p(x) = Ae^{i(\frac{p}{\hbar}x-\omega t)}$$

Now,

$$\hat{p}(\psi_p(x)) = p \cdot Ae^{i(\frac{p}{\hbar}x-\omega t)}$$

Also,

$$\frac{\partial}{\partial x}\psi_p(x) = i\frac{p}{\hbar} \cdot Ae^{i(\frac{p}{\hbar}x-\omega t)}$$

So,

$$\hat{p}\psi_p(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi_p(x)$$

Therefore,

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

Here, the 'p' is the eigenvalue of the operator, and $\psi_p(x)$ is the eigenstate. Similarly, the eigenstate for the given position and energy can be found.

4.2 Position Operator

Let $|\psi_{x_0}\rangle$ be a position eigenstate of a quantum system where the particle is localized at x_0. So, $\hat{x}\,|\psi_{x_0}\rangle = x_0\,|\psi_{x_0}\rangle$. Position eigenstate of a quantum system will be a Dirac-delta function[6] as probability of finding the particle is zero except for x_0. $\psi_{x_0}(x) = \delta(x - x_0)$. Now, $\int_{-\infty}^{\infty} x\delta(x - x_0)dx = x_0$. So, $\hat{x}$ is just multiplying by x.

4.3 Energy Operator

Again, let $\psi_E(x) = Ae^{i(kx-\omega t)}$ be the eigenstate for the quantum state with energy E. Since $E = \hbar\omega$, $\psi_E(x) = Ae^{i(kx-\frac{E}{\hbar}t)}$

$$\hat{E}\psi_E(x) = E\psi_E(x)$$

But also,

$$\frac{\partial}{\partial t}Ae^{i(kx-\frac{E}{\hbar}t)} = \frac{-iE}{\hbar}Ae^{i(kx-\frac{E}{\hbar}t)} = \frac{-i}{\hbar}E\psi_E(x)$$
$$\hat{E} = i\hbar\frac{\partial}{\partial t}$$

But, from classical mechanics, $E = \frac{p^2}{2m} + V(X)$. So, $\hat{E} = \frac{\hat{p^2}}{2m} + V(\hat{X})$

$$\hat{E} = \hat{E}$$
$$i\hbar\frac{\partial}{\partial t} = \frac{\hat{p^2}}{2m} + V(\hat{X})$$
$$i\hbar\frac{\partial}{\partial t} = \frac{1}{2m}(\frac{\hbar}{i}\frac{\partial}{\partial x})^2 + V(\hat{X})$$
$$i\hbar\frac{\partial}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(\hat{X})$$

which leads back to Schrödinger's equation.

Physical Quantity	**Operator**	**Eigenvalue**	**Eigenfunction**
Position	$\hat{x} = x$	x_0	$\delta(x - x_0)$
Momentum	$\hat{p} = -i\hbar\frac{\partial}{\partial x}$	p	$\psi_0 e^{i\frac{p}{\hbar}x}$
Energy	$\hat{p} = i\hbar\frac{\partial}{\partial t}$	E	$\psi_0(x,p)e^{-i\frac{E}{\hbar}t}$

Table 1: Measurement Operators

4.4 Hermitian Operator

Hermitian adjoint of any linear operator Ω is defined in following way:

$$\langle \Omega^\dagger u|v\rangle = \langle u|\Omega v\rangle$$

where $\Omega^\dagger$ is the adjoint of Ω. If $\Omega = \Omega^\dagger$, then the linear operator is called the Hermitian operator. Hermitian Operators have real eigenvalues. The operator discussed are Hermitian and therefore have real eigenvalues.

4.5 Measurement and collapse of Wave function

A quantum state can be linear combination or superposition of numerous eigenstate due to observer effect.[2] But, when any observation is done, the state collapses into one of its eigenstate. The probability of collapsing into that specific eigenstate is given by absolute square of associated co-efficient. For example, if $|\Psi\rangle = \sum_{i=1}^{n} \alpha_i |\psi_i\rangle$, given that $\sum_{i=1}^{n} \alpha_i^* \alpha_i = 1$, then the probability of collapsing into $|\psi_k\rangle$ is $\alpha_k^* \alpha_k$. The eigenvalue of the eigenstate after collapse is the measurement value.

4.6 Basis states

The eigenvalues of the measurement form the basis for the wavefunction. Let the position eigenfunction for the particle at x be $|x\rangle$. By definition, $|\psi\rangle = \int_{-\infty}^{\infty} \psi(x)\,|x\rangle\,dx$. Also, given that position eigenfunction is localized. $\langle x'|x\rangle = \delta(x - x')$.[6] So, the position are orthogonal.[7]

Now,

$$\begin{aligned}
\langle x|\psi\rangle &= \int_{-\infty}^{\infty} \langle x|\,\psi(x')\,|x'\rangle\,dx' \\
&= \int_{-\infty}^{\infty} \psi(x')\,\langle x|x'\rangle\,dx' \\
&= \int_{-\infty}^{\infty} \psi(x')\delta(x - x')dx' \\
&= \psi(x)
\end{aligned} \tag{2}$$

Again,

$$\begin{aligned}
|\psi\rangle &= \int_{-\infty}^{\infty} |x\rangle\,\psi(x)dx \\
&= \int_{-\infty}^{\infty} |x\rangle\,\langle x|\psi\rangle\,dx
\end{aligned}$$

Therefore,

$$\int_{-\infty}^{\infty} |x\rangle \langle x| \, dx = \mathbb{I} \tag{3}$$

Another way to break a continuous function is using Fourier series. Consider a complex-valued function in open interval L $f : \mathbb{R} \to \mathbb{C}$. It can be written as $f(x) = \frac{1}{L} \sum_k e^{ikx} \hat{f}(x)$, where $\hat{f}(x)$ is complex Fourier-coefficients and e^{ikx} are called Fourier modes that forms Fourier basis. Fourier modes are orthogonal to each other.[8] Inner Product $= \frac{1}{L} \int_I e^{i(k-k')x} = \delta(k-k')$. Delta function can be defined as $\delta(x) = \frac{1}{2\pi} \lim_{K\to\infty} \int_{-K}^{K} e^{ikx} dk$. Every L^2 function can be expanded as Fourier series. The wave function is a L^2 function. So, $N_k e^{ikx}$ can form orthonormal basis, where N_k is normalization constant. Now, the Fourier modes can be represented as momentum eigenstates $|p\rangle$.[2] The fourier modes are orthogonal.[8] And, similar to position eigenstates, momentum eigenstates show completeness.

5 Relation between Position and Momentum Space

The wavefunction $|\psi\rangle$ can be expressed in two different set of basis vector position basis ans momentum basis. The space formed by those basis are called position-space and momentum-space respectively. Let $|x\rangle$ and $|p\rangle$ the the position and momentum eigenvectors.Now, using the relation in equation 2, wavefunction can be expressed as $\psi(x) = \langle x|\psi\rangle$ in position domain and similarly, as $\widetilde{\psi}(p) = \langle p|\psi\rangle$ in momentum domain.

Given that $|p\rangle$ is a momentum eigenstate,

$$p(x) = \phi_0 e^{i\frac{p}{\hbar}x}$$

Where ϕ_0 is normalizing coefficient which equals $\frac{1}{\sqrt{2\pi\hbar}}$

From Equation 2

$$\begin{aligned} \langle x|p\rangle = p(x) &= \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x} \\ \langle p|x\rangle &= \frac{1}{\sqrt{2\pi\hbar}} e^{-i\frac{p}{\hbar}x} \end{aligned} \tag{4}$$

Now,

$$\widetilde{\psi}(p) = \langle p|psi\rangle$$

Using relation in Equation 3,

$$\widetilde{\psi}(p) = \int_{-\infty}^{\infty} \langle p|x\rangle \langle x|\psi\rangle \, dx$$
$$\widetilde{\psi}(p) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\hbar}} e^{-i\frac{p}{\hbar}x} \psi(x) dx$$

Similarly, it can be found that,

$$\psi(x) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x} \widetilde{\psi}(p) dx \tag{5}$$

The above equation looks like the Fourier transformation. In fact, it is exactly the Fourier transformation. This implies that a position eigenstate is linear combination or superposition of multiple position eigenstates and vice versa which is why one can not measure the position and the momentum of a quantum system at the same time.

5.1 Using commute of operators

Given A and B are linear operator, commute of A and B is defined as following:

$$[A, B] = AB - BA$$

In case of operators $\hat{X} and \hat{P}$,

$$[\hat{X}, \hat{P}]\psi = \hat{X}\hat{P}\psi - \hat{P}\hat{X}\psi$$

If $\hat{X} and \hat{P}$ is defined as position and momentum operator,

$$\begin{aligned}
[\hat{X}, \hat{P}]\psi &= x\left(-i\hbar\frac{\partial}{\partial x}\psi\right) + i\hbar\frac{\partial}{\partial x}(x\psi) \\
&= xp\psi + i\hbar\psi + -xp\psi \\
&= i\hbar\psi \\
[\hat{X}, \hat{P}] &= i\hbar \neq 0
\end{aligned}$$

Since the operators do not commute, the eigenstate can not be found simultaneously.

6 Modelling 1D Infinite-square-well

The time evolution of a quantum state with a given initial state is simulated using numerical methods. Here particle in a infinite-square-well is simulated. The potential energy outside the box is infinite and the potential energy inside the box is zero.

6.1 Discretization

Discretization is used to transform a continuous function or model to discrete for ease of computation.[9] In this project, a finite length of space is discretized into the desired number of evenly spaced nodes. Now, the wavefunction is discretized with the same density, so that there can be a one-to-one association between space vector and wavefunction vector.

6.2 Finite Difference Method for derivative

Since, differential operator is linear, it can be written as matrix. Now, let the inter-nodal length be h and D_- and D_+ be first order differential operators evaluated at same node but in different directions. The first order derivative can be approximated by:[10]

$$D_- : U(X) = \frac{U(X) - U(X-h)}{h}$$

$$D_+ : U(X) = \frac{U(X+h) - U(X)}{h}$$

Now the second order derivative(D^2) can be approximated by:[10]

$$\begin{aligned} D^2 : U(X) &= \frac{D_+ : U(X) - D_- : U(X)}{h} \\ &= \frac{\frac{U(X+h)-U(X)}{h} - \frac{U(X)-U(X-h)}{h}}{h} \\ &= \frac{U(X+h) - 2U(X) + U(X-h)}{h^2} \end{aligned}$$

Which is a linear operator. So, it can be written as:

$$D^2 : U(X) = \frac{1}{h^2}\mathbb{M}U$$

where,

$$\mathbb{M} = \begin{bmatrix} -2 & 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & 0 & 0 & 1 & -2 & 1 & 0 \\ \vdots & 0 & \dots & 0 & 1 & -2 & 1 \\ 0 & 0 & \dots & 0 & 0 & 1 & -2 \end{bmatrix}$$

For first node and last node, extra steps has to be taken by adding the boundary condition. However, in this specific case, boundary condition is zero as probability of particle in infinite energy level should be zero Therefore, the wavefunction must be zero at the boundary. Now in numerical form, Schroödinger's equation can be written as:

$$i\hbar\frac{\partial}{\partial t}U = -\frac{\hbar^2}{2m}\mathbb{M}U + V(X)U$$

where $U = \psi(x)$.
Since, $V(X) = 0$,

$$i\hbar\frac{\partial}{\partial t}U = -\frac{\hbar^2}{2m}\mathbb{M}U$$

Or,

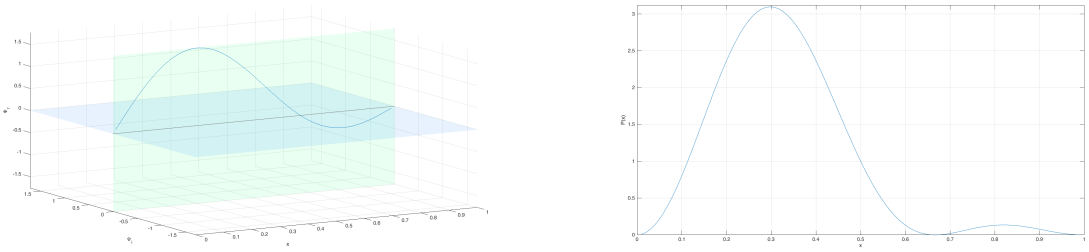
$$\frac{\partial}{\partial t}U = i\frac{\hbar}{2m}\mathbb{M}U$$

6.3 MATLAB implementation using the Finite Difference Method

Now, the time evolution can be solved using time stepping. A simple time-stepping would be Euler's Method. However, it is inefficient and produces inaccurate results. Instead, Adams-Bashforth-Moulton's Method, provided by MATLAB ode113 library, is used which produced a good result. A normalization constant of $\frac{2m}{\hbar}$ is multiplied to the derivative, so that wave function is normalized in every time step. The probability density function is calculated as $P_t(X) = U_t(X)^* U_t(X)$ for each time step.

6.3.1 Representation of vectors

Variables with data type of vector is used to represent $\psi(x)$, $\psi(p)$, x, p, and t. Simulation is done in position-space. Later Fourier transformation is used in order to convert to momentum-space. Initial State is chosen as such that it is values zero at the boundary. Sin wave is a good example.
For example, if the initial state is $\psi(x, 0) = sin(\pi x) + sin(2\pi x)$, the initial state can be given by figure 1(a). The probability distribution is given by figure 1(b). As time progresses, the probability density evolves as shown in figure 2. At a specific time, figure 3 shows the wavefunction and probability density function.



((a)) ((b))

Figure 1: (a) Initial Wave Function and (b) Initial Probability Density Function

Fourier transform is applied on the the solution in position space to get the wavefunction in momentum space. Another initial function is taken: $\psi(x, 0) = sin(10\pi x) + sin(20\pi x) + sin(30\pi x)$ is simulated. They have 3 distinct momentum which can be analytically calculated using $p = \hbar k$ in units of $J \cdot s \cdot m^{-1}$.

Function	k	momentum
$sin(10\pi x)$	10π	$p = \hbar \times 10\pi = 3.31 \times 10^{-33}$
$sin(20\pi x)$	20π	$p = \hbar \times 20\pi = 6.63 \times 10^{-33}$
$sin(30\pi x)$	30π	$p = \hbar \times 30\pi = 9.93 \times 10^{-33}$

Table 2: Momentum of functions

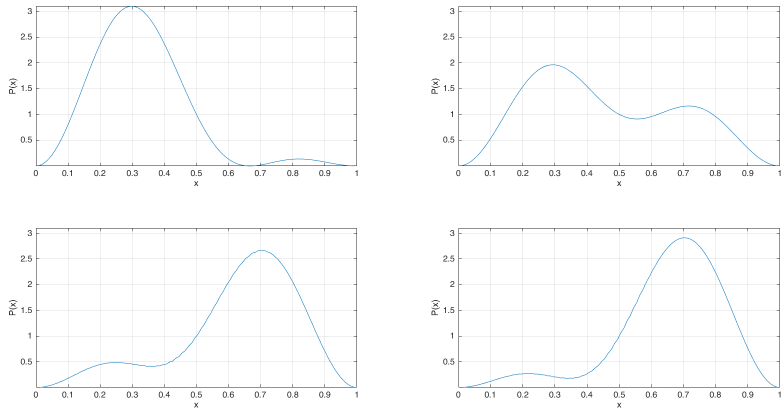
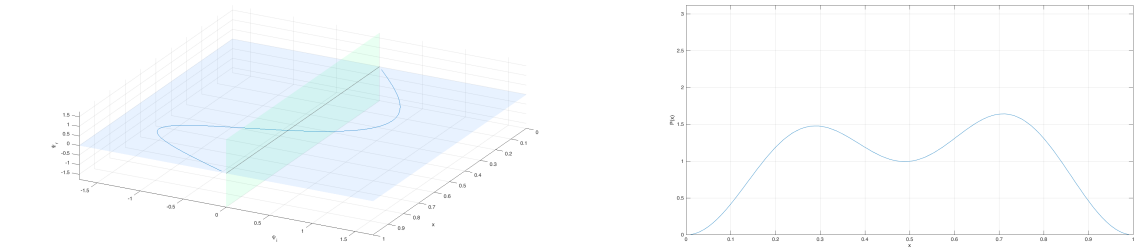


Figure 2: Evolution of PDF



((a)) ((b))

Figure 3: (a) Wave Function and (b) Probability Density Function

Figure 4 shows the Fourier transformation,as in equation 5, applied to wavefunction. The momentum of the wavefunction is similar to analytically calculated momentum in table 2

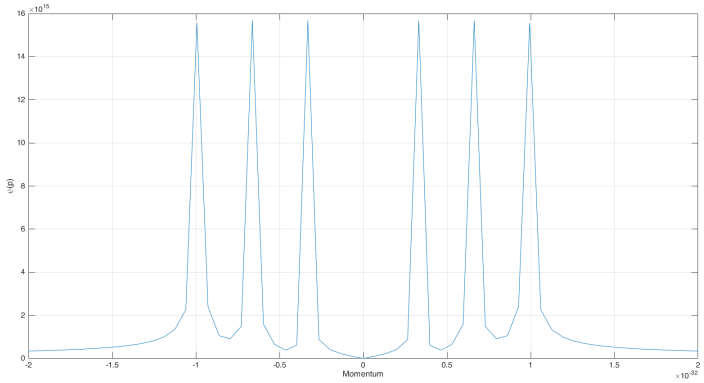


Figure 4: Fourier Transformation of wavefunction

7 Conclusion

Quantum Mechanics tries to model the phenomena that occur in sub-microscopic level and it is the best model that predicts those phenomena. Quantum Mechanics require a very high level of mathematics and is unintuitive. There are some phenomena that entirely defy the everyday nature. However, understanding those phenomena is important in order to understand and device smaller technology such as transistors, microchips. Also, the strange and unique nature of quantum mechanics opens up new possibilities of advancement such as quantum computing.

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