The Schrodinger Equation

Alexandre El-Masry

Department of Physics, Vanier College

Statics and Engineering Physics

Prof. Jicai Pan

Table of Contents

Abstract	
Abstract (French)	
Introduction	
History	5
Time-Independent Schrodinger equation derivation	7
Time Dependent Schrodinger equation	10
Finding the general solution	11
Time evolution	14
Wavefunction General Solution	15
The Infinite Square Well	16
Animation	22
Code	23
Conclusion	25
References	27

Abstract

In this paper, the famous Schrodinger equation is explained, derived, and used to solve an example problem to provide more insight on the basic concepts of Quantum Physics. In addition, an animation of the particle's wavefunction probability density is produced to better visualise how the particle behaves. However, this animation unfortunately has a few numerical errors but still captures the general ideas behind the evolution of the wavefunction. Schrodinger's equation, the equation that outputs the wavefunction of a particle as a solution, is a complex formula that is often very difficult to understand and interpret. To understand this formula, general ideas of differential equations and the methods used to solve them such as separation of variables are used and shown. The methods are then put to the test by solving the problem of a particle in an infinite square well whose solution is then used to produce a Python animation using Matplotlib. The solution to the problem of a particle in a potential V(x) = $\begin{cases} \infty; x \leq 0, x \geq a \\ 0; \ 0 < x < a \end{cases}$ was found to be $\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin{(\frac{n\pi}{a}x)} e^{-\frac{iE_nt}{\hbar}}$. In conclusion, this paper provides a concise and thorough introductory look at the Schrodinger equation and its representation for a particle which can hopefully be used to acquire a better understanding of the quantum world. In addition, this paper also provides a method for visually representing the multivariable expression obtained by solving the problem which must be further worked on to provide a completely accurate picture of the particle.

Abstract (French)

Dans cet article, la célèbre équation de Schrodinger est expliquée, dérivée et utilisée pour résoudre un exemple de problème afin de fournir plus d'informations sur les concepts de base de la physique quantique. De plus, une animation de la fonction d'onde de la particule est produite pour mieux visualiser le comportement de la particule. Cependant, cette animation a malheureusement quelques erreurs numériques mais capture toujours les idées générales derrière l'évolution de la fonction d'onde. L'équation de Schrodinger, l'équation qui produit la fonction d'onde d'une particule comme solution, est une formule complexe qui est souvent très difficile à comprendre et à interpréter. Pour comprendre cette formule, des idées générales d'équations différentielles et les méthodes utilisées pour les résoudre telles que la séparation des variables sont utilisées et montrées. Les méthodes sont ensuite mises à l'épreuve en résolvant le problème d'une particule dans un puits carré infini dont la solution est ensuite utilisée pour produire une animation Python à l'aide de Matplotlib. La solution au problème d'une particule dans un potentiel $V(x) = \begin{cases} \infty; x \le 0, x \ge a \\ 0; & 0 < x < a \end{cases} \text{ s'est avérée être } \Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin{(\frac{n\pi}{a}x)} e^{-\frac{iE_nt}{\hbar}}. \text{ En}$ conclusion, cet article fournit un aperçu concis et approfondi de l'équation de Schrodinger et de sa représentation d'une particule qui, espérons-le, peut être utilisée pour acquérir une meilleure compréhension du monde quantique. En outre, cet article fournit également une méthode pour représenter visuellement l'expression multivariable obtenue en résolvant le problème qui doit être travaillé plus loin pour fournir une image complètement précise de la particule.

Introduction

Throughout human history, humanity has constantly tried to understand the universe they reside in through discovery, research, exploration, etc. The Greeks were some of the first in recorded history to theorise how the world around us was composed. Upon centuries of research, the concept of the atom as the building block of the universe was further established. As the scientific method and technology allowed us to gain exponentially more knowledge on the atoms and the elements, some discoveries presented more questions than answers. Such was the case in the early 20th century when the study of quantum physics was born. In this research paper, I will be briefly covering the history of quantum physics, along with an overview of the Schrodinger Equation, and finally I will be demonstrating a python program that computes an animation of the wavefunction in a particular setup to demonstrate its evolution with respect to both position and time.

History

During the end of the 19th century and the beginning of the 20th century, the atomic model was undergoing collective revision and development by many scientists around the world. Models such as the Bohr-Rutherford atomic model—comprised of a large nucleus surrounded by small electrons in specific orbits that correspond to energy states—were developed. Despite this massive collective effort to learn more about the atom, the history of quantum mechanics starts a lot earlier, to the 18th and 19th century. In 1704, Isaac Newton published one of the most important books in the field of physics, *Optiks* (Hook & Norman 1991). In this book, Newton wrote about his various discoveries

of the behavior of light and his hypotheses of its nature. Newton believed that light had a "corpuscular" nature and that it essentially consisted of many small bodies of light (Hook & Norman, 1991). In 1790, a man called Thomas Young read Newton's work and pondered on his proposition that light was corpuscular rather than wave-like (Tretkoff, 2008). Young eventually performed the double-slit experiment, where he shined light through an obstacle with two slits of similar size to the wavelength of light. This subsequently produced an interference pattern behind the slits which served as proof that light was in fact a wave due to its property of interfering constructively and destructively. On December 14th, 1900, Max Planck, a German physicist, published a study where he demonstrated the phenomenon of Blackbody Radiation and showed that energy could sometimes behave like matter rather than a wave, this effectively marked the birth of Quantum Physics (History.com Editors, 2018). In fact, Planck theorised that energy was composed of small packets called quanta (singular quantum). Five years later, the world-renowned physicist Albert Einstein published his paper on the photoelectric effect based on the findings of Planck (History.com Editors, 2018a). The physics phenomenon of the photoelectric effect consists of the emission of electrons from a material when it is struck by electromagnetic radiation. Einstein proposed that this was possible if light itself was composed of quanta, like Planck's proposition, these quanta would come to be known as photons. Einstein's paper presented a monumental dilemma whereby both Young and Einstein both had evidence that light was a wave and quanta respectively. In addition, in 1924, Louis de Broglie proposed in a thesis that electrons had the characteristics of waves such as frequency and wavelength while also being matter (Barbara Lovett Cline, 2019). Both Einstein and de Broglie's findings lead to the notion

of wave-particle duality of both light and matter which is the basis of Quantum Physics as we know it. The following year, in December 1925, Erwin Schrodinger was attempting to combine de Broglie's findings about the wave nature of electrons with Einstein's Special Relativity, a task that has yet to be completed (Orzel, 2018). Schrodinger eventually decided to put special relativity aside and focused on de Broglie's findings which led him to create the Schrodinger equation, the equivalent of Newton's laws but for quantum mechanics, effectively starting a new era in the study of quantum physics.

Time-Independent Schrodinger equation derivation

Despite the title of this chapter, it is important to mention that the Schrodinger equation cannot be "derived" per say like other equations since it is a basic principle of quantum mechanics, like Newton's laws, that Schrodinger created through basic logical assumptions. However, I will still be using this word to describe the steps taken to get the equation. His equation was tested out experimentally, and it still works perfectly to this day (Knight, 2004). The derivation I will present is based on that of Randall D. Knight's derivation in *Physics for Scientists and* Engineers. As mentioned in the previous chapter, Schrodinger created his famed equation by partially basing himself on the de Broglie wavelength:

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{h}{\sqrt{2mK}}$$

Where h is Planck's constant, p is the momentum of the particle, v is the velocity, m is the mass and K is the kinetic energy. Using basic features of waves studied in physics such as SHM, the wavelength can characterise a wave function¹

$$f(x) = Asin(kx)$$

Where A is the amplitude, and k is the wave vector and is defined as $k = \frac{2\pi}{\lambda}$. To simplifying the derivation, I will adopt the conventional symbols of the Schrodinger equation tuning the function into

$$\psi(x) = \psi_0 \sin(kx)$$

(2)

Taking the second derivative as we would for SHM and inserting equations (1) and (2)

$$\frac{d^2\psi}{dx^2} = -k^2\psi_0 \sin(kx) = -k^2\psi(x) = -\frac{(2\pi)^2}{\lambda^2}\psi(x)$$

$$\frac{d^2\psi}{dx^2} = -\frac{(2\pi^2)2mK}{h^2}\psi(x)$$

Substituting Planck's reduced constant $\hbar = h/2\pi$

$$\frac{d^2\psi}{dx^2} = -\frac{2mK}{\hbar^2}\psi(x)$$

Finally, isolating for Kinetic Energy, K

¹ This short derivation will only consider the time-independent Schrodinger equation as the derivation of the time evolution of the equation is too complex for the scope of this paper.

$$K = -\frac{\hbar^2}{2m} \cdot \frac{1}{\psi(x)} \cdot \frac{d^2\psi}{dx^2}$$

(3)

Equation 3 expresses the kinetic energy of a particle in terms of its mass and wavefunction. It is important to remember that in the context of the time, Schrodinger was trying to find the wavefunction of the electron of a hydrogen atom to get a better picture of the atom as a whole and verify the most up to date models. As one learns in general chemistry, the electron of the atom can only be found at discrete energy states. Thus, conservation of energy will be involved. Assuming the electron is in a conservative environment such as an electric, gravitational, or magnetic field, the basic statement of conservation of energy is

$$E = K + V$$

Where E is the total energy of the system, K is the kinetic energy, and V is the potential energy. In general, the potential energy will be a function of both position and time of the form V(r,t) where r is the 3D position vector. Due to the limited scope of this paper, in addition to the method of solving the equation, I will only be covering 1D potentials that are independent of time of the form V=V(x). Substituting equation 3 into equation 4, we get

$$E = -\frac{\hbar^2}{2m} \cdot \frac{1}{\psi(x)} \cdot \frac{d^2\psi}{dx^2} + V(x)$$

From now on, to simplify the equation, I will be using $\psi = \psi(x)$ and V = V(x) (Note that small psi, ψ , is only dependent on position unlike the complete 1D wavefunction, $\Psi(x,t)$, that also depends on time. We will cover this function later). Multiplying both sides by ψ , we get

$$E\psi = -\frac{\hbar^2}{2m} \cdot \frac{d^2\psi}{dx^2} + V\psi$$
(5)

Equation 5 is the familiar time-independent Schrodinger equation (TISE). Using the classical Hamiltonian operator $\hat{H} = -\frac{\hbar^2}{2m} \cdot \frac{\partial^2}{\partial x^2} + V$, equation 5 can be rewritten in its simplest form (David Jeffrey Griffiths et al., 2018):

$$E\psi = \widehat{H}\psi$$

Time Dependent Schrodinger equation

Now that I have demonstrated a basic "derivation" of the TISE, I will be briefly covering the time dependent Schrodinger equation (TDSE) of the form (LibreTexts, 2014a):

$$i\hbar \frac{\partial \Psi(r,t)}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(r,t) \right] \Psi(r,t)$$

(7)

Equation 7 is actually the 3D Schrodinger equation where $\Psi(r,t)$ is the complete wavefunction that we mentioned earlier and ∇ is the Laplacian operator that is

² An operator is to a function what a function is to a number. They can be seen as functions that change functions, in this case, the Hamiltonian modifies the time-independent wavefunction (LibreTexts, 2014).

represented as $\nabla = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$ (LibreTexts, 2014a). Since I will only be covering 1D cases with constant potential in terms of time, equation 7 can be rewritten as

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left[-\frac{\hbar^2}{2m} \cdot \frac{\partial^2}{\partial x^2} + V(x) \right] \Psi(x,t)$$
Or
$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x) \Psi(x,t)$$

It is noticeable that the Right-Hand Side (RHS) of the TDSE is the same as equation 5 that we found for the TISE except for the wavefunction being multivariable rather than only dependent on position and partial differentials used instead of regular ones since the TDSE deals with both time and position. It is also noticeable that the LHS only deals with time in terms of the partial differential and the RHS only deals with position. This version of the Schrodinger equation is what we call a linear partial differential equation which is an equation that has the property of linearity (where every possible solution is a linear combination of elements). As mentioned, the RHS of the equation is similar to the TISE, so both sides of the equation can be made equal to $E\Psi$. This will allow us to find a general solution to the TDSE.

Finding the general solution

In the earlier chapters, I mentioned that I would only cover solutions were the potential energy function is only position dependent. This will allow us to find the general solution to the TDSE using the method of separation of variables. To do so, we must first look at the wavefunction itself. The wavefunction essentially describes the state

of a particle in time and space and is usually of sinusoidal form. On its own, the wavefunction does not really have a physical representation. To achieve a physical representation, the magnitude of the wavefunction must be squared as such: $|\Psi(x,t)|^2$. This is what is called the probability density and it represents the probability of finding a particle in space by analysing the maxima of the probability density function. In other words, if the function only has one maximum, then it is highly probable to find the particle at the position corresponding to that maximum, if the function has two equal maxima, then there is highly probably to find the particle at one of the two maxima. In any case, since we are dealing with probabilities, the sum of all possible probabilities to find the particle somewhere in space must logically add up to 100%. This is what is called normalization and is expressed as

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 = 1$$

$$|\Psi(x,t)|^2 = \Psi^*\Psi = \psi^* e^{\frac{iEt}{\hbar}} \cdot \psi e^{-\frac{iEt}{\hbar}} = \psi^* \psi = |\psi(x)|^2$$

When trying to find the solution to the Schrodinger equation, one essentially must find the wavefunction to then find the probability density which itself has a physical meaning and importance. To star this process, we must first separate the wavefunction into a product of two separate single-variable function:

$$\Psi(x,t) = \psi(x) \cdot f(t) = \psi f$$
(9)

Inserting equation 9 into equation 8, we get

$$i\hbar \frac{\partial \psi(x)f(t)}{\partial t} = -\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \psi(x)f(t)}{\partial x^2} + V(x)\psi(x)f(t)$$
(10)

The next step is to simplify the partial derivatives starting with the LHS followed by the RHS. Since we are dealing with partial derivatives, we can take out the functions that are not being differentiated as constants

$$\frac{\partial \psi(x)f(t)}{\partial t} = \psi(x) \cdot \frac{\partial f(t)}{\partial t}$$

$$\frac{\partial^2 \psi(x) f(t)}{\partial x^2} = f(t) \cdot \frac{\partial^2 \psi(x)}{\partial x^2}$$

Substituting these simplified derivatives into equation 10, we get

$$i\hbar \cdot \psi(x) \cdot \frac{\partial f(t)}{\partial t} = -\frac{\hbar^2}{2m} \cdot f(t) \cdot \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x)f(t)$$
(11)

Next, to make the equation easier, we need to make each side of the equation deal with one variable instead of two. The LHS should only be dealing with the time variable and the RHS should only deal with the position variable. This can be done by dividing both sides by $\psi(x)f(t)$ that we will rewrite as ψf

$$i\hbar \cdot \frac{1}{f} \cdot \frac{\partial f}{\partial t} = -\frac{\hbar^2}{2m} \cdot \frac{1}{\psi} \cdot \frac{\partial^2 \psi}{\partial x^2} + V = E$$

As mentioned earlier, both sides can be made equal to a constant that we will label E, this corresponds to the total energy. This allows us to separate equation 12 into two separate equations since both sides only deal with one variable. The LHS is the time evolution of the particle, and the RHS is the TISE

$$i\hbar \cdot \frac{1}{f} \cdot \frac{df}{dt} = E$$

$$(13)$$

$$-\frac{\hbar^2}{2m} \cdot \frac{1}{\psi} \cdot \frac{d^2\psi}{dx^2} + V = E$$

$$(14)$$

Since we now have two separate equations that both deal with single variables, the partial derivatives can be replaced with regular derivatives. Without the potential energy function V defined, equation 14 cannot be simplified any longer. Therefore, we will try to simplify equation 13 as much as we can by isolating for f(t).

Time evolution

Equation 13 is a simple differential equation that can be solved by isolating the differentials df and dt on either side of the equation and subsequently integrating to remove those differentials. This will allow us to define the time evolution of the particle.

$$i\hbar \cdot \frac{1}{f} \cdot \frac{df}{dt} = E$$

$$\frac{1}{f} \cdot df = \frac{E}{i\hbar} \cdot dt = -\frac{iE}{\hbar} \cdot dt$$

$$\int \frac{1}{f} \cdot df = \int -\frac{iE}{\hbar} \cdot dt$$

$$\ln(f) = -\frac{iEt}{\hbar} + C$$

$$f(t) = e^{-\frac{iEt}{\hbar} + C} = e^{-\frac{iEt}{\hbar}} \cdot e^{c} = Ae^{-\frac{iEt}{\hbar}}$$

In the last step, I made the exponential of the constant of integration, e^c , equal to the constant A. Since we defined the wavefunction as a product of two functions, $\Psi(x,t) = \psi(x)f(t)$, the constant A can be removed and absorbed into $\psi(x)$. The time evolution thus becomes

$$f(t) = e^{-\frac{iEt}{\hbar}}$$

This is the general solution for the time evolution of the particle and this function is the same in any case, thus, to solve the Schrodinger equation, we just need to find $\psi(x)$ and then multiply the time evolution f(t) to get the full wave equation.

Wavefunction General Solution

Now that the two functions have been simplified as much as possible, we can rewrite the wavefunction as

$$\Psi(x,t) = \psi(x)f(t) = \psi(x)e^{-\frac{iEt}{\hbar}}$$

As mentioned earlier, the Schrodinger equation is a linear equation, thus, the solution to it, the wavefunction, can be expressed as a linear combination of separate equations that we will call states in relation to the different energy states a quantum particle can be found in. This linear combination has the form

$$\Psi(x,t) = c_1 \psi_1(x) e^{-\frac{iE_1 t}{\hbar}} + c_2 \psi_2(x) e^{-\frac{iE_2 t}{\hbar}} + \dots + c_n \psi_n(x) e^{-\frac{iE_n t}{\hbar}}$$

As is normal with linear combinations, each element is the product of a constant that is labeled, c_n . This linear combination can then be simplified using summation notation of the form

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-\frac{iE_n t}{\hbar}} = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)$$

(16)

Equation 16 is the general solution to the time dependent Schrodinger equation for any situation where the potential energy is constant through time. We can now use this equation to solve many different situations of which I will cover one in the following chapter.

The Infinite Square Well

The infinite square well is a theoretical model of a particle bounded in an infinite potential well between x = 0, x = a. At the bottom of the well and at their bounds, the potential energy, V(x) = 0

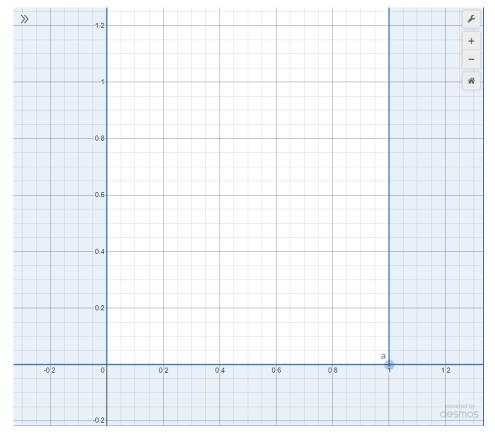


Figure 1: Infinite potential well (via Desmos)

Therefore, the potential well equation can be expressed as

$$V(x) = \begin{cases} \infty; x \le 0, x \ge a \\ 0; 0 < x < a \end{cases}$$

A particle will usually go towards the space with the least potential meaning that the particle cannot be found anywhere outside of the well bound by 0 and a. In other words, there is 100% chance to find the particle in the well, or as expressed by the normalisation of the wavefunction through its probability density

$$\int_0^a |\Psi(x,t)|^2 \, dx = 1$$

One important thing to notice is that this normalization also applies to the time independent wavefunction ψ which can be proven in the following manner

$$|\Psi(x,t)|^2 = \Psi^*\Psi = \psi^* e^{\frac{iEt}{\hbar}} \cdot \psi e^{-\frac{iEt}{\hbar}} = \psi^* \psi = |\psi(x)|^2$$

Therefore, it can also be said that

$$\int_0^a |\psi(x)|^2 dx = 1$$

This is property tells us that the particle will be found inside the well at any time given and we will use this to solve the problem later. In addition, the particle cannot be found at the border of the well since the potential is infinite, thus

$$\psi(0) = \psi(a) = 0$$

Since the potential inside the well is zero, the TISE, equation 5, can be rewritten as

$$E\psi = -\frac{\hbar^2}{2m} \cdot \frac{d^2\psi}{dx^2}$$

Since this is an ordinary differential equation, we will isolate the second derivative

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

To make the math easier, we set $k=\frac{\sqrt{2mE}}{\hbar}$, not to be confused with the wave-vector, k, that we used at the start of this paper. Thus, the previous equation becomes

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

Once again, this is the same format as SHM, which already has an established solution of the form

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

Using our boundary conditions, we can already simplify this solution since the wavefunction is zero at x=0

$$\psi(0) = Asin(k*0) + Bcos(k*0)$$

Since the argument of both sinusoidal functions will be equal to zero, and that sin(0) = 0 while cos(0) = 1, then the value of *B* must be zero. Thus

$$\psi(x) = Asin(kx)$$

Using our second boundary condition, we can find constraints on the argument of the sin function:

$$\psi(a) = 0 = Asin(ka)$$

The variable A cannot be zero since that would mean the particle cannot be found anywhere in the well. Therefore, the argument ka must equal zero. When studying the sin function, we can see that there are zeros at every integer multiple of π :

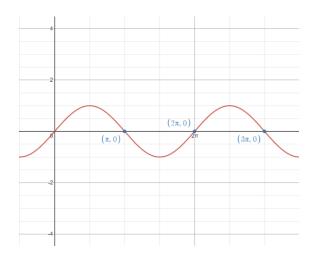


Figure 2: Sin function zeroes (via Desmos)

We can therefore make the assertion that the argument of the sin function corresponds to

$$ka = \{\pi, 2\pi, 3\pi, ..., n\pi\}$$

We do not include x = 0 since it is our boundary condition. We can isolate for k:

$$k_n = \frac{n\pi}{a} \ (n = 1, 2, 3, ...)$$

We can substitute this into our wavefunction to get

$$\psi(x) = Asin(\frac{n\pi}{a}x)$$

Using k_n , we can also find all the different allowed energy states where it becomes even more evident why $n \neq 0$ because that would mean the particle has zero energy which is impossible in this situation. The energy states can be found and expressed as:

$$k_n = \frac{n\pi}{a} \& k = \frac{\sqrt{2mE}}{\hbar}$$
$$\therefore E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

All that is left to do to find the general solution to the TISE is to find A. This can be done using the normalization condition that was shown earlier:

$$\int_0^a |\psi(x)|^2 dx = 1 = \int_0^a A^2 \sin^2(kx) dx = A^2 \int_0^a \sin^2(kx) dx = A^2 \cdot \frac{a}{2} = 1$$

$$\therefore A = \sqrt{\frac{2}{a}}$$

Finally, substituting A into our wavefunction, we get

$$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$

This is the general solution to the TISE. To get the general solution to the TDSE, we just have to substitute our $\psi(x)$, therefore

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-\frac{iE_n t}{\hbar}}$$

Finally, the coefficients c_n remains unknown, however, I will not be going through the steps of finding it since it involves higher level mathematics, such as Fourier series, that are beyond the scope of this paper's range. Nevertheless, David Griffiths and Darell Schroeter's textbook goes through all the steps to find the coefficients. As a general solution for the coefficients of the infinite square well problem they present:

$$c_n = \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a}x\right) \Psi(x,0) dx$$

Therefore, to fully solve the problem, all that is really needed is the length of the well, a, the mass of the particle, m, and the initial wavefunction, $\Psi(x, 0)$.

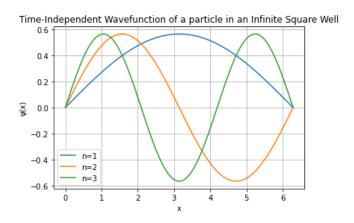


Figure 3: Plot showing the wavefunction at different energy states (via Python)

Animation

As mentioned previously, an animation of the final probability density of the particle in the infinite square well was animated using python code. Errors in the animation were also previously mentioned which include a reduced Planck's constant that is 31-fold larger than the actual constant as smaller values "broke" the wave and made it constant due to unknown errors in the code. It is important to note that this program was written with very rudimentary knowledge of python programming leading to multiple errors. Another notable error that is immediately visible is the lack of normalization of the probability density function as it is larger than 1. This obviously does not make physical sense since probability cannot surpass 1. Nevertheless, this animation provides a reasonable estimate of what the actual solution of the multivariable function would look like with the x-axis capturing the position variable and the animation progression capturing the time variable. As we can see, the probability of finding the particle at a certain area of the well is highly variable by sometimes peaking at the center, peaking at two opposite ends, and sometimes even being spread out through the whole well. This animation really captures the core principle of quantum physics that a particle can be at many places at the same time in a state of superposition. Hopefully this animation can be used to better understand the nature of a quantum particle. More work would need to be put into this code to correct the mentioned issues and it would also be interesting to develop an algorithm that could solve and animate the wavefunction for any arbitrary potential instead of being bound to the infinite square well case. The code for this program is included below for reference with some brief comments.

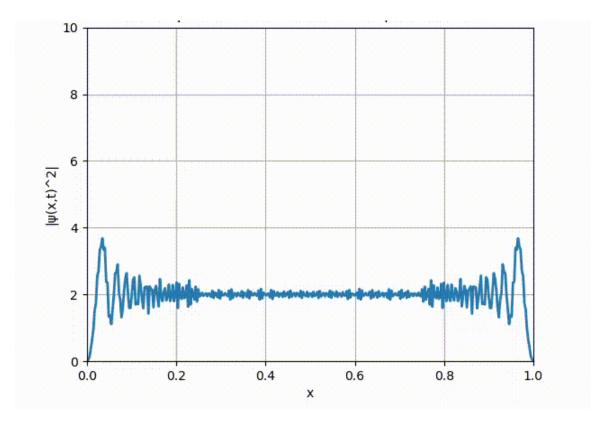


Figure 4: Animation of wavefunction probability density of a particle in a box

Code

```
Animation of probability density of a particle in an infinite square well

Created on Tue Mar 29 21:35:14 2022

@author: Alexandre El-Masry

"""

import numpy as np

import matplotlib.pyplot as plt

import scipy.integrate as integrate

from matplotlib import animation

pi=np.pi

L=1 #length of box set to 1 for visual simplicity

Nx=350 #number of divisions set to 350 because it is the ideal number before

wavefunction because meaningless

tvals=np.linspace(0,100,Nx)

A=np.sqrt(2/L)

c=np.empty(Nx) #linear combination coefficients

hbar=1.05457182E-3 #hbar set to 10e-3 because the wavefunction becomes meaningless when

smaller,this is one of the flaws mentioned in the paper.
```

```
E=np.empty(Nx) #Energy states
m=1 #mass set to 1 for simplicity
#animation plot configuration
fig = plt.figure()
ax = plt.axes(xlim=(0, 1), ylim=(0, 10))
line, = ax.plot([], [], lw=2)
plt.rcParams["figure.figsize"] = [7.50, 3.50]
plt.rcParams["figure.autolayout"] = True
#time independent wavefunction solution to infinite square well (small psi)
def psi(x,Nx):
    wf=A*np.sin(Nx*pi*x/L)
    return wf
#loop to compute the sum of all linear coefficients and energy states
for i in range(Nx):
    c[i]=A*integrate.quad(psi,0,L, args=(i,))[0]
    E[i]=(i**2*pi**2*hbar**2/(2*m*L**2))
def init():
   line.set_data([], [])
   return line,
#animation body
def animate(tvals):
   x=np.linspace(0,L,Nx)
    y=sum(c[i]*(A*np.sin(i*pi*xvals/L))*np.exp(-1j*E[i]*tvals/hbar)for i in
range(1,Nx))
   f=np.abs(y**2)
    line.set_data(x,f)
    return line,
#plotting fucntion calls
anim = animation.FuncAnimation(fig, animate, init_func=init, frames=20000,
interval=150, blit=False)
plt.title("Time-dependent Wavefunction of a particle in a box")
plt.ylabel("|\u03C8(x,t)^2|")
plt.xlabel("x")
plt.grid()
plt.show()
```

Conclusion

In conclusion, humankind is constantly seeking to learn more about the surrounding universe and how it operates on a macro and micro level. This perpetual exploration and curiosity have led to the discoveries of a modern field in Physics that has completely upended and changed the way we see the universe. For centuries, we assumed that the universe operated on a deterministic level which was grounded upon Newton's laws of motion. With the advent of Quantum Physics, a probabilistic model of the universe became equally possible due to the evidence associated to it. Both models came into conflict due to their antagonistic nature despite both having clear evidence. Nowadays, this has become one of the biggest unsolved mysteries in the world, with classical and modern physics being incompatible together. Nevertheless, these two models still represent the world as we know it accurately at the levels they are best fit to operate in. Through this paper, the basic concepts that led to the discovery of the Schrodinger equation were explored, along with the computation of its general solution, and an application of the equation in a problem providing insight on the way it can be used to model the world around us. In addition, an animation of the wavefunction probability density was produced to help visualise the particles behavior. Despite numerous attempts, the method used did not yield a completely accurate model since the function was not normalised ($\Psi(x,t)^2 > 1$), and some of the constants such as Planck's constant did not have the correct units. Nevertheless, the animation does successfully provide a fairly accurate model of how the particle would behave inside an infinite square well. To improve this model, a better understanding of python programming, in addition to differential equations would be required. Finally, this is only a raindrop in the storm

that is the quantum world, and there is much more to be discovered and explained. In particular, quantum physics becomes crucial when trying to understand how black holes function. These cosmic bodies will forever catch the attention of humanity since all the laws of physics break down at their center, the Singularity. Will our development ever allow us to comprehend these amazing phenomena? Only time will tell.

References

- Barbara Lovett Cline. (2019). Louis de Broglie | French physicist. In *Encyclopædia Britannica*. https://www.britannica.com/biography/Louis-de-Broglie
- David Jeffrey Griffiths, Schroeter, D. F., & Cambridge University Press. (2018). *Introduction to quantum mechanics*. Cambridge University Press.
- History.com Editors. (2018a, August 21). *Albert Einstein*. HISTORY; A&E Television Networks. https://www.history.com/topics/inventions/albert-einstein
- History.com Editors. (2018b, December 14). *The birth of quantum theory*. HISTORY. https://www.history.com/this-day-in-history/the-birth-of-quantum-theory
- Knight, R. D. (2004). *Physics for scientists and engineers with modern physics : with modern physics : a strategic approach*. Pearson, Addison Wesley.
- LibreTexts. (2014a, June 17). 3.1: The Schrödinger Equation. Chemistry LibreTexts. https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Te xtbook_Maps/Physical_Chemistry_(LibreTexts)/03:_The_Schrödinger_Equation_and_a_Particle_in_a_Box/3.01:_The_Schrödinger_Equation
- LibreTexts. (2014b, June 17). 3.2: Linear Operators in Quantum Mechanics. Chemistry LibreTexts.
 - https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Te xtbook_Maps/Physical_Chemistry_(LibreTexts)/03:_The_Schrodinger_Equation_and_a_Particle_in_a_Box/3.02:_Linear_Operators_in_Quantum_Mechanics
- Norman, J. (n.d.). *Opticks: Isaac Newton's Theories of Light & Color*. History of Information. https://historyofinformation.com/detail.php?id=1724

- Orzel, C. (2018, February 6). Why Vacations Are Essential For Physics. Forbes. https://www.forbes.com/sites/chadorzel/2018/02/06/why-vacations-are-essential-for-physics/?sh=6074e3e02367
- Tretkoff, E. (2008). *May 1801: Thomas Young and the Nature of Light*. APS Physics. https://www.aps.org/publications/apsnews/200805/physicshistory.cfm