TIME EVOLUTION OF FREE PARTICLE

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Project Report Submitted to

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Contents

1 OBJECTIVE

The objective of this project is to :-

- study the Schrödinger Equation for a free particle.
- understand that a wave packet can represent a free particle.
- study the time evolution of a given wave packet numerically

2 FREE PARTICLE

One of the simplest problems in Quantum Mechanics is : **the free particle (*V(x)=0 everywhere*)**. A classical free particle obeys the kinematic equation: $x = x_0 + v_0 t$. Classical particles obey Newton's second law, $F = ma$, and when there is no net force, there is no acceleration. So this would just mean motion at constant velocity.
But the problem is not the same quantum mechanically .
The time independent Schrödinger Equation for a free particle

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

(1)

or

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

where $k = \dfrac{\sqrt{2mE}}{\hbar}$
The general solution of the given equation is of the form:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

Since, there are no boundary conditions ,So there is no restriction on the value of k.Thus a free particle, even in quantum mechanics, can have any non-negative value of the energy in the range 0 to ∞.

$$E = \frac{k^2\hbar^2}{2m} \geq 0$$

The energy levels in this case are not quantized and correspond to the same continuum of kinetic energy shown by a classical particle.
Adding the time dependence, $e^{-iEt/\hbar}$,

$$\Psi(x,t) = Ae^{ik(x-\frac{\hbar k}{2m}t)} + Be^{-ik(x+\frac{\hbar k}{2m}t)} \tag{3}$$

So, any function of x and t that depends upon these variables in the special combination $(x \pm vt)$, for some constant v represents a wave of fixed profile, travelling in $\mp$ x-direction, at a speed v. The shape of the wave doesn't change as it propagates because every point on the waveform is moving along with same velocity.

The first term in the equation 3 represents a wave travelling to the left and the second term represents a wave moving to the right. We can write,

$$\Psi_k(x,t) = Ae^{i(kx - \frac{\hbar k^2}{2m} t)} \tag{4}$$

where : $k = \pm \frac{\sqrt{2mE}}{\hbar}$, with

$$\begin{cases} k > 0 & \text{travelling to the right} \\ k < 0 & \text{travelling to the left} \end{cases} \tag{5}$$

So, the stationary states of a free particle are propagating waves with wavelength $\lambda = 2\pi/|k|$.

DIMENSIONLESS FORM

Let $\xi = x/x_0$ and $e = E/\epsilon$

then $\frac{2mx_0^2\epsilon}{\hbar^2} = 1$

$x_0 = 1$

$\epsilon = \frac{\hbar^2}{2m}$

$$\frac{d^2u}{d\xi^2} + eu = 0$$

Let $k^2 = e$

$$\frac{d^2u}{d\xi^2} + k^2u = 0$$

And it's solution (including time dependence) is

$$u_k(x,t) = Ae^{i(k\xi - k^2\xi)}$$

Is this wavefunction normalizable ?

This wavefunction is not normalizable.

$$\int_{-\infty}^{+\infty} \Psi_k^* \Psi_k \, dx = |A|^2 \int_{-\infty}^{+\infty} dx = |A|^2(\infty)$$

This means that the separable solutions do not represent physically realisable states i.e. a free particle cannot exist in stationary states .

3 WAVEPACKETS

The separable solutions play a mathematical role , which is entirely independent of its physical interpretation.The general solution to the time independent Schrödinger Equation in this case is a linear combination of separable solutions(integral over continuous variable k):

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)} \, dk \tag{6}$$

This wave function can be normalised for appropriate values of $\phi(k)$.It carries a range of k's and thus a range of energies and speeds.We call it ***WAVEPACKET***.

The idea is : A wave packet is a superposition of sinusoidal functions whose amplitude is modulated by ϕ and it consists of ripples contained within the envelope. What corresponds to the particle velocity is the speed of the envelope **(group velocity)** whereas the speed of the individual ripples is called the **phase velocity**. Phase velocity , depending upon the nature of the waves , can be greater than , less than or equal to the phase velocity.

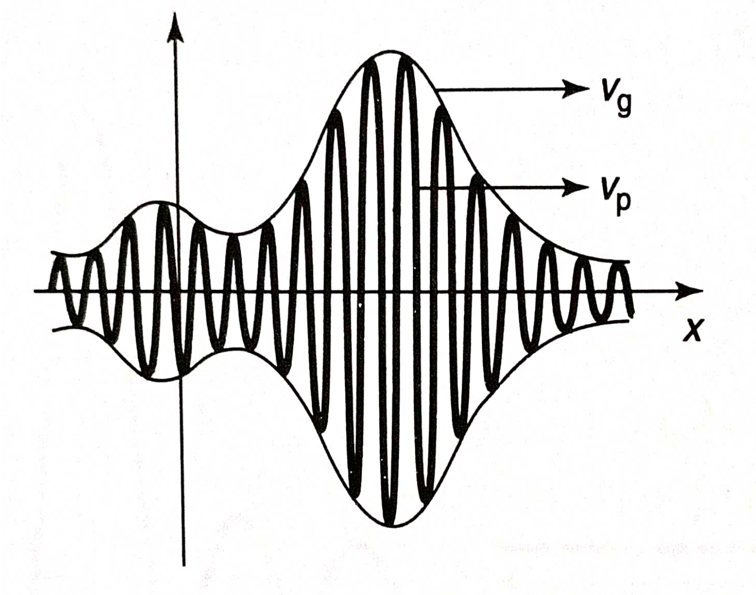

Figure 1: **A Wave Packet. The "envelope" travels at group velocity and the "ripples" travel at phase velocity**

For the wave function of a free particle in quantum mechanics, the group velocity is twice the phase velocity.

$$v_{classical} = v_{group} = 2v_{phase}$$

4 TIME EVOLUTION OF A WAVE PACKET

The general solution to the time independent Schrödinger Equation :

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)} \, dk \tag{7}$$

Now we need to determine $\phi(k)$ such that

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} \, dk \tag{8}$$

To determine $\phi(k)$, we use Fourier and Fourier Inverse transform, i.e.

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0) e^{-ikx}\, dx \tag{9}$$

We put this in Eq. 7 to get time evolution of a wave packet.

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} (\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0) e^{-ikx}\, dx) e^{i(kx - \dfrac{\hbar k^2}{2m} t)}\, dk \tag{10}$$

5 PROBLEM

This is based on Problem 2.22 from Griffiths, Introduction to Quantum Mechanics 2ed

THE GAUSSIAN WAVE PACKET A free particle has the initial wavefunction

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

where A and a are constants.(a is real and positive)

1. Normalize $\psi(x,0)$ and determine A.
2. Find $\psi(x,t)$
3. Find $\psi(x,t)$ and $|\psi(x,t)|$. Express your answer in terms of the quantity

$$w = \sqrt{\frac{a}{1 + (2\hbar a t/m)^2}}$$

. Sketch $|\psi|^2$ as a function of x for different t.

Solution

1.

$$1 = |A|^2 \int_{-\infty}^{+\infty} e^{-2ax^2}\, dx = |A|^2 \sqrt{\frac{\pi}{2a}}$$

$$A = (\frac{2a}{\pi})^{1/4}$$

2.

$$\phi(k) = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ax^2} e^{-ikx}\, dx$$

$$\phi(k) = \frac{e^{-k^2/4a}}{(2\pi a)^{1/4}}$$

3.

$$\psi(x,t) = (\frac{2a}{\pi})^{1/4} \frac{e^{-ax^2/(1+2i\hbar a t/m)}}{1 + 2i\hbar a t/m}$$

$$|\psi(x,t)|^2 = \sqrt{\frac{2}{\pi}} w e^{-2w^2x^2}$$

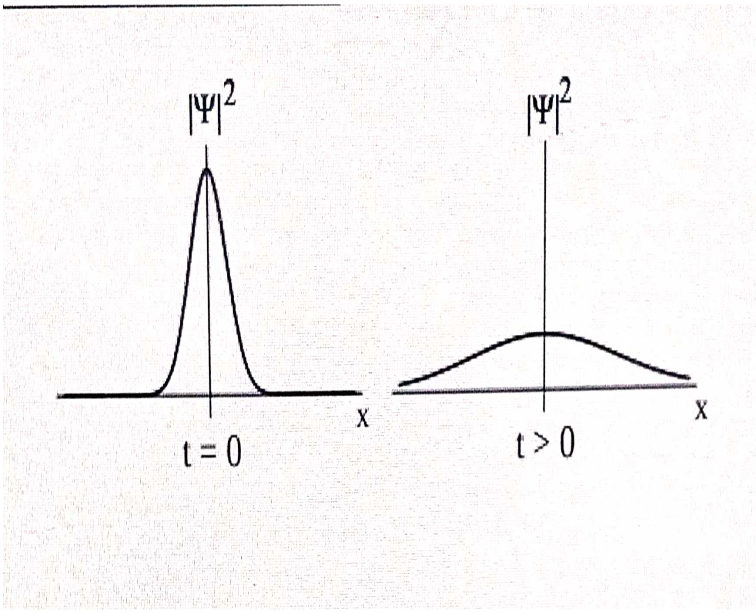

Figure 2: **The plot of $|\psi|^2$ with respect to x for two different t.**

where

$$w = \sqrt{\frac{a}{1 + (2\hbar a t/m)^2}}$$

As t increases, the graph of $|\psi|^2$ flattens out and broadens.

6 Program

```
'''
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'''
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
import scipy.integrate as integrate
import imageio.v2 as imageio


a=1 #arbitrarily taken 1
A=(2*a/np.pi)**(1/4) #constant A calculated using normalisation

#function to calculate psi(x,0)
def psi_0(x1,a):
        psi=[]
        for x in x1:
           psi.append(A*np.exp(-a*x*x))
        return x1,np.array(psi)

#function to calculate phi(k)
def phi_k(x,psi_,k):
    value=[]
    for i in k:
        value_=np.exp(-1j*i*x)
        m_v=psi_*value_/np.sqrt(2*np.pi)
        d=integrate.simps(m_v,x)
        value.append(d)
    a=integrate.simps(np.power(value,2),x)
    value1=(value)/(a)
    return k,np.array(value1)

#function to calculate phi(x,t)
def time_evolution(phi_,x,t,k):
    psi_x_t=[]
    for i in range(len(x)):
        factor=np.exp((-1j*(k*x[i] -(k**2)*t)))
        value=np.array(phi_)*factor/np.sqrt(2*np.pi)
        d=integrate.simps(value,k)
        psi_x_t.append(d)
    norm=integrate.simps(np.power(psi_x_t,2),k)
    psi_norm=psi_x_t/np.sqrt(norm)
    return psi_norm

N=1000
x1=np.linspace(-4,4,N)
x,psi_=psi_0(x1,1)
k=np.linspace(-10,10,N)
k,phi_=phi_k(x,psi_,k)

#probability density at t=0
fig, (ax1, ax2) = plt.subplots(1, 2)
fig.suptitle('Probability Density plot at t=0')
ax1.plot(x,np.power(psi_,2))   #position basis
ax1.grid()
ax1.set(xlabel="x",ylabel="$U(x)^2$",title="Probability Density in position basis")

ax2.plot(k, abs(phi_**2))  #momentum basis
```

```
ax2.grid()
ax2.set(xlabel="k",ylabel="$U(k)^2$",title="Probability Density in momentum basis")
plt.show()
#plt.savefig('Prob_density.png', dpi=72)
#plt.close()


t1=np.linspace(0,5,50)   #time frames
dpi = 72
s=np.arange(0,50,1)

#plotting psi(x,t) in different time frames
for (i,f) in zip(t1,s):
    m=time_evolution(phi_,x,i,k)
    fig = plt.figure(figsize=(600/dpi, 450/dpi), dpi=dpi)
    ax = fig.add_subplot(111)

    ax.plot(k, abs(np.power(m,2)), c='b', lw=3, alpha=0.8)
    ax.set_ylim(0, 0.4)
    ax.grid()
    # Fill under the line with reduced opacity
    ax.fill_between(k,abs(np.power(m,2)), facecolor='b', alpha=0.5)
    ax.yaxis.set_tick_params(width=2, length=5)
    ax.spines['left'].set_position('center')
    ax.spines['left'].set_linewidth(2)
    ax.spines['right'].set_visible(False)
    ax.spines['top'].set_visible(False)
    ax.yaxis.set_ticks_position('left')
    ax.xaxis.set_ticks_position('bottom')
    ax.spines['bottom'].set_linewidth(2)
    ax.annotate(text='$\ tau=${:.2f} '.format(i), xy=(0.8, 0.8),xycoords='axes
   fraction', ha='center', va='center')
    ax.set_xlabel('x')
    ax.set_ylabel("psi(x,t)")
    ax.set_label("NUMERICAL")
    plt.savefig('psi2-{0}.png'.format(f), dpi=dpi)
    plt.close()

# Creating the animation from png images
with imageio.get_writer('psi2_num.gif', mode='i') as writer:
    for i in s:
        image = imageio.imread('psi2-{0}.png'.format(i))
        writer.append_data(image)


#ANALYTIC SOLUTION
'''
The code below generates the frames in the above animation of |  (x,t)|^2 for an
   electron with a=1bohr^( 1 /2). We will work in atomic units so me=1 and hbar=1,
   but convert the time to attoseconds (as) for the annotation.
'''
# Grid of times t1 is in atomic units
hbar, Eh = 1.054571726e-34, 4.35974417e-18 # hbar and hartree in SI units for the
   time conversion
def plot_psi2(ax, i, t, psi2):
    # Plot |psi|^2 on Axes ax for frame i, time t
    ax.plot(x, psi2, c='r', lw=3, alpha=0.8)
    # Fill under the line with reduced opacity
    ax.fill_between(x, psi2, facecolor='r', alpha=0.5)
    ax.set_ylim(0, 0.8)
    ax.grid()
    ax.yaxis.set_tick_params(width=2, length=5)
```

```
    ax.spines['left'].set_position('center')
    ax.spines['left'].set_linewidth(2)
    ax.spines['right'].set_visible(False)
    ax.spines['top'].set_visible(False)
    ax.yaxis.set_ticks_position('left')
    ax.xaxis.set_ticks_position('bottom')
    ax.spines['bottom'].set_linewidth(2)
    ax.xaxis.set_tick_params(width=2, length=5, direction='out')
    ax.yaxis.set_ticklabels([])

    # Add x-axis label and annotate with time in attoseconds
    t_in_as = t * hbar/Eh * 1.e18
    ax.annotate(text='{:.2f} as'.format(t_in_as), xy=(0.8, 0.8),xycoords='axes fraction', ha='center', va='center')
    ax.set_xlabel('$x$ / bohr')
    ax.set_label("ANALYTIC")

# Creating the animation frames at 72 dpi, 600x450 pixels as PNG images

for i, t in enumerate(t1):
    w = np.sqrt(a/(1+(2*a*t)**2))
    psi2 = np.sqrt(2/np.pi) * w * np.exp(-2*w*x**2)
    fig = plt.figure(figsize=(600/dpi, 450/dpi), dpi=dpi)
    ax = fig.add_subplot(111)
    plot_psi2(ax, i, t, psi2)
    plt.savefig('psi2_ana-{0}.png'.format(i), dpi=dpi)
    plt.close()


with imageio.get_writer('psi2_ana.gif', mode='i') as writer:
    for i in s:
        image = imageio.imread('psi2_ana-{0}.png'.format(i))
        writer.append_data(image)
```

7 RESULTS

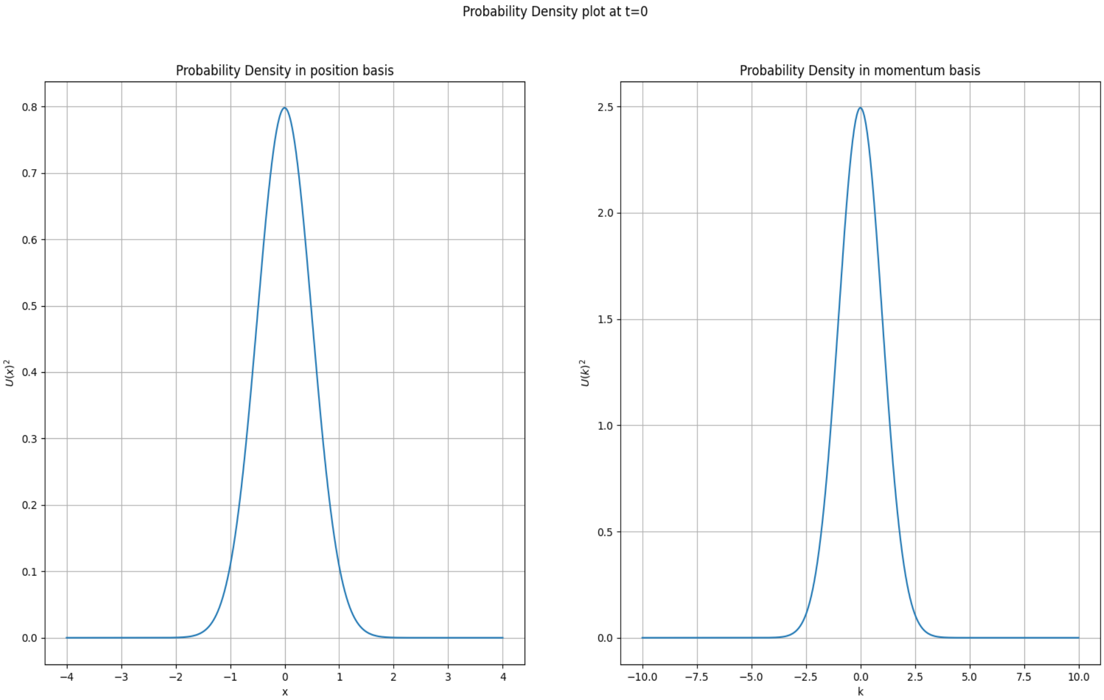

Figure 3: **The plot of $|\psi|^2$ for t=0**

The animation created to visualise time evolution :- Numerical and Analytic

The given below are plots of $|\psi|^2$ with respect to x for two different values of t.

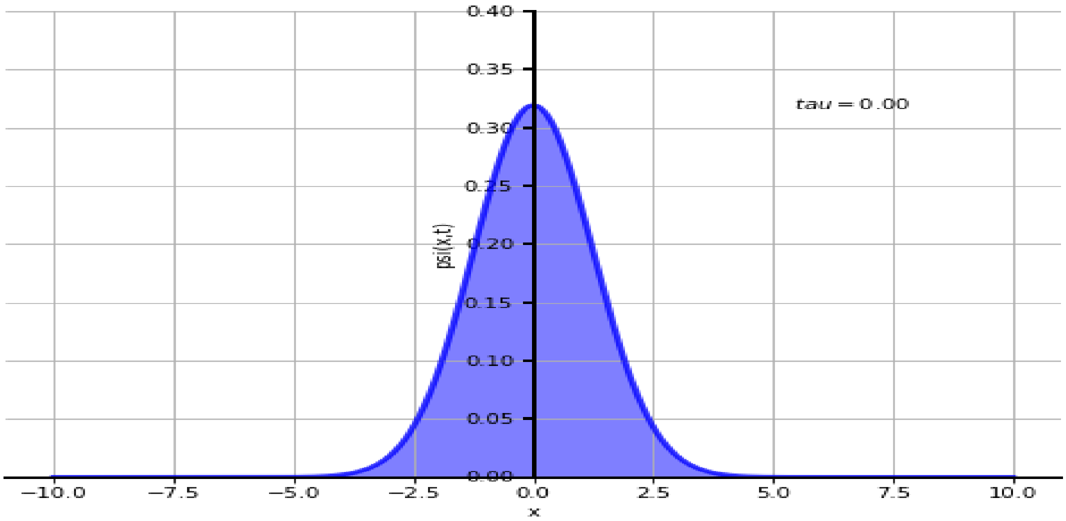

Figure 4: **The plot of $|\psi|^2$ for t=0**

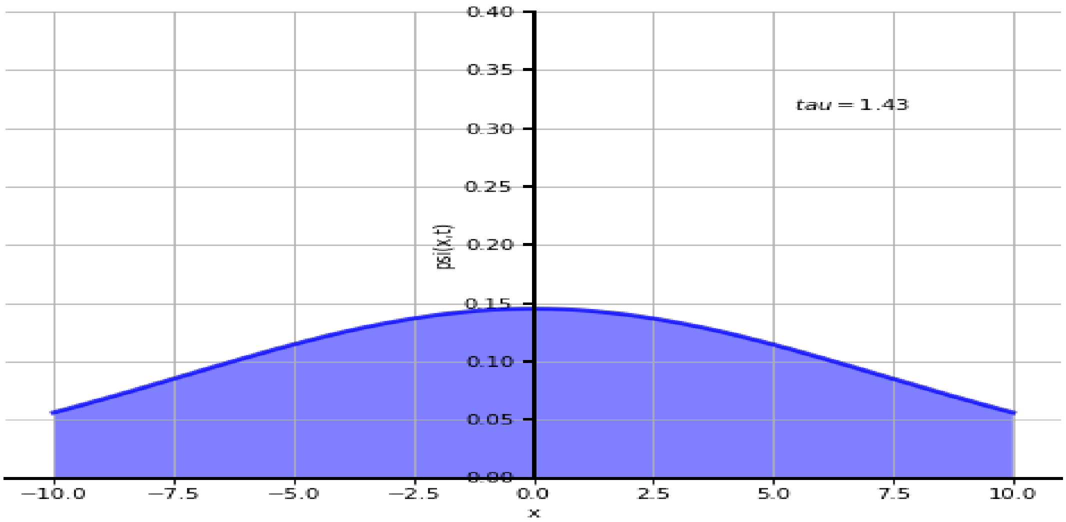

Figure 5: **The plot of $|\psi|^2$ for t=1.43**

8 REFERENCES

1. Griffiths -Introduction to Quantum Mechanics (View)

2. Solutions-of-quantum-mechanics-by-griffith (View)

3. The Quantum Mechanical Free Particle Chemistry Libre Texts (View)

4. animate-your-python-plots (View)