WAVE PACKETS
(GAUSSIAN WAVE PACKET AND ITS SPREAD WITH TIME)

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"32221501 - Quantum Mechanics and its Applications"

1 WAVE PACKETS

A localized wave function is known as a wavepacket.

A wave packet consists of a group of waves of slightly different wavelengths, with phases and amplitudes chosen such that they interfere constructively over a small region of space and destructively elsewhere.

2 GAUSSIAN WAVE PACKET AND ITS SPREAD WITH TIME

The Gaussian wave packet is a coherent state and can be expressed as a superposition of oscillator states.

Let us consider that the wave packet is given by

$$\psi(x,t) = A\int_{-\infty}^{+\infty} g(x)e^{i(kx-w(k)t)}dk \tag{1}$$

with the Gaussian form of the function g(k) given by

$$g(k) = e^{-a(k-k_0)^2} \tag{2}$$

The wave function $\psi(x,t)$., Eq (1), becomes (taking A = 1)

$$\psi(x,t) = \int_{-\infty}^{+\infty} e^{-a(k-k_0)^2}e^{i(kx-w(k)t)}dk \tag{3}$$

at t=0, we have

$$\psi(x,0) = \int_{-\infty}^{+\infty} e^{-a(k-k_0)^2}e^{ikx}dk \tag{4}$$

with k' = k - k_0, we get

$$\psi(x,0) = e^{ik_0x}\int_{-\infty}^{+\infty} e^{-a(k)^2}e^{ik'x}dk' \tag{5}$$

$$= e^{ik_0x}\int_{-\infty}^{+\infty} e^{-a(k'-\frac{ix}{2a})^2}e^{-\frac{x^2}{4a}}dk'$$

$$\psi(x,0) = e^{ik_0x}e^{-\frac{x^2}{4a}}\int_{-\infty}^{+\infty} e^{-aq^2}dk' \tag{6}$$

$$\text{with } q = k' - \frac{(ix)}{2a}$$

Using theory of complex variables, the integral may be evaluated to give

$$\psi(x,0) = e^{\frac{-x^2}{4a}}\sqrt{\frac{\pi}{a}}e^{ik_0x} = B(x)e^{ik_0x} \tag{7}$$

Here B(x) $= e^{\frac{-x^2}{4a}}\sqrt{\frac{\pi}{a}}$ is the amplitude of the wave packet and $e^{ik,x}$ is its phase factor. The absolute sqaure of $\psi(x,0)$,given by

$$|\psi(x,0)|^2 = B^2 = \frac{\pi}{a}e^{-\frac{x^2}{2a}} \tag{8}$$

has its peak value at x = 0. It may be notes that the wave packet is narrow for small values of a and broad for large values of a. Before we discuss propagation of this wave packet of this wave packet, let us see the relation of wave packet width with the width of Gaussian function g(k) used in the formation of the wave packet[Eq.(2)].

We can see the schematic plots of g(k) and B(k) for two different values of a. From Figure(1) we can see that for a = 4 and in Figure(2) for a = 1. It is clear that in Figure(2) that the effective width of the wave packet B(x) is quite large if only a narrow range of plane wave [i.e. narrow Gaussian g(k)] are taken in the formation of the wave packet. However, if a wide range of plane waves are used in the formation of wave packet, the resulting wave packet is narrow(i.e. sharply peaked) as seen in the figures.

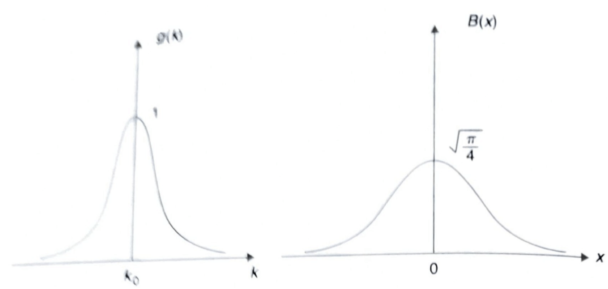


Figure 4.1 Plots of g(k) and B(x) for $a = 4$

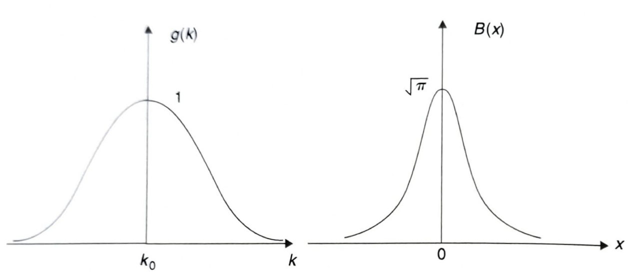


Figure 4.2 Plots of g(k) and B(x) for $a = 1$

3 Time-Development of the wave packet

Let us know study the time-development of the wave packet, that is, the propagation of the wave packet. The wave packet $\psi(x,0)$ has been formed of a continuous superposition of simple displacements e^{ikx} in a certain k - range with weight factor g(k) = $e^{-a(k-k_0)^2}$. To see how this wave packet propagates in time, we should superpose, instead of displacement e^{ikx}, the propagating plane waves, $e^{i[kx-w(k)t}$, with the same weight factor g(k). So,

$$\psi(x,t) = \int_{-\infty}^{+\infty} e^{-a(k-k_0)2} e^{i[kx-w(k)t]} dk \tag{9}$$

It may be easily checked if $\omega(k)$ is linear in k (just like in case of light wave propagating in vacuum, [Eq. (2)] may be written as

$$\begin{aligned} \psi(x,t) &= A \int_{-\infty}^{+\infty} e^{-a(k-k_0)^2 e^{ik(x-ct)} dk} \\ &= \psi(x-ct,0) \end{aligned}$$

This equation is similar to Eq(4), except that x in Eq(4) is replaced by (x - ct)here. Therefore we can easily get

$$|\psi(x-ct,0)|^2 = \frac{\pi}{a} e^{-\frac{(x-ct)^2}{2a}} \tag{10}$$

So, the wave function $\psi(x,t)[= \psi(x-ct,0)]$ is having the same shape as that of the staring wave function $\psi(x,0)$; but, instead of being peaked at x = 0, it is now peaked at x = ct. Thus, in case of light, the wave packet of light waves in vacuum propagates with the velocity of the light c, without any sort of distortion. However, the case of propagation of wave packet of matter waves may not be that simple. Let us reconsider Eq(2) representing propagation of wave packet of particle waves. Let the wave packet, we consider, be strongly localized in k-shape about k = k_0 [i.e. let a be large in the Gaussian function]

$$e^{-} a(k-k_0)$$

appearing in equation(2). We see the above figures). Then ,it is not hard to see that the integrand in Eq(2) will peak around k = k_0 and it is reasonable to expand $\omega(k)$ about k = k_0; we are implicitly assuming $\omega(k)$ to be a slowly varying function of k, So we may write -

$$\omega(k) = \omega(k_0) + (k-k_0)\frac{\partial\omega}{\partial k}_{k_0} + \frac{1}{2}(k-k_0)^2 \left(\frac{\partial^2\omega}{\partial k^2}\right)_{k0} + ... \tag{11}$$

The first term being independent of k, is a constant. The quantity

$$\frac{\partial\omega}{\partial k}_{k=0}$$

appearing in the second term is the group velocity of the wave packet.

Let

$$v_g = \frac{\partial \omega}{\partial k}_{k_0} \tag{12}$$

and

$$\beta = \frac{\partial^2 \omega}{\partial k^2}_{k_0} \tag{13}$$

then Eq(2) may be written as

$$\psi(x,t) = \int_{-\infty}^{+\infty} e^{-a(k-k_0 2} e^i[kx - \omega(k_0)t - (k-k_0)v_g t - \frac{1}{2}\beta(k-k_0)^2 t]dk$$

$$= e^{i[k_0 x - \omega(k_0)t]} \int_{-\infty}^{+\infty} e^{-ak'^2 e^{i[k'(x-v_g t)]} e^{ik'^2 \beta \frac{t}{2}}} dk' d \tag{14}$$

where k - $k_0 = k'$

This equation looks like Eq(5) with a replaced by [a + i$\frac{(\beta t)}{2}$] and x replaced by (x - v_g t). So just like Eq(5), Eq(14) may be integrated to give,

$$\psi(x,t) = e^{i[k_0 x - \omega(k_0)t]} \sqrt{\frac{\pi}{(a + \beta t/2)}} e^{-\frac{(x-v_g t)^2}{4(a+i\beta t/2)}}$$

absolute square of $\psi(x,t)$ is

$$|\psi(x,t)|^2 = \sqrt{\frac{\pi^2}{(a^2 + \beta^2 t^2/4)}} e^{-\frac{(x-v_g t)^2}{2(a+\frac{\beta^2 t^2}{4a})}} \tag{15}$$

Obviously equation(15) represents a propagating wave packet with its peak moving with velocity v_g. It may, however, be noted here that the width of the wave packet is not fixed. Comparing the two equations Eq(8) and Eq(15), one notices that the quantity a at t = 0[in Eq(8)] is replaced by $[a^2 + \frac{\beta^2 t^2}{4}]^{\frac{1}{2}}$ at time t [in Eq(15)]. So the width of the wave packet grows as it propagates, but is, the wave packet spreads as it progates.

4 Program

```
'''RAVNEET KAUR
2020PHY1064'''

```

```python
from math import sin, pi,cos
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import matplotlib.cm as cm
from matplotlib.widgets import Slider
from matplotlib.widgets import CheckButtons

def psi(t): #Calculation of wave function as a function of time
  global x
  v = alpha*k0
  w = (a**4 + ((alpha*t)**2)/4)
  wComplex = a**2 + 1j*alpha*t/4
  omega = (k0**2)*alpha/2
  probCompl = np.exp(1j*(k0*x - t*omega))*((pi/wComplex)**0.5)*np.exp(-((x - v*t)**2)/(4*wComplex))
  return probCompl

#Functions for Plots
def plot(A,B,C,D,E,F,G,H):
     fig,ax = plt.subplots(1, 2, squeeze=False, figsize=(10,5))
     ax[0,0].set(xlabel = 'Displacement (x)',ylabel="g(k)",title = "Gaussian form of the Function g(x) v/s Displacement(x)")
     ax[0,0].plot(B, C, c='midnightblue',label = 'g(k) = 1 for a = 1')
     ax[0,0].plot(B, E,c='mediumvioletred',label = 'g(k) = 1 for a = 4')
     ax[0,0].plot(B, G,c='mediumturquoise',label = 'g(k) = 1 for a = 8')
     ax[0,0].legend(loc = 'best')
     ax[0,0].grid()
     ax[0,1].plot(A,D , c = 'magenta' , label = 'B(x) =      /1 = 1.78 for a = 1')
     ax[0,1].plot(A,F,c ='sienna', label = 'B(x) =      /4 = 0.89 for a = 4')
     ax[0,1].plot(A,H,c ='yellowgreen', label = 'B(x) =      /8 = 0.22 for a = 8')
     ax[0,1].set(ylabel="Amplitude of the wavepacket B(k)")
     ax[0,1].legend(loc = 'best')
     ax[0,1].set(xlabel = "Displacement (x)",ylabel="Amplitude of the wavepacket B(k)",title = "Gaussian Wavepacket for B(x)")
     ax[0,1].legend(loc = 'best')
     ax[0,1].set(xlabel ="Displacement (x)",ylabel="Amplitude of the wavepacket B(k)",title = "Amplitude of the wavepacket B(x) v/s Displacement(x)")
     ax[0,1].grid()
     ax[0,1].legend(loc = 'best')
```

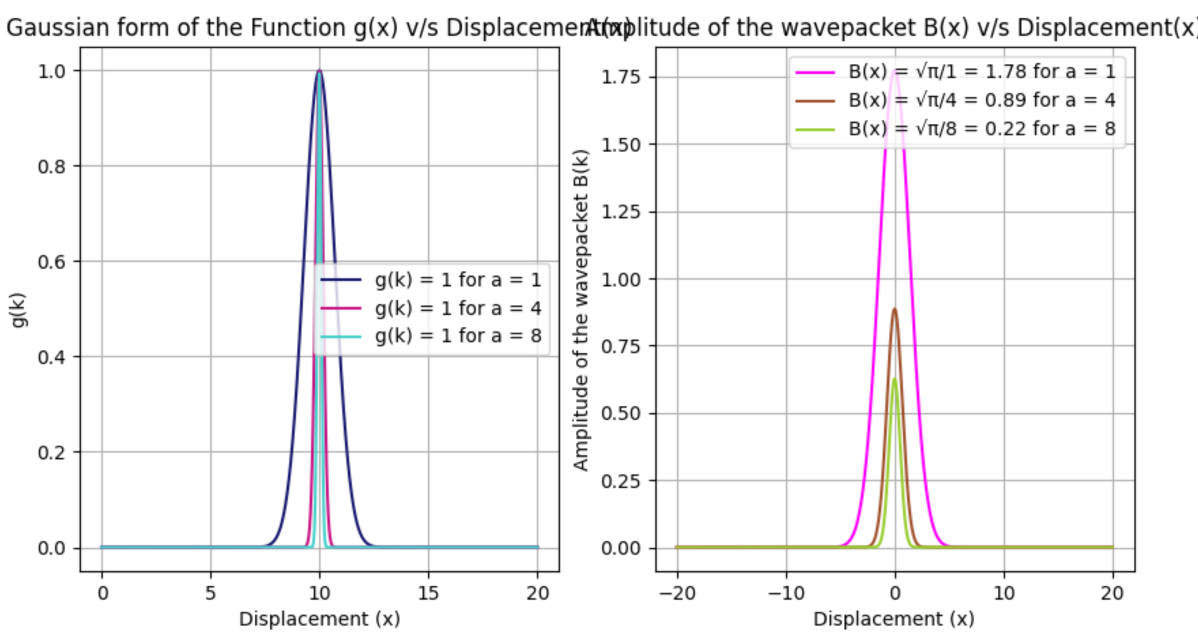
```python

def plot_1(A1,B1,C1,D1):
      fig,axe = plt.subplots(2,2)
      axe[0,0].plot(A1, B1, label = '$\operatorname{Re}(\psi)$',c='navy')
      axe[0,0].plot(A1, C1, label = '$\operatorname{Im}(\psi)$',c='pink')
      axe[0,0].plot(A1, D1, label = '$\psi \psi^{\dag} $',c='limegreen')
      axe[0,0].set_title("Gaussian Wavepacket for $\operatorname{Re}(\psi)$,$\operatorname{Im}(\psi)$ and $\psi \psi^{\dag}$")
      axe[0,0].set(xlabel = "Time (t)")
      axe[0,0].grid()
      axe[0,0].legend(loc='best')
      axe[0,1].plot(A1, B1,c='navy')
      axe[0,1].set(xlabel = "Time (t)",ylabel = '$\operatorname{Re}(\psi)$' , title = 'For Real part of Wave Function')
      axe[0,1].grid()
      axe[1,0].plot(A1, C1,c='pink')
      axe[1,0].grid()
      axe[1,0].set(xlabel = "Time (t)",ylabel = '$\operatorname{Im}(\psi)$',title = 'For Imagine part of Wave Function')
      axe[1,1].plot(A1,D1,c='limegreen')
      axe[1,1].set(xlabel = "Time (t)",ylabel = '$\psi \psi^{\dag}$',title = 'For modulus of Wave Function $\psi \psi^{\dag}$')
      axe[1,1].grid()

if __name__ == "__main__" :
    a = 1
    a0 = 4  #Gaussian distribution factor
    a1 = 8
    k0 = 10 #Central wavenumber of the Gaussian packet
    alpha = 1 #alpha = hbar/m => v = alpha*k
    x = np.linspace(-20,20,1000) #Displacement
    x1 = np.linspace(0,20,1000)
    y = np.exp(-(a**2)*(k0-x1)**2) #distribution some frequencies
    y1 = np.exp(-(a0**2)*(k0-x1)**2)
    y2 = np.exp(-(a1**2)*(k0-x1)**2)
    B_x = np.exp(-(x**2)/4*a)*np.sqrt(pi/a)  #amplitude of the wavepacket
    B_x1 = np.exp(-(x**2)/4*a0)*np.sqrt(pi/a0)
    B_x2 = np.exp(-(x**2)/4*a1)*np.sqrt(pi/a1)
    # ###################################################################################

    t=np.linspace(-1,1,1000) #time
```

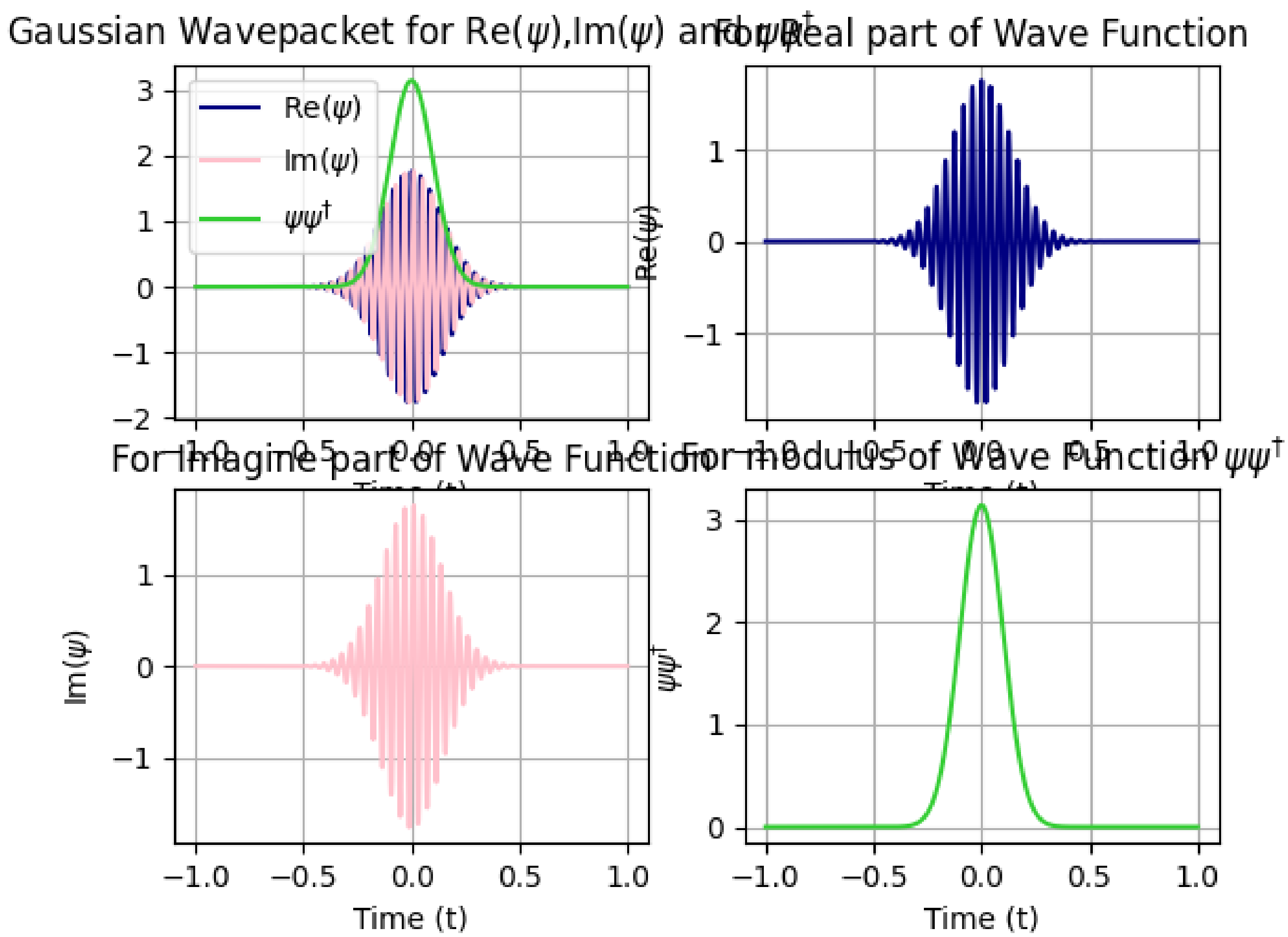
```
    probCompl = psi(t) #Wave Function

fig = plt.figure()
ax1 = fig.add_subplot(211)
ax2 = fig.add_subplot(212)
plt.subplots_adjust(left=0.12, bottom=0.35)
is_color = False
ax_a = plt.axes([0.1, 0.05, 0.8, 0.03])
a_slider = Slider(ax_a, '$t$', 0, 10, valinit=0) #slides the time
a_slider.label.set_size(20)

ax_b = plt.axes([0.1, 0.15, 0.8, 0.03])
b_slider = Slider(ax_b, '$a$', 0.01, 5, valinit=a) #slider for a
b_slider.label.set_size(20)

ax_c = plt.axes([0.1, 0.25, 0.8, 0.03])
c_slider = Slider(ax_c, '$k_0$', 1, 15, valinit=k0)#slider for k0
c_slider.label.set_size(20)

rax = plt.axes([0.01, 0.45, 0.08, 0.1]) #Color control button
check = CheckButtons(rax,['color'], [False])


def update_phase(val_):
  global a
  a = b_slider.val
  y = np.exp(- (a**2)*(k0-x)**2) #distribution some frequencies
  B_x = np.exp(-(x**2)/4*a)*np.sqrt(pi/a)
  ax1.clear()
  ax1.set_title('Gaussian Wavepacket')
  ax1.plot(x, y,label='g(k)')
  ax1.plot(x,B_x,label='B(x)')
  ax1.grid()
  ax1.legend()
  fig.canvas.draw_idle()
  update_temps(0)

def update_temps(val_): #Drawing the wave function

  probCompl = psi(a_slider.val)
  ax2.clear()
  ax2.set_xlim([-20,20])
```

```
  ax2.set_ylim([-4, 4])
  ax2.set_title('Wavefunction')

  if(is_color): #Color Display
    X = np.array([x,x])
    y0 = np.zeros(len(x))
    y = [abs(i) for i in probCompl]
    Y = np.array([y0,y])
    Z = np.array([probCompl,probCompl])
    C = np.angle(Z)
    ax2.pcolormesh(X, Y, C, cmap=cm.hsv, vmin=-np.pi, vmax=np.pi)
    ax2.plot(x, np.abs(probCompl), label = '$|\psi|$', color='black')
    ax2.grid()

  else: #Display of real and complex games
    ax2.plot(x, np.real(probCompl), label = '$\operatorname{Re}(\psi)$')
    ax2.plot(x, np.imag(probCompl), label = '$\operatorname{Im}(\psi)$')
    ax2.plot(x, np.absolute(probCompl)**2, label = '$\psi \psi^{\dag} $')
    ax2.legend(loc='best')
    ax2.grid()

  ax2.legend(fontsize=15)
  fig.canvas.draw_idle()

def update_k(val_): #changing k0
  global k0
  k0 = c_slider.val
  update_phase(0)
  update_temps(0)

def on_check(label): #when you click on the button
  global is_color
  is_color = not is_color
  update_temps(0)
update_phase(0) #Creation of the first frame

#Associating functions with sliders
a_slider.on_changed(update_temps)
b_slider.on_changed(update_phase)
c_slider.on_changed(update_k)

check.on_clicked(on_check)
```

```

plot(x,x1,y,B_x,y1,B_x1,y2,B_x2)
plot_1(t,np.real(probCompl),np.imag(probCompl),np.absolute(probCompl)**2)
plt.show()

#Printing Data for the results
data1 = {"Displacement(x)":x,"Gaussian form of the Function g(k) for a = 1":y,"
    Gaussian form of the Function g(k) for a = 4":y1,"Gaussian form of the
    Function g(k) for a = 8":y2}
print(pd.DataFrame(data1))
data2 = {"Displacement(x)":x1,"Amplitude of the wavepacket B(k) for a = 1":B_x,"
    Amplitude of the wavepacket B(k) for a = 4":B_x1,"Amplitude of the wavepacket
    B(k) for a = 8":B_x2}
print(pd.DataFrame(data2))
data3 = {"Time (t)":t,"Real(  )":np.real(probCompl), "Imaginary(  )":np.imag(
    probCompl),"    +":np.absolute(probCompl)**2}
print(pd.DataFrame(data3))
pd.set_option('display.expand_frame_repr',False)
pd.set_option('display.max_rows', None)
```

5 Output





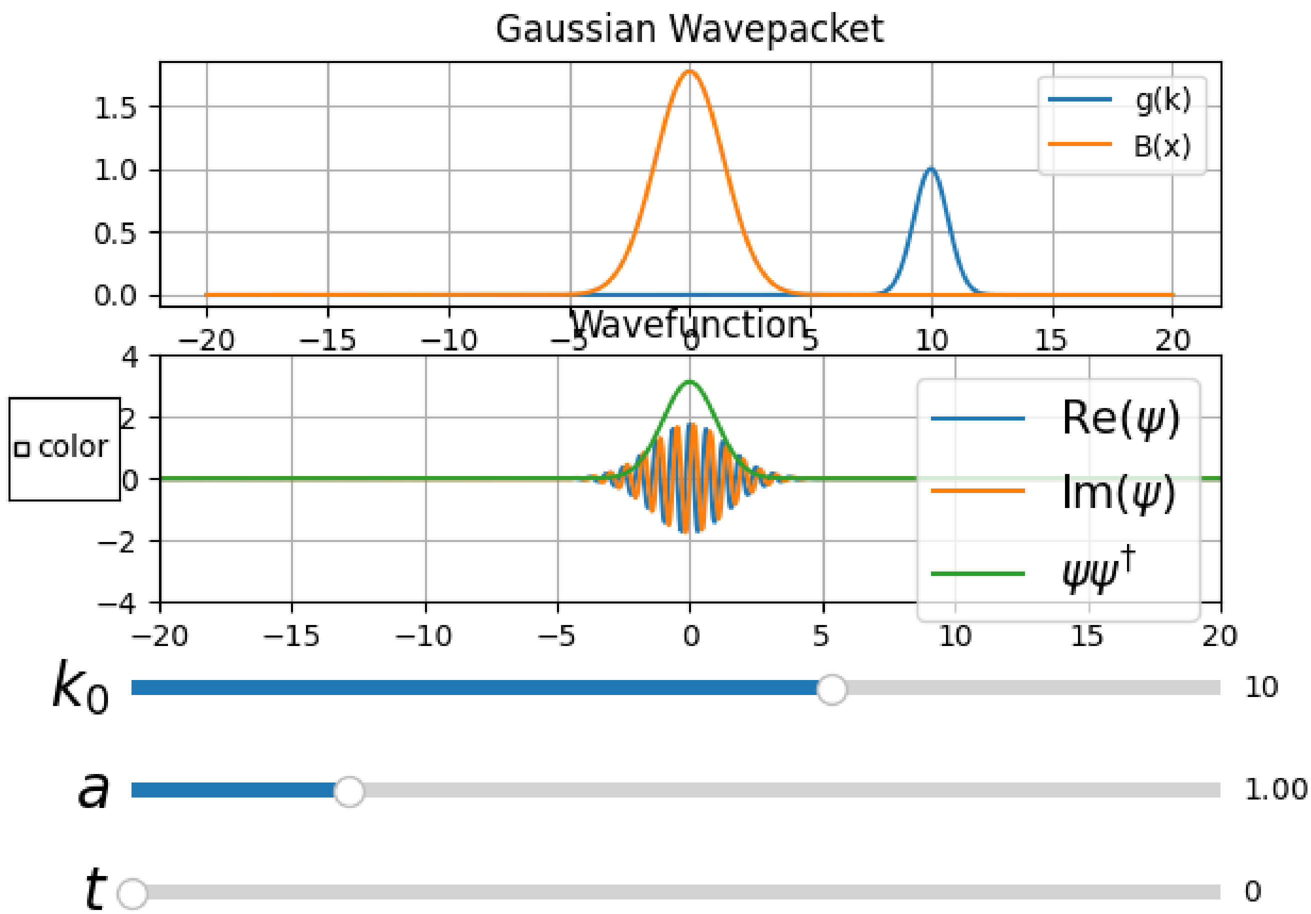
6 Results

Since we have plotted various plots for the wave packets.

PLOT-1 We have observed that for different values of a,the Gaussian Distribution Factor the peak points change. for small a, the peak point is broad but in case of large values of a, the peak becomes narrow. Similar is the case for amplitude of the Gaussian function.

PLOT-2 In graph 2, we can see the spreading of the wave packet w.r.t time for the wave function. We have plotted the real, imaginary and the magnitude of the wave function for a = 1 and divided the axis with a itself.

PLOT-3 In graph 3, we have used the sliders in order to illustrate the change in behaviour of the of the wave corresponding to the wave number,distribution factor and time. This will perfectly



depict the Gaussian Wave packet.

7 References

1. Principles of Quantum Mechanics by Dr. Ishwar Singh Tyagi.
2. Quantum Mechanics Concepts and Applications by Nouredine Zetli.
3. http://www.softsea.com/screenshot/Gaussian-Wave-Packet-Step-Scattering.html
4. https://youtu.be/pB4$_{G}eY5f_{o}5.https : //github.com/Azercoco/gaussian_{w}ave_{p}acket/blob$ $/master/gaussian_{w}ave_{p}acket.py$

dell@dell-Inspiron-3593: ~/Desktop

```
dell@dell-Inspiron-3593:~/Desktop$ python3 shukla.py
dell@dell-Inspiron-3593:~/Desktop$ python3 rav.py
     Displacement(x)  Gaussian form of the Function g(k) for a = 1  Gaussian form of the Function g(k) for a = 4  Gaussian form of the Function g(k) for a =
0          -20.00000                                  3.720076e-44                                           0.0                                           0
1          -19.95996                                  5.549699e-44                                           0.0                                           0
2          -19.91992                                  8.272541e-44                                           0.0                                           0
3          -19.87988                                  1.232141e-43                                           0.0                                           0
4          -19.83984                                  1.833722e-43                                           0.0                                           0
..               ...                                           ...                                           ...                                           .
995         19.83984                                  1.833722e-43                                           0.0                                           0
996         19.87988                                  1.232141e-43                                           0.0                                           0
997         19.91992                                  8.272541e-44                                           0.0                                           0
998         19.95996                                  5.549699e-44                                           0.0                                           0
999         20.00000                                  3.720076e-44                                           0.0                                           0

[1000 rows x 4 columns]
     Displacement(x)  Amplitude of the wavepacket B(k) for a = 1  Amplitude of the wavepacket B(k) for a = 4  Amplitude of the wavepacket B(k) for a = 8
0            0.00000                                6.593663e-44                               1.697275e-174                                         0.0
1            0.02002                                9.836585e-44                               8.406644e-174                                         0.0
2            0.04004                                1.466270e-43                               4.150502e-173                                         0.0
3            0.06006                                2.183912e-43                               2.042613e-172                                         0.0
4            0.08008                                3.250188e-43                               1.002026e-171                                         0.0
..               ...                                         ...                                         ...                                         ...
995         19.91992                                3.250188e-43                               1.002026e-171                                         0.0
996         19.93994                                2.183912e-43                               2.042613e-172                                         0.0
997         19.95996                                1.466270e-43                               4.150502e-173                                         0.0
998         19.97998                                9.836585e-44                               8.406644e-174                                         0.0
999         20.00000                                6.593663e-44                               1.697275e-174                                         0.0

[1000 rows x 4 columns]
     Time (t)       Real(Ψ)  Imaginary(Ψ)          ΨΨ+
0   -1.000000  2.620892e-11  1.022043e-10  1.113264e-20
1   -0.997998 -9.549182e-12  1.148971e-10  1.329254e-20
2   -0.995996 -5.098887e-11  1.151838e-10  1.586717e-20
3   -0.993994 -9.384241e-11  1.006426e-10  1.893533e-20
4   -0.991992 -1.328440e-10  7.030701e-11  2.259059e-20
..        ...           ...           ...          ...
995  0.991992 -1.328440e-10 -7.030701e-11  2.259059e-20
996  0.993994 -9.384241e-11 -1.006426e-10  1.893533e-20
997  0.995996 -5.098887e-11 -1.151838e-10  1.586717e-20
998  0.997998 -9.549182e-12 -1.148971e-10  1.329254e-20
999  1.000000  2.620892e-11 -1.022043e-10  1.113264e-20

[1000 rows x 4 columns]
dell@dell-Inspiron-3593:~/Desktop$
```