Assignment 11 - Time Evolution of Wave Packet

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Theory

(a) Write Schrodinger Wave Eqn for free particle in dimensionless form & determine stationary states?

Ans. The TISE is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\,\psi(x) = E(x)$$

for free particle $V(x) = 0$

$$+\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + E(x) = 0$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}E(x) = 0 \qquad -(1)$$

To this Equation dimensionless,

Take $\xi\, x = \frac{x}{L}$

$$\frac{\partial^2\psi}{\partial x^2} = \frac{1}{L^2}\frac{\partial^2\psi}{\partial \xi^2}$$

Put $\frac{\partial^2\psi}{\partial x^2}$ in (1)

$$\frac{\partial^2\psi}{\partial \xi^2} + \frac{2mL^2}{\hbar^2}E(\xi) = 0$$

Now take $e = \frac{\hbar^2}{2m\hbar^2}$

$$\frac{\partial^2\psi}{\partial \xi^2} + e\,E(\xi) = 0$$

which is dimensionless.

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(b) Discuss why stationary state can't represent physical state?

Ans The wave function is not normalisable in stationary state, so it can't represent physical state.

(c) what is wave packet? Show that group velocity of wave packet corresponds to speed of free particle.

Ans 'Wave packet is linear combination of ~~well defined~~ individual waves with well defined frequency.

As we know from schrodinger Eqn for wave particle

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

Taking $k = \frac{\sqrt{2mE}}{\hbar}$

The solⁿ is

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

For particular k, $E_k = \frac{\hbar^2 k^2}{2m}$

As we know $E = h\nu = \frac{h\omega}{2\pi} = \frac{\hbar^2 k^2}{2m}$

So, $\omega = \frac{\hbar k^2}{2m}$

phase velocity $v_p = \frac{\omega}{k} = \frac{\hbar k}{2m}$

speed of free particle from K.E

$$v = \sqrt{\frac{2E}{m}} = \frac{\hbar k}{m} = \frac{v_p}{2}$$

Wave packet is made of individual ripples ~~made of~~ which are contained in envelope. The speed of envelope is group velocity.

Let's take

$$\psi'(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \phi(k)\, e^{i(kx-\omega t)}$$

From Taylor expansion

$\omega(k) \simeq \omega_0 + \omega_0'(k-k_0)$

Take $s = k - k_0$

Now, $\psi'(x,t)$ becomes at $k = k_0$

$$\psi'(x,t) = \frac{1}{\sqrt{2\pi}} e^{i(k_0 x - \omega_0 t)} \int_{-\infty}^{\infty} ds\, \phi(k_0+s)\, e^{is(x-\omega_0' t)}$$

From above expression, we can see

$$v_{group} = \frac{d\omega}{dk} = \frac{\hbar k \times 2}{2 \hbar m} = \frac{\hbar k_0}{m} = \frac{\omega_0'}{k} \qquad \left[\text{here } \omega = \frac{\hbar k^2}{2m}\right]$$

Relating it with velocity of free particle, we found they both are same

(d) How wavepacket evolves with time?

The above expression

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} e^{i(k x-\omega_0 t)} \int_{-\infty}^{\infty} ds\, \phi(k_0+s)\, e^{is(x-\omega_0' t)}$$

gives time evolution of wave packet.

(e)

$$\psi(x,0) = \begin{cases} A & |x| < b \\ 0 & |x| > b \end{cases}$$

Normalising $\psi(x,0)$

$$\int_{-\infty}^{\infty} |\psi(x,0)|^2 dx = |A|^2 \times 2b = 1 \rightarrow \boxed{A = \frac{1}{\sqrt{2b}}}$$

As $\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} a(k)\, e^{ikx}\, dk$

So, $a(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,0)\, e^{-ikx}\, dx$

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$$a(k) = \frac{1}{\sqrt{2\pi}} \times \frac{1}{\sqrt{2b}} \int_{-\infty}^{\infty} e^{-ikx}\, dx$$

$$= \frac{1}{(-ik)2\sqrt{\pi b}} \left[e^{-ikx} \right]_{-b}^{b} \rightarrow \frac{1}{\sqrt{\pi b}\, k} \left(\frac{e^{ikb} - e^{-ikb}}{2i} \right)$$

$$= \frac{1}{\sqrt{\pi b}\, k} \sin(kb)$$

(F) $$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} a(k)\, e^{ik\left(x - \frac{\hbar k^2 t}{2m}\right)}\, dk$$

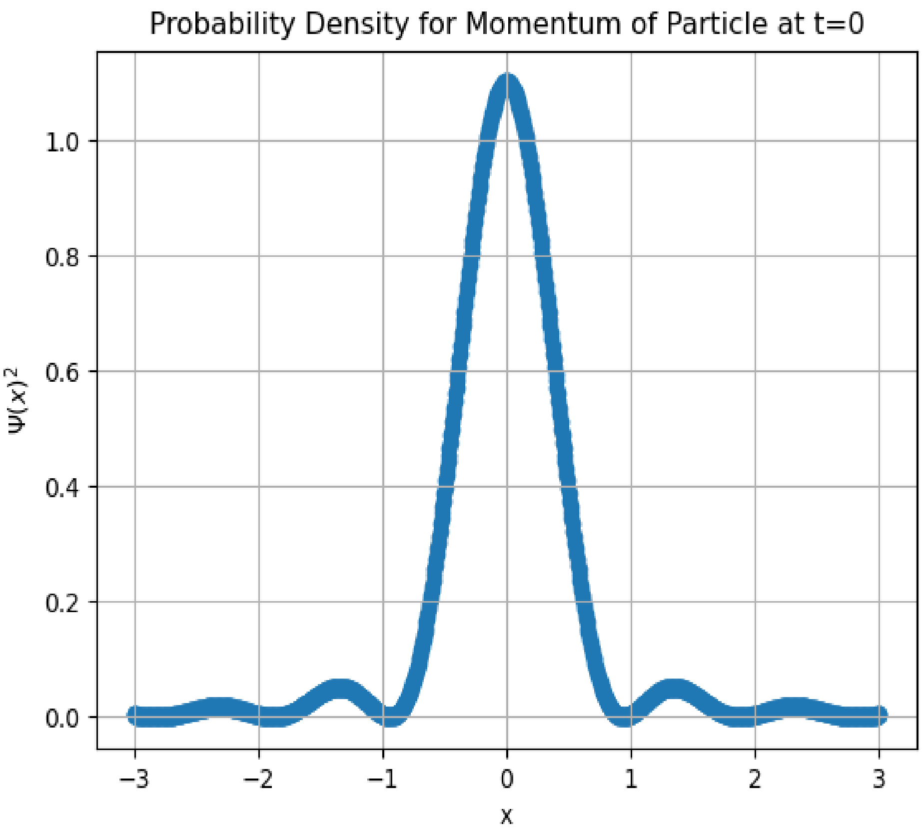
$$\psi(x,t) = \frac{1}{\sqrt{\pi b}\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\sin(kb)}{k}\, e^{ik\left(x - \frac{\hbar k^2 t}{2m}\right)}\, dk$$

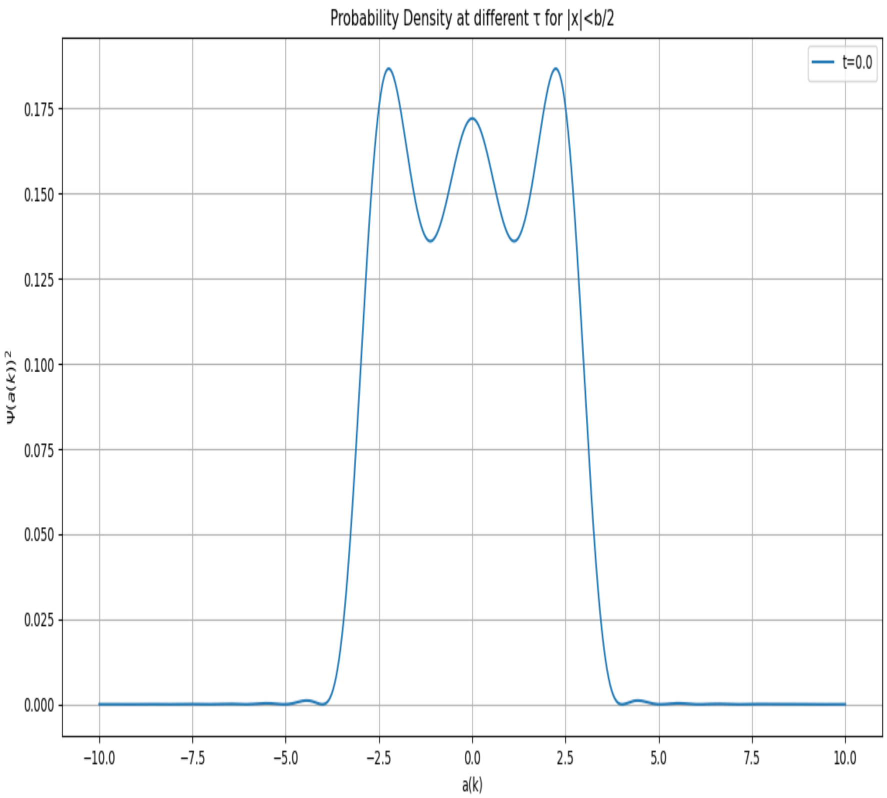
Programming

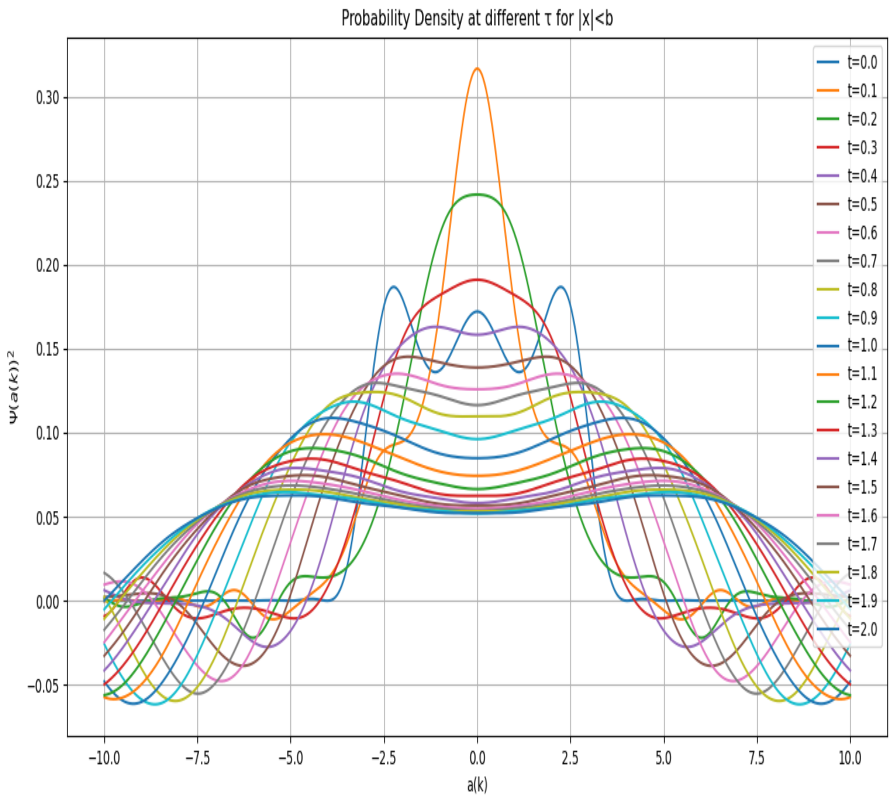
```
import numpy as np
import matplotlib.pyplot as plt
import math
import scipy.integrate as integrate
from scipy import optimize,stats
from scipy.optimize import fsolve
import pandas as pd
from scipy.integrate import solve_ivp
import array

# def a_k(xi,xf,N,B):
#     array=[];psi=[]
#     x=np.linspace(xi,xf,N)
#     k=np.linspace(-10,10,N)
#     for i in x:
#         if abs(i)<=B:
#             psi.append(1/np.sqrt(2*B))
#         else:
#             psi.append(0)
#     for i in k:
#         array_=(1/np.sqrt(2*np.pi))*integrate.simps(psi*np.exp(complex(0,-1)*x*i),x)
#         array.append(array_)
#     u_norm=array/np.sqrt(integrate.simps(np.power(array,2),x))
#     # plt.scatter(x,u_norm**2)
#     # plt.xlabel("x")
#     # plt.ylabel("$  (x)^2$")
#     # plt.grid()
#     # plt.title("Probability Density for Momentum of Particle at t=0")
# #     plt.show()
#     return u_norm, x

# def wv_fn(xi,xf,t,N,B):
#     k=np.linspace(-10,10,N)
#     u_norm,x = a_k(-3,3,N,1)
#     for j in t:
#         wv_fn=[]
#         for i in x:
#             wv_fn_=(1/np.sqrt(2*np.pi))*integrate.simps(u_norm*np.exp(complex(0,-1)*(i*k-(k**2)*j)),k)
#             wv_fn.append(wv_fn_)
#         wv_norm=wv_fn/np.sqrt(integrate.simps(np.power(wv_fn,2),k))
#         plt.plot(k,wv_norm**2,label=f't={np.round(j,2)}')
#         plt.grid()
#         plt.xlabel("a(k)")
#         plt.ylabel("$  (a(k))^2$")
#         plt.title("Probability Density at different    for |x|<b/2")
#         plt.legend()
#     plt.show()

'''-----------------------------------------Q(a)---------------------------------------------------'''
# xi=-3;xf=3;N=1000;B=1
# t=np.arange(0,0.1,0.1)
# wv_fn(xi,xf,t,N,B/2)

'''-------------------------------------------Q(b)-----------------------------------------------'''
# xi=-3;xf=3;N=1000;B=1
# t=np.arange(0,2.1,0.1)
# wv_fn(xi,xf,t,N,B/2)

def a_k_gaussian(xi,xf,N,A,a):
    array=[];psi=[]
    x=np.linspace(xi,xf,N)
```

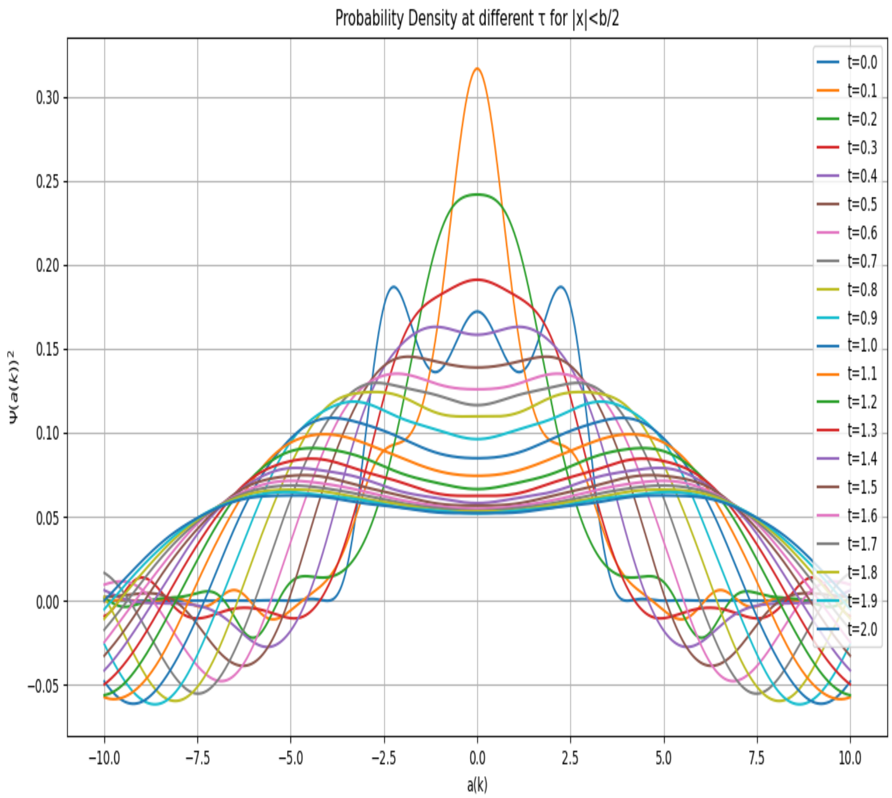
```
    k=np.linspace(-10,10,N)
    for i in x:
        psi.append(np.power(2*a/np.pi,1/4))
    for i in k:
        array_=(1/np.sqrt(2*np.pi))*integrate.simps(psi*np.exp(-a*(x**2))*np.exp(complex(0,-1)*i*x),x)
        array.append(array_)
    u_norm=array/np.sqrt(integrate.simps(np.power(array,2),x))
    plt.scatter(x,u_norm**2)
    plt.xlabel("x")
    plt.ylabel("$  (x)^2$")
    plt.grid()
    plt.title("Probability Density for Momentum of Particle at t=0")
    plt.show()
    return u_norm, x

def wv_fn_gaussian(xi,xf,t,N,A,a):
    k=np.linspace(-10,10,N)
    u_norm,x = a_k_gaussian(xi,xf,N,A,a)
    for j in t:
        wv_fn=[]
        for i in x:
            wv_fn_=(1/np.sqrt(2*np.pi))*integrate.simps(u_norm*np.exp(complex(0,-1)*(i*k-(k**2)*j)),k)
            wv_fn.append(wv_fn_)
        wv_norm=wv_fn/np.sqrt(integrate.simps(np.power(wv_fn,2),k))
        plt.plot(k,wv_norm**2,label=f't={np.round(j,2)}')
        plt.grid()
        plt.xlabel("a(k)")
        plt.ylabel("$  (a(k))^2$")
        plt.title("Probability Density at different    for |x|<b/2")
        plt.legend()
    plt.show()
xi=-3;xf=3;N=1000;B=1;a=1
t=np.arange(0,2.1,0.1)
wv_fn_gaussian(xi,xf,t,N,B,a)
```

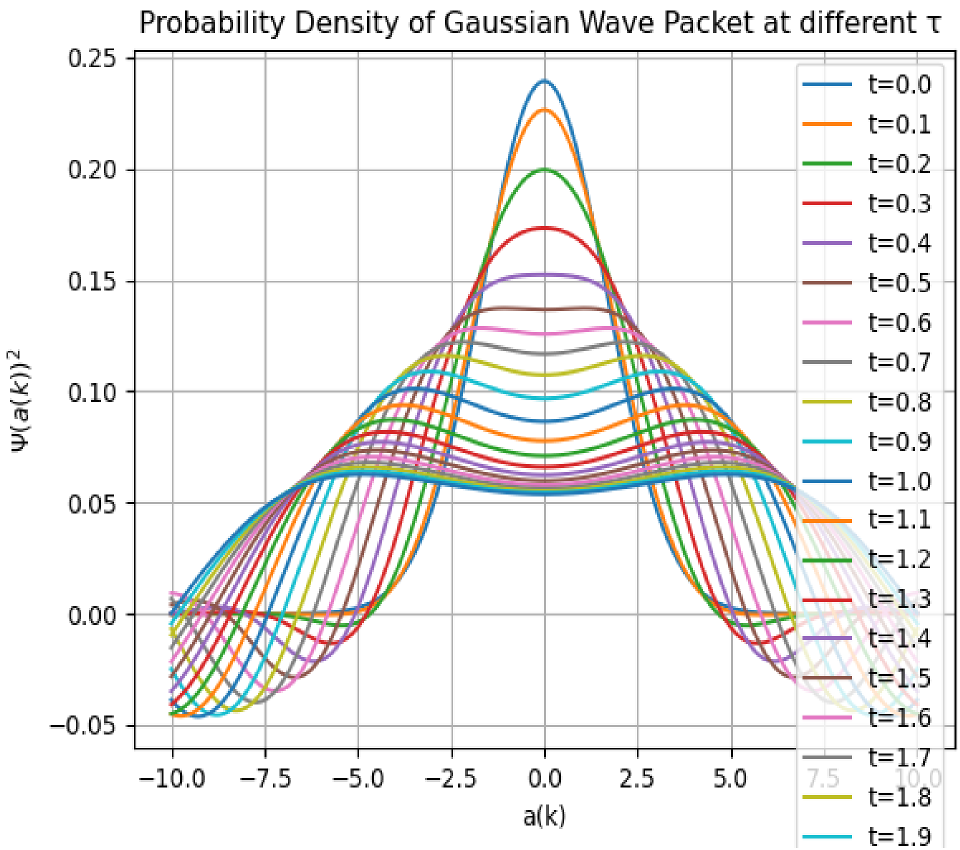
Result and Discussion




Probability Density at different τ for |x|<b/2
t=0.0
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0
a(k)
Ψ(a(k))²


Probability Density at different τ for |x|<b
$\Psi(a(k))^2$
a(k)
0.30
0.25
0.20
0.15
0.10
0.05
0.00
−0.05
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0
t=0.0
t=0.1
t=0.2
t=0.3
t=0.4
t=0.5
t=0.6
t=0.7
t=0.8
t=0.9
t=1.0
t=1.1
t=1.2
t=1.3
t=1.4
t=1.5
t=1.6
t=1.7
t=1.8
t=1.9
t=2.0


Probability Density at different τ for |x|<b/2
$\Psi(a(k))^2$
a(k)
t=0.0
t=0.1
t=0.2
t=0.3
t=0.4
t=0.5
t=0.6
t=0.7
t=0.8
t=0.9
t=1.0
t=1.1
t=1.2
t=1.3
t=1.4
t=1.5
t=1.6
t=1.7
t=1.8
t=1.9
t=2.0


Probability Density of Gaussian Wave Packet at different τ
0.25
0.20
0.15
0.10
0.05
0.00
−0.05
$\Psi(a(k))^2$
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0
a(k)
t=0.0
t=0.1
t=0.2
t=0.3
t=0.4
t=0.5
t=0.6
t=0.7
t=0.8
t=0.9
t=1.0
t=1.1
t=1.2
t=1.3
t=1.4
t=1.5
t=1.6
t=1.7
t=1.8
t=1.9