IISER Kolkata

PH3203 Advanced Quantum Mechanics

Project Report

Non Spreading Wave Packets in Free Space - Airy Packets

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Abstract

This project is about non-spreading wave packets in quantum mechanics.Initially the Airy function and the different concepts of motion and spreading of wave packets are introduced. Then non-spreading wave packets in free space are discussed.

Contents

Chapter 1

Background

1.1 The Airy function

The Airy function and few of its important properties are introduced here.

1.1.1 Airy differential equation and solutions

The Airy differential equation is given by

$$y'' - xy = 0 \tag{1.1}$$

This is a second order non-linear differential equation in x.We want solutions over $\mathbb{R}$. There are no singular points in the domain. Hence we can use a power series expansion for y(x)

$$y = \sum_{n=0}^{\infty} a_n x^n \tag{1.2}$$

With this we obtain the recurrence relation connecting the a_n as given below. Note a_2 comes out to be zero.

$$\sum_{t=1}^{\infty} [(t+2)(t+1)a_{t+2} - a_{t-1}]x^t = 0 \tag{1.3}$$

This gives the relation $a_{t+2} = \frac{a_{t-1}}{(t+1)(t+2)}$ with t taking values from 1 to ∞. With this we finally define the 2 linearly independent solutions

$$f(x) = \sum_{k=1}^{\infty} \frac{x^{3k}}{(2.3)(5.6)....((3k-1).(3k))} + 1 \tag{1.4}$$

$$g(x) = x + \sum_{k=1}^{\infty} \frac{x^{3k+1}}{(3.4)(6.7)....((3k).(3k+1))} \tag{1.5}$$

The general solution to the differential equation is given by $y(x) = c_1 f(x) + c_2 g(x)$. Choosing particular values of the constants we get the well known airy functions $Ai(x)$ and $Bi(x)$. Define:

$$Ai(x) := c_1 f(x) - c_2 g(x) \tag{1.6}$$

$$Bi(x) := \sqrt{3}(c_1 f(x) - c_2 g(x)) \tag{1.7}$$

$$c_1 := \frac{1}{3^{2/3}\Gamma(2/3)} \tag{1.8}$$

$$c_2 := -\frac{1}{3^{1/3}\Gamma(2/3)} \tag{1.9}$$

In this report, only the $Ai(x)$ is of relevance. Its graph is given below.

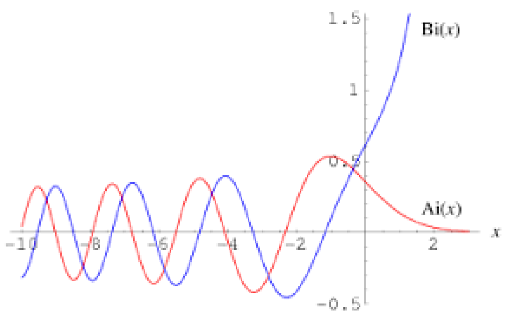

Figure 1.1: The red line corresponds to $Ai(x)$ which is of relevance

1.2 Properties

The airy function has several important properties of which a few shall be stated here without proof.The proofs of the relevant claims to the discussion can be found in the appendix.

- Suppose we start with the differential equation (1.1). By using the technique of the

Laplace Transform,we can also construct the solution in the following manner.

$$y = \int_C e^{-xz} v(z) dz \tag{1.10}$$

$$\implies v' + z^2 v = 0 \tag{1.11}$$

$$\implies y = \int_C e^{xz - \frac{z^3}{3}} dz \tag{1.12}$$

With a suitable choice of the contour C in the complex plane(A contour such that v(z) should vanish at the boundaries and the integral should stay finite no matter how large x is.), we obtain the following expression.

$$Ai(x) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} e^{xz - \frac{z^3}{3}} dz \tag{1.13}$$

- Another important transformation equation is given below.It is a consequence of the the above representation.

$$\int_{\infty}^{\infty} e^{i[\frac{z^3}{3} + az^2 + bz]} dz = 2\pi Ai(b - a^2) e^{ia(\frac{2a^2}{3} - b)}$$

- The fourier transform of $Ai(x)$ is given below. The proof is in the appendix. We have

f(x)	$\int_{-\infty}^{\infty} f(x) e^{(-iwx)}$
Ai(x)	$e^{i\frac{w^3}{3}}$

1.3 Wavepackets

1.3.1 Introduction

We know that the solution for a free particle Hamiltonian in the time dependent wave equation results in plane wave functions of the form:

$$\psi(\vec{r}, t) = A e^{i(\vec{k} \cdot \vec{r} - \omega t)} \tag{1.14}$$

where $\omega = \frac{\hbar|\vec{k}|^2}{2m}$. The linearity of the wave equation tells us that a superposition of all the solutions is also a solution of the wave equation.Such a superposition can be written as follows:

$$\psi(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \int g(\vec{k}) e^{i(\vec{k}\cdot\vec{r}-\omega(k)t)} d^3\vec{k} \tag{1.15}$$

where $d^3\vec{k}$ is the volume element in k-space and $g(\vec{k})$ is the weight function. A wave function represented as above is known as a 3-dimensional "wave packet". In the one dimensional case:

$$\psi(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} g(k) e^{i(kx-\omega(k)t)} dk \tag{1.16}$$

$g(k)$ now is just the Fourier transform of $\psi(x,0)$.

It is to be noted here that a particular plane wave solution is not square integrable whereas a superposition of plane waves is square integrable.

1.3.2 Motion and spreading of wave packets

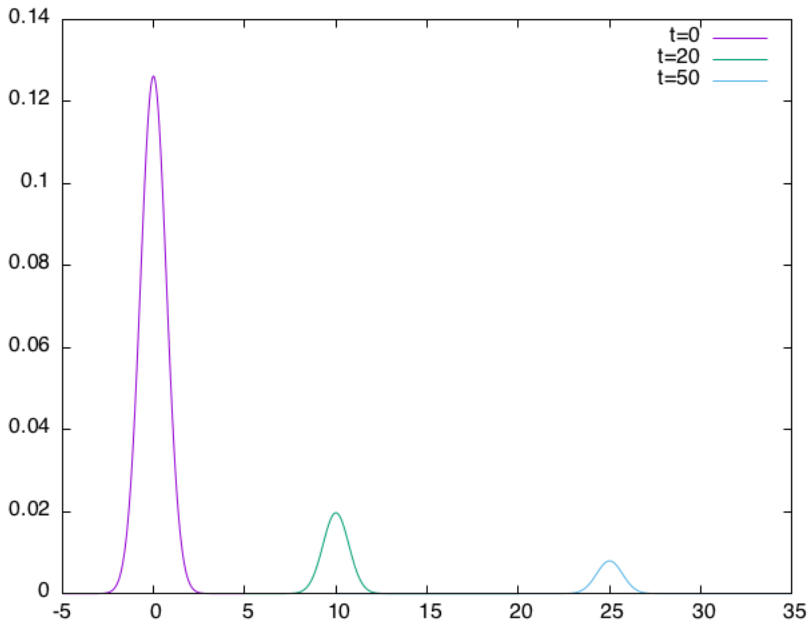

Figure 1.2: A Gaussian wave packet spreading in time

In the limit $h \to 0$, we expect the Schrodinger equation to give us the known results of classical mechanics.One of the most important classical approximations is treating particles as wave packets. At any given time, a dynamical system is represented by its position and velocity.However, we know that,since q(position) and p(momentum) are non-commuting observables in quantum mechanics, the best we can do is form a minimum uncertainty wave packet and associate the mean values of q and p with a particle.This should satisfy a couple of important requirements:

- The mean values obey the laws of classical physics.
- The dimensions of the wave packet are small compared to the physical situation and they remain small as time progresses

As we shall soon see, atleast in free space, the classical approximation is limited by the fact that requirement 2 cannot be satisfied for all time. Let us restrict the treatment to a one dimensional case.The Ehrenfest theorem states that for any observable A(p,q)

$$i\hbar\frac{d<A>}{dt} =<[A,H]> \tag{1.17}$$

$$\frac{d<q>}{dt} =<\frac{\partial H}{\partial p}> \tag{1.18}$$

$$\frac{d<p>}{dt} =-<\frac{\partial H}{\partial q}> \tag{1.19}$$

Let $H=\frac{p^2}{2m}+V(q)$. This is the well known Hamiltonian of a particle moving in a potential V(q). Introducing the the force as $F=-\frac{\partial V}{\partial x}$, we get the equations

$$\frac{d<q>}{dt}=\frac{<p>}{m} \tag{1.20}$$

$$\frac{d<p>}{dt}=\frac{<F>}{m} \tag{1.21}$$

These equations closely resemble the well known classical equations with a small difference.The point is <q> would obey the classical equations if I could replace if the average <F(q)> could be replaced by F(<q>). This, as we shall soon see, is not a trivial requirement. Define the variable $\chi=(\Delta q)^2 =<q^2>-<q>^2$ and $\varpi=(\Delta p)^2 =<p^2> - <p>^2$. In the classical approximation, this represents a particle with position <q> and momentum <p>.$E_{cl}=\frac{p^2}{2m}+V(<q>)$ gives the classical energy of the system.Define $\epsilon =<H> -E_cl$.Since the extension of the wave packet, $\sqrt{\chi}$ is small, let us taylor expand V(q) and V'(q) around the point <q>.Hence

$$V(q)=V_{cl}+(q-<q>)V'_{cl}+\frac{1}{2}(q-<q>)^2V"(<q>)_{cl}+.... \tag{1.22}$$

$$V'(q)=V'_{cl}+(q-<q>)V"_{cl}+\frac{1}{2}(q-<q>)^2V"'_{cl} \tag{1.23}$$

When we average these 2 equations, the average of terms like (q-<q>) goes to zero. Hence, our equations reduce to,

$$< V >= V_{cl} + \frac{\chi}{2} V"_{cl} \tag{1.24}$$

$$< V' >= V'_{cl} + \frac{\chi}{2} V"'_{cl} \tag{1.25}$$

With this,we see that a sufficient condition for the Ehrenfest theorem to completely behave classically is $V"'_{cl} = 0$. This is definitely justified for cases like the harmonic oscillator or the free particle. In general, we want V"' to be a very slowly varying function. Since χ is itself a mean value, using the ehrenfest theorem we compute $\frac{d\chi}{dt}$ and $\frac{d^2\chi}{dt^2}$. Also, the quantity ϵ can now be written as

$$\epsilon =< H > -E_{cl} \tag{1.26}$$

$$< H >= \frac{p^2}{2m} + < V(q) > \tag{1.27}$$

$$\frac{p^2}{2m} = \frac{\varpi + < p >^2}{2m} \tag{1.28}$$

$$\epsilon = \frac{\varpi + m\chi V"_{cl}}{2m} \tag{1.29}$$

For studying how χ changes with time, we get the following equations

$$\frac{d\chi}{dt} =< [\chi, H] > \tag{1.30}$$

$$\frac{d\chi}{dt} = \frac{1}{m}(< pq + qp > -2 < p >< q >) \tag{1.31}$$

$$\frac{d^2\chi}{dt^2} = \frac{2}{m^2}(\varpi - mV"_{cl}\chi) \tag{1.32}$$

$$\frac{d^2\chi}{dt^2} = \frac{4}{m}(\epsilon - V"_{cl}\chi) \tag{1.33}$$

In our case $V"_{cl} = 0$ as V $=$ 0. In the free particle case, therefore, we list the results.

$$< V >= 0 \quad (1.34)$$
$$< p >= k \quad (1.35)$$
$$< q >= \frac{< p > t}{m} \quad (1.36)$$
$$\varpi = 2m\epsilon(constant) \quad (1.37)$$
$$\frac{d^2\chi}{dt^2} = \frac{2\varpi}{m^2} \quad (1.38)$$
$$\chi = \chi_0 + \ddot{\chi}_0 t + \frac{\varpi}{m^2}t^2 \quad (1.39)$$

We see that the wavepacket always spreads(coefficient of t^2 is positive). If it does not spread, we have to satisfy 2 equations.One of them is $\varpi = 0$ which only means that the wavepacket does not have a spread in the momentum space. This means the wavepacket is made of a single frequency wave or a linear combination of waves. Of course, this is not physical. Finally, upon suitably recasting, we get the following equation.

$$(\Delta q) = \sqrt{(\Delta q_0)^2 + (\frac{\Delta p_0 t}{m})^2} \quad (1.40)$$

1.4 Further Classical Approximations

Another approximation we need is to understand that,in the classical limit, $\psi(\mathbf{r}, t)$ could represent the velocity field of a stream of classical particles. To see this, let the potential in the Schrodinger equation is V(r). Hence, we have,

$$[\frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r})]\psi(\mathbf{r}, t) = i\hbar\frac{\psi(\mathbf{r}, t)}{t} \quad (1.41)$$

We start, with setting, $\psi(\mathbf{r}, t) = A(\mathbf{r})e^{(\frac{i}{\hbar}S(\mathbf{r}))}$. On substitution, we get 2 equations. We segregate the real and imaginary parts, to get,

$$(\frac{\delta S}{\delta t}) + V(\mathbf{r}) + \frac{(\nabla S)^2}{2m} = \frac{\hbar^2}{2m}\frac{\nabla^2(A(\mathbf{r}))}{A(\mathbf{r})} \quad (1.42)$$
$$m(\frac{\delta A}{\delta t}) + (\nabla A)(\nabla S) + \frac{A}{2}\nabla^2 S = 0 \quad (1.43)$$

The second equation is just the equation of continuity, recast. Multiplying by 2A, throughout, we get the equation of continuity. Setting $\hbar = 0$, we get the classical limit in the first case. Thus , we have,

$$\frac{\delta S}{\delta t} + \frac{(\nabla S)^2}{2m} + V = 0 \tag{1.44}$$

$$m\frac{\delta A^2}{\delta t} + \nabla.(A^2 \nabla S) = 0 \tag{1.45}$$

The equation 1.45 gives us another interpretation of ψ. If I think of a fluid of classical particles with mass m and moving in a potential V(r), by equation 1.45, the density of the fluid is A^2 and its current density $A^2\nabla S$. But, A^2 is the probability density of $\psi(|\psi|^2)$ and the current density $A^2\nabla S$ is nothing but the probability current J. Hence the velocity field of the fluid is

$$\mathbf{v} = \frac{\mathbf{J}}{\mathbf{P}} = \frac{\nabla S}{m} \tag{1.46}$$

$$m\frac{d\mathbf{v}}{dt} = -\nabla V \tag{1.47}$$

Chapter 2

Derivation of Airy Wave Function

2.1 Integral form of $\psi(x,t)$

The Schrodinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = i\hbar\frac{\partial\psi}{\partial t} \tag{2.1}$$

We assume that at time t = 0, the wave form is the Airy function.

$$\psi(x,0) = Ai\left(\frac{Bx}{\hbar^{2/3}}\right) \tag{2.2}$$

where B is an arbitrary constant taken to be positive for convenience. Let us take the Fourier transform of $\psi(x,0)$ and call it $\phi(k)$

$$\psi(x,t) = \frac{1}{2\pi}\int \phi(k)e^{i(kx-\omega t)}dx \tag{2.3}$$

$\psi(x,0)$ is the inverse transform of $\phi(k)$:

$$\psi(x,0) = \frac{1}{2\pi}\int \phi(k)e^{ikx}dk \tag{2.4}$$

The Fourier transform of $Ai(x)$ has the form[1] $e^{\frac{ik^3}{3}}$.

$$\int_{-\infty}^{\infty} Ai(x)e^{-i\omega x}dx = e^{i\omega^3/3} \tag{2.5}$$

In our case, we have $Ai(Bx/\hbar^{2/3})$ hence by doing a change of variables, we find that $\phi(k)$ is:

$$\phi(k) = \frac{\hbar^{2/3}}{2\pi B}e^{i\frac{\hbar^2}{B^3}k^3} \tag{2.6}$$

[1] Olivier Vallee - "Airy functions and its Applications to Physics" pg. 87

Substituting $\phi(k)$ and $\omega = \frac{\hbar^2 k^2}{2m}$ into equation (2.3) we get the integral form of the wave function.

$$\psi(x,t) = \frac{\hbar^{2/3}}{2\pi B} \int_{-\infty}^{\infty} exp\left[i\left(\frac{\hbar^2}{3B^3}k^3 - \frac{\hbar t}{2m}k^2 + kx\right)\right] dk \tag{2.7}$$

2.2 Converting to Airy function

We make use of the following formula[2]

$$\int exp\left[i\left(\frac{z^3}{3} + az^2 + bz\right)\right] dz = 2\pi e^{ia\left(\frac{2a^2}{3} - b\right)} Ai(b - a^2) \tag{2.8}$$

In our integral form, we do a simple change of variable from k to $z = \frac{\hbar^{2/3}}{B}k$ and apply the above formula by substituting $a = -\frac{B^2 t}{2m\hbar^{1/3}}$ and $b = \frac{Bx}{\hbar^{2/3}}$ to get:

$$\psi(x,t) = Ai\left(\frac{B}{\hbar^{2/3}}\left[x - \frac{B^3 t^2}{4m^2}\right]\right) e^{i\frac{B^3 t}{2m\hbar}\left(x - \frac{B^3 t^2}{6m^2}\right)} \tag{2.9}$$

This equation satisfies the time dependent Schrödinger equation (2.1) A few graphs of the function are given below.

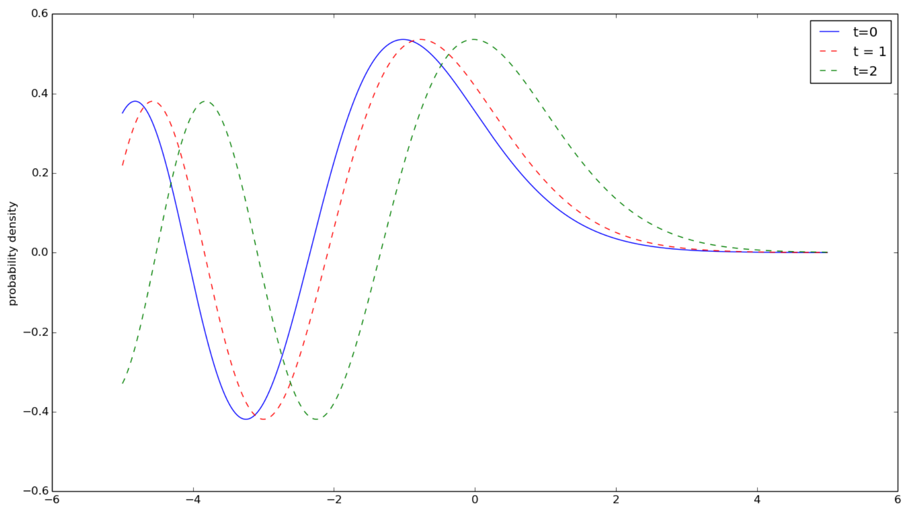

Figure 2.1: $Ai(x - \frac{t^2}{4})$ B=$\hbar$ = m = 1.0

[2]Olivier Vallee pg. 10

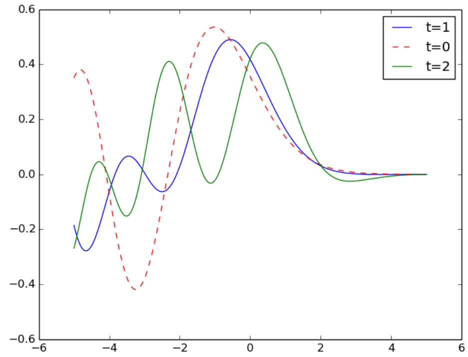

Figure 2.2: $\psi(x,t)$ at different times

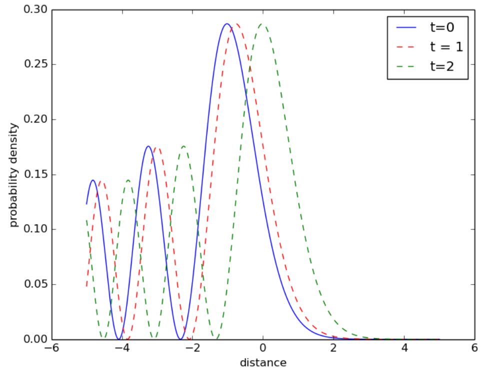

Figure 2.3: Probability density at different times

2.3 Wave velocity

From the wave form, we can gather that the wave is not stationery and is moving to the right with a definite velocity.Also, from the graph above(Fig:2.3), it is clear that the probability density propagates in time without distortion.If we compare the exponential part of the final form of the wave function to the plane wave equation $e^{k'x-\omega' t}$, by comparison of coefficients, we can see that: $k' = \frac{B^3 t}{2m\hbar}$ and $\omega' = \frac{B^6 t^2}{12m^3\hbar}$ Therefore the wave velocity is[3]:

$$v = \frac{w'}{k'} = \frac{B^3 t}{6m^2} \tag{2.10}$$

[3]In the paper by Berry, the velocity was reported as $\frac{B^3 t^2}{2m^2}$. This answer is not of the correct dimension.

Conclusion

For any wave packet to translate in its unchanged form, its semi-classical representation must propagate rigidly along x as time passes. In the free particle case, an initial point (x_0, p_0)moves in the phase space according to the following equation:

$$x = x_0 + \frac{p_0 t}{m} \tag{2.11}$$

This corresponds to simple shear in the phase space with the x axis as the pivotal axis. If $X_t(p)$ represents the family of orbits translating rigidly in phase space, then it deforms as:

$$x = X_t(p) = X_0(p) + \frac{pt}{m} \tag{2.12}$$

Only two curves translate rigidly under this deformation:

- Straight line parallel to the x axis. This implies constant momentum which is precisely the case corresponding to the plane wave.
- Any parabola whose axis is parallel to the x axis. This corresponds to the Airy wave packet.

Hence the Airy packet remains undistorted as it progresses.

Since the Airy packet is not square integrable, it does not represent the probability distribution of a single particle. Instead it corresponds to an infinite number of particles just life the plane wave. One cannot define a proper centre of gravity for the wave packet. Therefore the supposed acceleration of the packet cannot contradict the Ehrenfest theorem which states that the center of gravity of a packet moves with constant speed. Instead, what accelerates is the critical point of the parabola $X_t(p)$ in phase space which corresponds to the maximum value of $|\psi|^2$.

The analysis done here is only for the free particle Hamiltonian. Whereas a modified, more complicated for of Airy function is a solution of the Hamiltonian when a force is applied on this particle. This problem was tackled in the Berry paper but due to time constraints we are not able to present that here.

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