Quantum Mechanics and Applications

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Contents

0.1 Basic Quantum Mechanics II

In this lecture, we will continue our discussions on wave particle duality and we will give a very heuristic derivation of the Schrodinger equation. Then, we will discuss the Dirac delta function and Fourier transform that will be a bit of mathematics, but that is necessary to understand the solutions of the Schrodinger equation.
As I mentioned in my previous talk, de Broglie wrote that:

I was convinced that the wave particle duality discovered by Einstein in his theory of light quanta was absolutely general and extended to all of the physical world, and it seemed certain to me that therefore, the propagation of a wave is associated with the motion of a particle of any sort photon, electron, proton or any other.

Actually after de Broglie wrote this, the experiments, the diffraction pattern by electrons, were observed much later. So that is why de Broglie's contribution is considered to be outstanding. He predicted wave nature of electrons; he said that it could not just be for protons; it would be for electrons, protons, neutrons or whatever. And it was only later, he made this prediction around 1922 and the experiments were carried out only in 1926 (the famous diffraction experiments of electron).
The wave particle duality, led to the development of quantum mechanics in 1926. It lead to the famous Schrodinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi \tag{1}$$

If you ask me the question: what is an electron? What is a proton? Is it a particle or a wave? Some people would answer that it is both; that answer is not quite correct. The correct answer is that it is neither. So the electron or the proton is neither a wave nor a particle; it is described by a wave function Ψ which is solution of Schrodinger equation. In 1926 itself, Max Born formulated the new standard interpretation of the probability density function for $\Psi^*\Psi$, for which, he was awarded the 1954 Nobel Prize in Physics.
So $|\Psi|^2 d\tau$ represent the probability of finding the particle in the volume element $d\tau$, and since the particle has to be found out somewhere, the total probability (total integral) must be equal to 1

$$\int |\Psi|^2 d\tau = 1 \tag{2}$$

This condition is known as the normalization condition. We will discuss that, but first we would like to give a heuristic derivation of the Schrodinger equation. Let take a one dimensional plain wave; a plain wave propagating in the positive x directiob, is described by a wave function Ψ as follow:

$$\Psi(x,t) = Ae^{i(kx-\omega t)} \tag{3}$$

In this equation, we can somehow inject the wave particle duality. By de-Broglie relation, the momentum of a particle is related to the wave length by the Planck constant h as:

$$p = \frac{\hbar}{\lambda} \tag{4}$$

Now multypling and divide by 2π:

$$p = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \hbar\, k \tag{5}$$

where $\hbar = \frac{\hbar}{2\pi}$ and $k = \frac{2\pi}{\lambda}$. The Einstain equation is:

$$E = h\nu \tag{6}$$

Now, multiplyng and dividing by 2π:

$$E = \frac{h}{2\pi} 2\pi\nu = \hbar\omega \tag{7}$$

So we arrive to the conclusion that

$$k = \frac{p}{\hbar} \quad , \quad \omega = \frac{E}{\hbar} \tag{8}$$

Substituting now (8) into (3) we get:

$$\Psi(x,t) = Ae^{\frac{i}{\hbar}(px - Et)} \tag{9}$$

Doing the partial derivative of (9) with respect to x and then multiplying by $-i\hbar$, yields:

$$-i\hbar\frac{\partial\Psi}{\partial x} = -i\hbar\frac{i\,p}{\hbar}\Psi = p\,\Psi \tag{10}$$

From this equation we can understand that the p operator, operating on Ψ, is th same as $-i\hbar\frac{\partial}{\partial x}$.
Differentiating again (10) with respect to x and then multiplying by $-i\hbar$

$$(-i\hbar)^2\frac{\partial^2\Psi}{\partial x^2} = p^2\,\Psi \tag{11}$$

From this equation we can understand that the p^2 operator, operating on Ψ, is th same as $(-i\hbar)^2\frac{\partial^2}{\partial x^2}$. Now dividing (11) by $2m$, where m is the mass of the particle:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = \frac{p^2}{2m}\,\Psi \tag{12}$$

Now, we want to partially differentiate (9) with respect to time t and then multiplying and dividing by $i\hbar$, yields:

$$i\hbar\frac{\partial\Psi}{\partial t} = i\hbar\left(-\frac{i\,E}{\hbar}\right)\Psi = E\,\Psi \tag{13}$$

Now, for a free particle, the total energy is the kinetic energy, classically, and so:

$$E = \frac{p^2}{2m} \tag{14}$$

which implies that (13) and (12) are equal:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} \tag{15}$$

Where (15) is the 1-D Schrodinger equation for a free particle.

If the particle is in a potential field $V(x)$, the total energy is:

$$E = \frac{p^2}{2m} + V(x) \tag{16}$$

where

$$E\Psi = \left(\frac{p^2}{2m} + V(x)\right)\Psi \tag{17}$$

and we get the following equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi \tag{18}$$

Where, the operator in the bracket, is called Hamiltonian and is defined with the letter H. Richard Feynman, as we all know his noble one of the outstanding physicist of the 20th century. He writes:

Where did we get that equation from ? Nowhere. It is not possible to derive it from anything you know; it came out of the mind of Schrödinger ...

So we have given a very heuristic derivation which lacks rigger. Somehow, we have been able to reach the Schrödinger equation and then, we will try to get results by solving the Schrödinger equation.
This equation was first obtained by Erwin Schrödinger in 1926, and we will obtain the solutions and then we will find that this compares very well with experimental data. So that is the success of quantum mechanics. That is the success of the Schrödinger equations for which Schrödinger got the noble prize in 1933. Now, we will use the Schrödinger equation

to study its solution. However, we will digress here for a moment and we will do a little bit of mathematics and in this mathematics, we will try to define what is Dirac delta function, and we will also discuss what we mean by the furrier transform of a function.
Let us evaluate the following integral

$$\begin{aligned} I^2 &= \int_{-\infty}^{+\infty} e^{-x^2} dx \int_{-\infty}^{+\infty} e^{-y^2} dy \\ &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} e^{-\left(x^2+y^2\right)} dx dy \end{aligned} \tag{19}$$

This integral in polar coordinates becomes:

$$I^2 = \int_0^{2\pi} d\theta \int_0^{\infty} e^{-\rho^2} \rho \, d\rho = \pi \tag{20}$$

and so we have that:

$$I = \int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{\pi} \tag{21}$$

Thanks to this integral, now we can evaluate the following integral:

$$\begin{aligned} \int_{-\infty}^{+\infty} e^{-\alpha x^2 + \beta x} dx &= \int_{-\infty}^{+\infty} e^{-\alpha\left[x^2 - \frac{\beta}{\alpha}x + \frac{\beta^2}{4\alpha^2} - \frac{\beta^2}{4\alpha^2}\right]} dx = \\ = e^{\beta^2/4\alpha} \int_{-\infty}^{+\infty} e^{-\alpha\left[x - \frac{\beta}{2\alpha}\right]^2} dx &= e^{\beta^2/4\alpha} \int_{-\infty}^{+\infty} e^{-\alpha\, z^2} dz \end{aligned} \tag{22}$$

and if we call $\sqrt{\alpha}z = y$ we get:

$$= e^{\beta^2/4\alpha} \frac{1}{\sqrt{\alpha}} \int_{-\infty}^{+\infty} e^{-y^2} dy = \sqrt{\frac{\pi}{\alpha}}\, e^{\beta^2/4\alpha} \tag{23}$$

We will now discuss the Dirac delta function and the simplest representation of this Dirac delta function is like this:

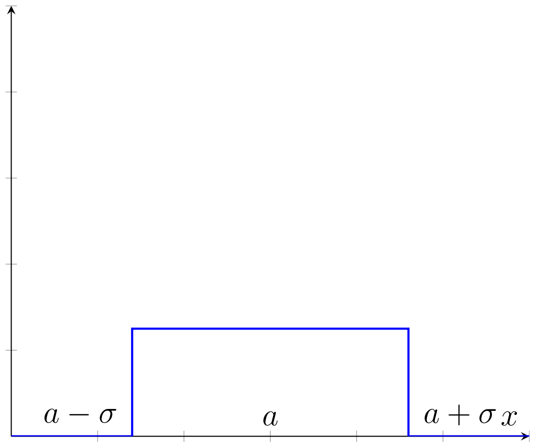


Figure 1: Rectangular representation of the Dirac delta function centered at $x = a$ with width 2σ and height $1/2\sigma$.

where the rectangle function can be expressed as:

$$R_\sigma(x) = \begin{cases} \dfrac{1}{2\sigma} & -\sigma < x - a < \sigma \\ 0 & |x-a| > \sigma \end{cases} \qquad \int_{-\infty}^{+\infty} R_\sigma(x) dx = 1$$

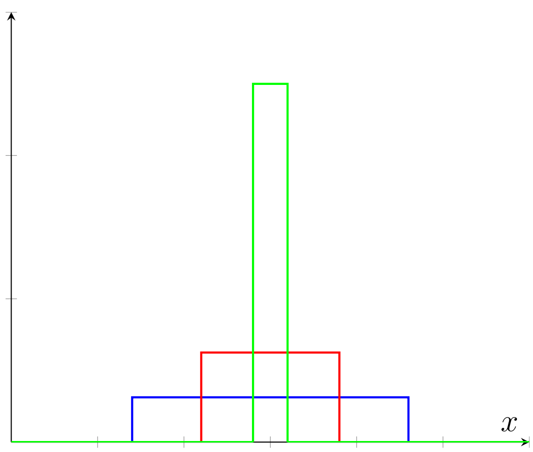


Figure 2: Blue is for $\sigma = 0.8$, red is for $\sigma = 0.4$ and green is for $\sigma = 0.1$

The area of the rectangle is 1 independent of σ and in the limit of σ tending to 0, then we have the representational of the Dirac delta function:

$$\delta(x-a) = \lim_{\sigma \to 0} R_\sigma(x) \tag{24}$$

The product of the Dirac delta function times a generic function $f(x)$ and making the integral is:

$$\int_{-\infty}^{+\infty} f(x)\delta(x-a) = \lim_{\sigma\to 0}\int_{-\infty}^{+\infty} f(x)R_\sigma(x) = \lim_{\sigma\to 0}\frac{1}{2\sigma}f(a)\int_{a-\sigma}^{a+\sigma} dx = f(a) \tag{25}$$

Since that the in the limit of $\sigma \to 0$ the function $f(x)$ does not vary to much in the interval $-\sigma < x-a < \sigma$ and is considered constant and equal to $f(a)$ in such a way to bring out off the integral.

Let us suppose a ramp function which is described by the following equation:

$$T_\sigma(x) = \begin{cases} \frac{1}{2\sigma}\left[x-(a-\sigma)\right] & -\sigma < x-a < \sigma \\ 0 & |x-a| > \sigma \end{cases} \qquad \frac{dT_\sigma(x)}{dx} = R_\sigma(x)$$

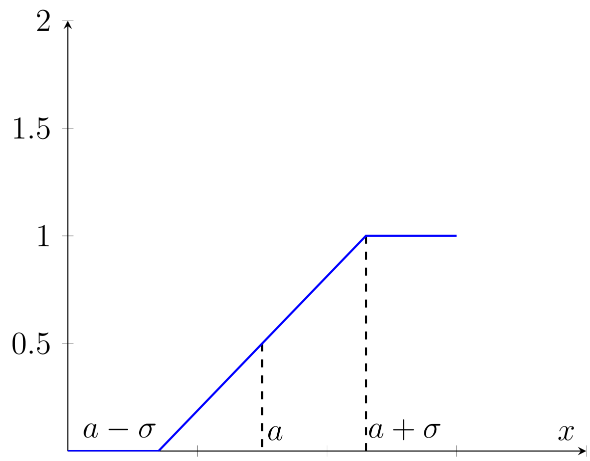


Figure 3: Ramp function

In the limit of $\sigma \to 0$ we have the Heaviside step function $H(x-a)$ and the derivative of this one is the Dirac delta function.
Let us consider the Gaussian function centered at $x = a$:

$$G_\sigma(x) = \frac{1}{\sigma\sqrt{2\pi}}e^{-(x-a)^2/2\sigma^2} \tag{26}$$

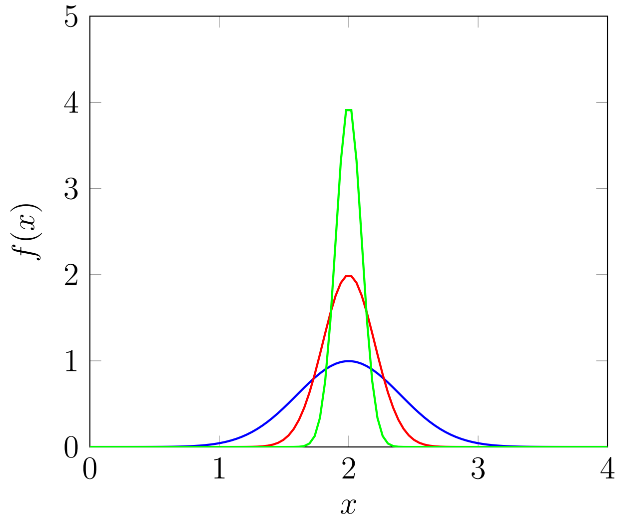


Figure 4: Gaussian function centered at $x = a = 2$ for $\sigma = 0.4$ (blue), $\sigma = 0.2$ (red) and $\sigma = 0.1$ (green)

and we can see that:

$$\frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{-(x-a)^2/2\sigma^2} dx = 1 \tag{27}$$

an we can say that the Dirac delta function is viewed as the Gaussian function when $\sigma \to 0$.

Now, we will consider yet another representation of the Dirac delta function and that is known as the integral representation of the Dirac delta function.
There is a definite integral which is equal to

$$\int_{-\infty}^{+\infty} \frac{sin(g\,x)}{x} dx = \pi \qquad g > 0 \tag{28}$$

$$\int_{-\infty}^{+\infty} \frac{sin(g\,x)}{\pi x} dx = 1 \qquad g > 0 \tag{29}$$

and it is possible to see that:

$$\lim_{x\to 0} \frac{sin(g\,x)}{\pi x} = \frac{g}{\pi} \tag{30}$$

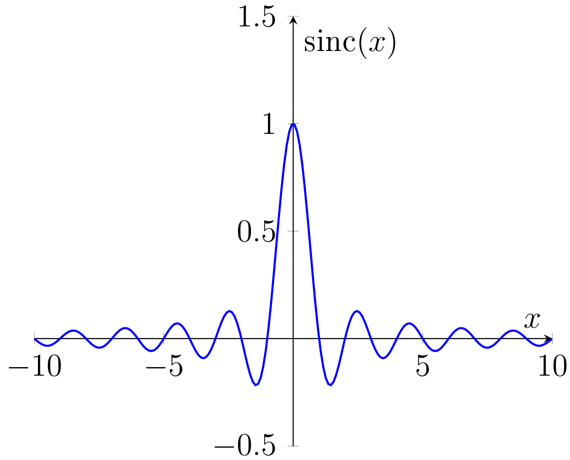


Figure 5: Plot of $sinc(x) = \frac{sin(\pi x)}{\pi x}$

and so the Dirac delta function can be seen as the limit of $g \to \infty$ of $\frac{sin(g\,x)}{\pi x}$.

$$\frac{1}{2\pi}\int_{-g}^{+g} e^{ikx}dk = \frac{1}{2\pi}\frac{e^{ikx}}{ix}\Big|_{-g}^{+g} = \frac{1}{2\pi x}\frac{e^{igx}-e^{-igx}}{i} = \frac{1}{\pi x}\frac{e^{igx}-e^{-igx}}{2i} = \frac{sin(g\,x)}{\pi x} \tag{31}$$

and so the integral representation of the Dirac delta function is:

$$\delta(x-x') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{ik(x-x')}dk \tag{32}$$

Consider any arbitrary well behaved function $f(x)$, we can say that:

$$f(x) = \int_{-\infty}^{+\infty} \delta(x-x')f(x')dx' \tag{33}$$

and inserting (32) inside (33)

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} e^{ik(x-x')}f(x')dx'dk \tag{34}$$

Let us define the following function:

$$F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(x')e^{-ikx'}dx' \tag{35}$$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} dk \tag{36}$$

These two equations describe what is known as the Fourier integral theorem, the function $F(k)$ is the Fourier transform of $f(x)$ and (36) is the inverse Fourier transform.
Since that in (35) x' is a defined integral, we can remove the prime ans write:

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx \tag{37}$$

Let us assume to have the Gaussian function:

$$f(x) = Ae^{-\frac{x^2}{2\sigma^2}} \tag{38}$$

the Fourier transform is:

$$F(k) = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-\frac{x^2}{2\sigma^2}} e^{-ikx} dx = \frac{A}{\sqrt{2\pi}} \sqrt{\pi 2\sigma^2} e^{-\frac{k^2\sigma^2}{2}} = A\sigma e^{-\frac{k^2\sigma^2}{2}} \tag{39}$$

The Fourier transform of the Gaussian function is a Gaussian function. We can notice that the width of $f(x)$ is of the order of $\Delta x \sim \sigma$, instead in the k space, the width of $F(k)$ is of the order of $\Delta k \sim 1/\sigma$. We can say that $\Delta x \Delta k \sim 1$.

Let us take the complex conjugate of (36):

$$f^*(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F^*(k) e^{-ikx} dk \tag{40}$$

And let us evaluate:

$$\int_{-\infty}^{+\infty} |f|^2 dx = \int_{-\infty}^{+\infty} f^* f dx = \frac{1}{2\pi} \int \int \int_{-\infty}^{+\infty} F(k') F^*(k) e^{ix(k'-k)} dx\, dk\, dk' \tag{41}$$

We already know that:

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ix(k'-k)} dx = \delta(k'-k) \tag{42}$$

$$\int_{-\infty}^{+\infty} F(k') \delta(k-k') dk' = F(k) \tag{43}$$

Finally, we can say that:

$$\int_{-\infty}^{+\infty} |f(x)|^2 dx = \int_{-\infty}^{+\infty} |F(k)|^2 dk \tag{44}$$

This is known as Parseval's Theorem.
Considering now a time dependent function $f(t)$. For such function, we write the Fourier transform in the following form:

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(t) e^{-i\omega t} dt \tag{45}$$

where this is known as frequency spectrum.

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(\omega) e^{i\omega t} d\omega \tag{46}$$

Basically, (46) represent the sum over all the frequencies. If the time dependent function has only one frequency, the the corresponding $F(\omega)$ is the Dirac delta function $\delta(\omega - \omega_0)$. Then, carry out the integration, we obtain a monochromatic wave:

$$f(t) = \frac{1}{\sqrt{2\pi}} e^{i\omega_0 t} \tag{47}$$

with:

$$F(\omega) = \delta(\omega - \omega_0) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{i(\omega - \omega_0)t} dt \tag{48}$$

Let us consider the following function:

$$f(t) = A e^{-\frac{t^2}{2\tau^2}} e^{i\omega_0 t} \tag{49}$$

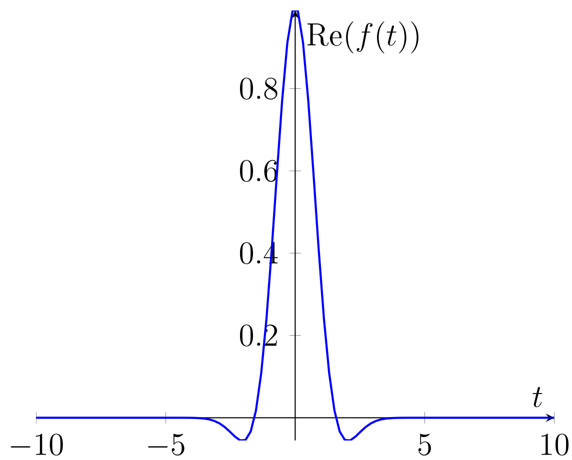


Figure 6: Plot of the real part of $f(t)$ for $\omega_0 = A = \tau = 1$

Now, using (45) we have:

$$F(\omega) = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-\frac{t^2}{2\tau^2}} e^{i(\omega-\omega_0)t} dt = \frac{A}{\sqrt{2\pi}} \sqrt{\pi 2\tau^2} e^{-\frac{(\omega-\omega_0)^2}{4} 2\tau^2} = \\ = A\tau e^{-\frac{(\omega-\omega_0)^2}{2}\tau^2} \tag{50}$$

We will be continuing our discussion on the use of the Dirac delta function, and specifically we will consider the solution of the Schrodinger equation for the free particle problem. And we will show that the solution of the Schrodinger equation contains the uncertainty principle. Let us introduce a mathematical variable $p = \hbar k$ and from this equation we can get $dk = \frac{dp}{\hbar}$. If we substitute it inside the integral representation od the Dirac delta function, we get:

$$\delta(x - x') = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{i\frac{p}{\hbar}(x-x')} dp \tag{51}$$

From the definition of the Dirac delta function, we can write that:

$$\Psi(x) = \int_{-\infty}^{+\infty} \Psi(x')\delta(x - x')dx' \tag{52}$$

and substituting (51) we get:

$$\Psi(x) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx' dp \, \Psi(x') e^{i\frac{p}{\hbar}(x-x')} \tag{53}$$

We can define the following function:

$$a(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \Psi(x')e^{-\frac{i\,p\,x'}{\hbar}} dx' \tag{54}$$

where, since is a defined integral, we can remove the prime. Now, substituting into (53):

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} a(p)e^{\frac{i\,p\,x}{\hbar}} dp \tag{55}$$

where we can say that:

$$\int_{-\infty}^{+\infty} |\Psi(x)|^2 dx = 1 = \int_{-\infty}^{+\infty} |a(p)|^2 dp \tag{56}$$

We can say that (54) is the Fourier transform of $\Psi(x)$ in the momentum space.
We can solve the Schrodinger equation (15) using the method of separation variables and so we will assume that:

$$\Psi(x,t) = \psi(x)T(t) \tag{57}$$

and substituting (57) into (15):

$$i\hbar\psi(x)\frac{dT}{dt} = -\frac{\hbar^2}{2m}T(t)\frac{d^2\psi}{dx^2} \tag{58}$$

Dividing (58) by (57):

$$i\hbar\frac{1}{T(t)}\frac{dT}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi}{dx^2} \tag{59}$$

We can see that on the left we have a function of time that is equal to the right that is a function of position. These two cannot be equal unless both of them are equal to a constant that we call $E = \frac{p^2}{2m}$, where p is a number.
Solving the left equation, integrating it, we get:

$$ln(T(t)) = -\frac{i}{\hbar}\frac{p^2}{2m}t \;\;\Rightarrow\;\; T(t) = const \cdot e^{-\frac{i}{\hbar}\frac{p^2}{2m}t} = const \cdot e^{-\frac{i\,E\,t}{\hbar}} \tag{60}$$

Solving the right equation, we get:

$$\psi(x) = e^{\frac{i}{\hbar}p\,x} \tag{61}$$

The total solution will be:

$$\Psi(x,t) = const \cdot e^{\frac{i}{\hbar}\left(p\,x - \frac{p^2}{2m}t\right)} \tag{62}$$

where p is a number that can take values between $-\infty < p < +\infty$ and so the most general solution will be a superposition of all solutions, what is known as wave packet:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} a(p) e^{\frac{i}{\hbar}\left(p\,x - \frac{p^2}{2m}t\right)} dp \tag{63}$$

where $a(p)$ will be determined by the initial form of the wave function, that is the following:

$$\Psi(x,0) = \psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} a(p) e^{\frac{i}{\hbar}p\,x} dp \tag{64}$$

and so $a(p)$ will be the inverse Fourier transform of the function (64):

$$a(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(x) e^{-\frac{i\,p\,x}{\hbar}} dx \tag{65}$$

where $|\psi(x)|^2 dx$ is the probability of funding the particle between x and $x+dx$, and $|a(p)|^2 dp$ is the probability of funding the momentum between p and $p+dp$.
For example let us assume that:

$$\psi(x) = \frac{1}{(\pi\sigma_0^2)^{1/4}} e^{-\frac{x^2}{2\sigma_0^2}} e^{\frac{i}{\hbar}p_0 x} \tag{66}$$

$$a(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(x) e^{-\frac{i}{\hbar}px} dx = \left(\frac{\sigma_0^2}{\pi\hbar^2}\right)^{1/4} e^{\left[-\frac{(p-p_0)^2\sigma_0^2}{2\hbar^2}\right]} \tag{67}$$

0.2 3d equation

For a classical plane wave we can write the 3-dimensional wave function propagating in the direction of $\vec{k}$, by:

$$\Psi(\vec{r},t) = A\, e^{i(\vec{k}\cdot\vec{r} - \omega\, t)} \tag{68}$$

where

$$p_x = \hbar\, k_x \quad p_y = \hbar\, k_y \quad p_z = \hbar\, k_z \tag{69}$$

and so:

$$\Psi(x,y,z,t) = A\, e^{\frac{i}{\hbar}(p_x\, x + p_y\, y + p_z\, z - E\, t)} \tag{70}$$

$$\Psi(x,y,z,t) = A\, e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{r} - E\,t)} \tag{71}$$

$$\begin{aligned}
-i\hbar\frac{\partial\Psi}{\partial x} &= p_x\Psi \qquad & p_x &\Leftrightarrow -i\hbar\frac{\partial}{\partial x} \\
-\hbar^2\frac{\partial^2\Psi}{\partial x^2} &= p_x^2\Psi \qquad & p_x^2 &\Leftrightarrow -\hbar^2\frac{\partial^2}{\partial x^2} \\
-i\hbar\frac{\partial\Psi}{\partial y} &= p_y\Psi \qquad & p_y &\Leftrightarrow -i\hbar\frac{\partial}{\partial y} \\
-\hbar^2\frac{\partial^2\Psi}{\partial y^2} &= p_y^2\Psi \qquad & p_y^2 &\Leftrightarrow -\hbar^2\frac{\partial^2}{\partial y^2} \\
-i\hbar\frac{\partial\Psi}{\partial z} &= p_z\Psi \qquad & p_z &\Leftrightarrow -i\hbar\frac{\partial}{\partial z} \\
-\hbar^2\frac{\partial^2\Psi}{\partial z^2} &= p_z^2\Psi \qquad & p_z^2 &\Leftrightarrow -\hbar^2\frac{\partial^2}{\partial z^2}
\end{aligned} \tag{72}$$

we will finally obtain that:

$$-\hbar^2\left[\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right] = (p_x^2 + p_y^2 + p_z^2)\Psi = p^2\Psi \tag{73}$$

dividing everything by $2m$:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi = \frac{p^2}{2m}\Psi \tag{74}$$

differentiating (71) and multiplying by $i\hbar$:

$$i\hbar\frac{\partial\Psi}{\partial t} = E\Psi = \left[\frac{p^2}{2m} + V\right]\Psi \tag{75}$$

and comparing (75) with (74) we get the 3-D time dependent shrodinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(x,y,z)\Psi \tag{76}$$

We know that V is the potential energy function which is necessary real. Taking the complex conjugate of (76):

$$i\hbar\frac{\partial\Psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi^* + V(x,y,z)\Psi^* \tag{77}$$

Now, we multiplay (76) by Ψ^* and (77) by Ψ, and then we subtract them, we obtain:

$$i\hbar\left[\Psi^*\frac{\partial\Psi}{\partial t}+\frac{\partial\Psi^*}{\partial t}\Psi\right]=-\frac{\hbar^2}{2m}\left[\Psi^*\nabla^2\Psi-\Psi\nabla^2\Psi^*\right] \tag{78}$$

which can be written as:

$$i\hbar\frac{\partial}{\partial t}\left(\Psi^*\Psi\right)=\frac{\hbar^2}{2m}div\left[\Psi\nabla\Psi^*-\Psi^*\nabla\Psi\right] \tag{79}$$

we know that:

$$div(\Psi\,\vec{F})=\Psi\,div\vec{F}+\nabla\Psi\cdot\vec{F} \tag{80}$$

We will call the function $\rho=\Psi^*\Psi=|\Psi|^2$ and dividing by $i\hbar$ (79), we obtain:

$$\frac{\partial\rho}{\partial t}+\frac{i\,\hbar}{2m}div\left[\Psi\nabla\Psi^*-\Psi^*\nabla\Psi\right]=0 \tag{81}$$

Let us define the following vector:

$$\vec{J}=\frac{i\,\hbar}{2m}\left[\Psi\nabla\Psi^*-\Psi^*\nabla\Psi\right] \tag{82}$$

and know from the Shrodinger equation we can arrive to the continuity equation:

$$\frac{\partial\rho}{\partial t}+div\,\vec{J}=0 \tag{83}$$

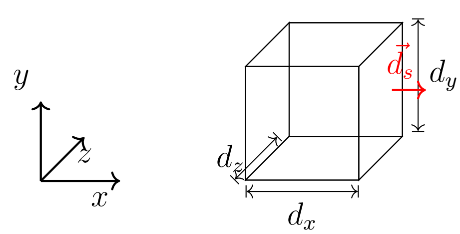
We may assume that ρ is proportional to the position probability density per unit volume:

$$\rho\,d\tau=|\Psi|^2d\tau \tag{84}$$

Since that the Shordinger equation is linear, if Ψ is a solution, multiple of them if always a solution and we can choose the multiplicative constant in such a way that the following Normalization condition is satisfied:

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}|\Psi|^2d\tau=1 \tag{85}$$

Let us consider a room as in the figure, in which particles are flowing:



There are particles in the room and let me try to find out the number of particles that are coming out of the surface area $d_y d_z$. If there is a current density $\vec{J}$ which represents number of particles crossing per unit area per unit time, then $\vec{J} \cdot d_s$ will represent the number of particles crossing the area d_s per unit time. Since d_s vector normal to the surface $d_y d_z$ is along the positive x axis

$$\text{Numb. of particles coming out per second from the RX area} = J_x(x + d_x) d_y d_z \tag{86}$$

$$\text{Numb. of particles entering per second from the LX area} = J_x(x) d_y d_z \tag{87}$$

$$\text{Net out flow} = \left[\frac{J_x(x + d_x) - J_x(x)}{d_x}\right] d_x d_y d_z = \frac{\partial J_x}{\partial x} d\tau \tag{88}$$

$$\text{Total net out flow} = \left(\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z}\right) d\tau = div \vec{J}\, d\tau \tag{89}$$

We know that ρ represent the number of particle per unit volume.
Let us consider a plane wave solution:

$$\Psi = A\, e^{\frac{i}{\hbar}(p\,x - E\,t)} \tag{90}$$

$$\nabla \Psi = \frac{i\,p}{\hbar} \Psi\, \hat{x} \tag{91}$$

$$\Psi^* = A^*\, e^{-\frac{i}{\hbar}(p\,x - E\,t)} \tag{92}$$

$$\nabla \Psi^* = -\frac{i\,p}{\hbar} \Psi^*\, \hat{x} \tag{93}$$

Substitutin these four equations into (82):

$$\vec{J} = \frac{i\,\hbar}{2m}\left[-\frac{i\,p}{\hbar}|\Psi|^2 \hat{x} - \frac{i\,p}{\hbar}|\Psi|^2 \hat{x}\right] = \frac{p}{m}|\Psi|^2 \hat{x} = v|\Psi|^2 \hat{x} \tag{94}$$

This result is for a infinitely extend plane wave which is really a practical impossibility because it is not normalizable.
A normalizable wave function is a something like a Gaussian wave packet

$$\Psi(x) = \frac{1}{\left(\pi\sigma^2\right)^{1/4}} e^{-\frac{x^2}{2\sigma^2}} e^{\frac{i}{\hbar}p_0 x} \tag{95}$$

$$\Psi^*(x) = \frac{1}{\left(\pi\sigma^2\right)^{1/4}} e^{-\frac{x^2}{2\sigma^2}} e^{-\frac{i}{\hbar}p_0 x} \tag{96}$$

$$\nabla\Psi = \left[-\frac{x}{\sigma^2} + \frac{i}{\hbar}p_0\right]\Psi\hat{x} \tag{97}$$

$$\nabla\Psi^* = \left[-\frac{x}{\sigma^2} - \frac{i}{\hbar}p_0\right]\Psi^*\hat{x} \tag{98}$$

$$\vec{J} = \frac{p_0}{m}|\Psi|^2\hat{x} = v|\Psi|^2\hat{x} \tag{99}$$

Now we can define a commutator between two operators α and β, is defined as:

$$[\alpha, \beta] := \alpha\beta - \beta\alpha \tag{100}$$

Let us assume that we want to calculate the following commutator operating on any function Ψ:

$$[x, p_x]\,\Psi = [x\,p_x - p_x\,x]\,\Psi = -i\hbar\left[x\frac{\partial\Psi}{\partial x} - \frac{\partial}{\partial x}\left(x\,\Psi\right)\right] = -i\hbar\left[x\frac{\partial\Psi}{\partial x} - x\frac{\partial\Psi}{\partial x} - \Psi\right] = i\hbar\Psi \tag{101}$$

Since that this is valid for every Ψ, we obtain the commutation relation, because does not commute with p_x:

$$[x, p_x] = i\hbar \tag{102}$$

$$[y, p_y] = i\hbar \tag{103}$$

$$[z, p_z] = i\hbar \tag{104}$$

We can see instead that all the following commute to each other:

$$[x, y] = 0 \tag{105}$$

$$[x, p_y] = 0 \tag{106}$$

$$[y, p_z] = 0 \tag{107}$$

$$[p_x, p_y] = 0 \tag{108}$$

0.3 Expectation Values and The Uncertainty Principle

Associated with the particle if we want to find out the expectation value of any quantity x then we just have to multiply by the probability density function and integrate over the entire space:

$$\langle x \rangle = \frac{\int\int\int x|\Psi|^2 d\tau}{\int\int\int |\Psi|^2 d\tau} \tag{109}$$

From now on we will assume that the wave function Ψ is normalized, which means $\int\int\int |\Psi|^2 d\tau = 1$ and so we can write the expectation value as:

$$\langle x \rangle = \int\int\int \Psi^* \, x \, \Psi \, d\tau \tag{110}$$

Now we have the time dependent Schrodinger equation in 3 dimensional:

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi \tag{111}$$

If we multiply (111) by Ψ^* and integrating over the entire 3D space, we obtain

$$\int \Psi^* \left(i\hbar\frac{\partial}{\partial t}\right) \Psi \, d\tau = \int \Psi^* \left(-\frac{\hbar^2}{2m}\nabla^2\right) \Psi \, d\tau + \int \Psi^* \, V \, \Psi \, d\tau \tag{112}$$

Where the second term on the right is the expectation value of the potential energy $\langle V \rangle$. Classically we know that the total energy is sum of the kinetic energy plus the potential energy and so the expectation value of the total energy is:

$$\langle E\rangle = \left\langle \frac{p^2}{2m} \right\rangle + \langle V\rangle \tag{113}$$

Therefore we can conclude that:

$$\begin{aligned} \langle E\rangle &= \int \Psi^* \left(i\hbar \frac{\partial}{\partial t} \right) \Psi \, d\tau \\ \left\langle \frac{p^2}{2m} \right\rangle &= \int \Psi^* \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \Psi \, d\tau \end{aligned} \tag{114}$$

where the term in the bracket correspond to the operator of E and $\frac{p^2}{2m}$ respectively.
For example, if we want to find the expectation value of p_x:

$$\langle p_x\rangle = \int \Psi^* \, p_x \, \Psi \, d\tau = \int \Psi^* \left(-i\,\hbar \, \frac{\partial}{\partial x} \right) \Psi \, d\tau \tag{115}$$

In statistical theories, if there is a variation of a parameter x, then the spread is measured in terms of mean square deviation (uncertainty in x)

$$\Delta x = \sqrt{\langle x^2\rangle + \langle x\rangle^2} \tag{116}$$

Now we want to prove an inequality known as Schwartz inequality:

$$\int f^* \, f \, d\tau \int g^* \, g \, d\tau \geq \frac{1}{4} \left[\int (f^* \, g + f \, g^*) \, d\tau \right]^2 \tag{117}$$

for simplification we will call

$$\begin{aligned} a &= \int f^* \, f \, d\tau \\ c &= \int g^* \, g \, d\tau \\ b &= \int f^* \, g \, d\tau \\ b^* &= \int f \, g^* \, d\tau \end{aligned} \tag{118}$$

In other to prove that we will consider a real parameter λ, and we know that the following integral is valid:

$$\int |\lambda f + g|^2 \, d\tau \geq 0 \tag{119}$$

we know that we can write:

$$|\lambda f + g|^2 = (\lambda \, f + g) \, (\lambda \, f^* + g^*) = \lambda^2 \, f^* \, f + \lambda \, (f^* \, g + f \, g^*) + g^* \, g \tag{120}$$

and so:

$$\lambda^2 \int f^* \, f \, d\tau + \lambda \int (f^* \, g + f \, g^*) \, d\tau + \int g^* \, g \, d\tau \geq 0 \tag{121}$$

$$\lambda^2 a + \lambda \, (b + b^*) + c > 0 \tag{122}$$

There are no real roots for λ equation and so this means that the discriminant must be negative, so the following is valid:

$$(b + b^*)^2 < 4 \, a \, c \quad \Rightarrow \quad a \, c > \frac{1}{4} \, (b + b^*)^2 \tag{123}$$

and this is proved.
Now let us assume that:

$$\begin{aligned} f &= p\Psi = -i\hbar \frac{\partial \Psi}{\partial x} \\ g &= i \, x \, \Psi \end{aligned} \tag{124}$$

we can see that:

$$\begin{aligned} &\int g^* \, g \, d\tau = \int \Psi^* x^2 \Psi d\tau = \left\langle x^2 \right\rangle \\ &\int f^* f d\tau = \int i\hbar \frac{\partial \Psi^*}{\partial x} \left(-i\hbar \frac{\partial \Psi}{\partial x} \right) dxdydz = \hbar^2 \int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial x} \frac{\partial \Psi}{\partial x} dxdydz = \\ &\quad = \hbar^2 \left[\cancel{\Psi^* \frac{\partial \Psi}{\partial x}\Big|_{-\infty}^{+\infty}} - \int \Psi^* \frac{\partial^2 \Psi}{\partial x^2} dx \right] = \int \Psi^* \left(-\hbar^2 \frac{\partial^2 \Psi}{\partial x^2} \right) dx = \left\langle p^2 \right\rangle \end{aligned} \tag{125}$$

The term was canceled because we have a localized wave packet (the particle is localized in a small region in the space), the wave function should vanish at infinity.

$$I = \frac{1}{4} \, (f^* \, g + f \, g^*) = \frac{1}{4} \left[-i\hbar \frac{\partial \Psi^*}{\partial x} \, i \, x \, \Psi + i\hbar \frac{\partial \Psi}{\partial x} \, i \, x \, \Psi^* \right] = -\frac{\hbar}{4} \left[\frac{\partial \Psi^*}{\partial x} \, x \, \Psi + \frac{\partial \Psi}{\partial x} \, x \, \Psi^* \right] \tag{126}$$

we can see that

$$\frac{\partial}{\partial x}\left(\Psi^* \, x \, \Psi\right) = \frac{\partial \Psi^*}{\partial x} \, x \, \Psi + \Psi^* \left[\Psi + x\frac{\partial \Psi}{\partial x}\right] = \frac{\partial \Psi^*}{\partial x} \, x \, \Psi + \Psi^* \Psi + \Psi^* x \frac{\partial \Psi}{\partial x} \tag{127}$$

and so we can rewrite (126):

$$I = -\frac{\hbar}{4}\left[\frac{\partial}{\partial x}\left(\Psi^* \, x \, \Psi\right) - \Psi^* \Psi\right] \tag{128}$$

integrating (128) the first term will vanish because at infinity the wave function is zero and the second term is equal to 1 because the wave function is normalized. If we will assume that the expettation value of p and x are zero, which means $\langle x \rangle = \langle p \rangle = 0$, we can say that:

$$\begin{aligned} \Delta p &= \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\langle p^2 \rangle} \\ \Delta x &= \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\langle x^2 \rangle} \end{aligned} \tag{129}$$

Using the relation (117) we can get the uncertainty relation:

$$\Delta p \Delta x \geq \frac{\hbar}{2} \tag{130}$$

Let us consider a one dimensional wave packet at initial condition

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} a(p) e^{\frac{i}{\hbar} p \, x} dp \tag{131}$$

we know that

$$\langle p \rangle = \int \Psi^* \, p \, \Psi \, d\tau = -i \, \hbar \int \Psi^* \, \frac{\partial \Psi}{\partial x} \, dx \tag{132}$$

Substituting (131) into (132)

$$\begin{aligned} \langle p \rangle &= -\frac{i\hbar}{2\pi\hbar} \int_{-\infty}^{+\infty} dx \left[\int_{-\infty}^{+\infty} a^*(p') e^{-\frac{i}{\hbar} p' \, x} dp'\right] \int_{-\infty}^{+\infty} \frac{i}{\hbar} \, p \, a(p) e^{\frac{i}{\hbar} p \, x} dp = \\ &= \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dp \int_{-\infty}^{+\infty} dp' a^*(p') \, p \, a(p) \int_{-\infty}^{+\infty} dx \, e^{\frac{i}{\hbar}(p \, x - p' x)} \end{aligned} \tag{133}$$

we already know that:

$$\frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}(p-p')x} dx = \delta(p - p') \tag{134}$$

and so we obtain:

$$\langle p \rangle = \int_{-\infty}^{+\infty} dp\, p\, a(p) \int_{-\infty}^{+\infty} a^*(p')\delta(p-p')dp' = \int_{-\infty}^{+\infty} p\, |a(p)|^2\, dp \tag{135}$$

Carry out the same procedure, we cn arrive that:

$$\left\langle p^2 \right\rangle = \int_{-\infty}^{+\infty} p^2\, |a(p)|^2\, dp \tag{136}$$