Quantum Mechanics and Applications

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Dedication

The creation of this book was made thanks to the collection of notes from the precious video lessons of the Quantum Mechanics and Applications, Prof. Ajoy Ghatak, Department of Physics, IIT Delhi and my thanks go to him.

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:

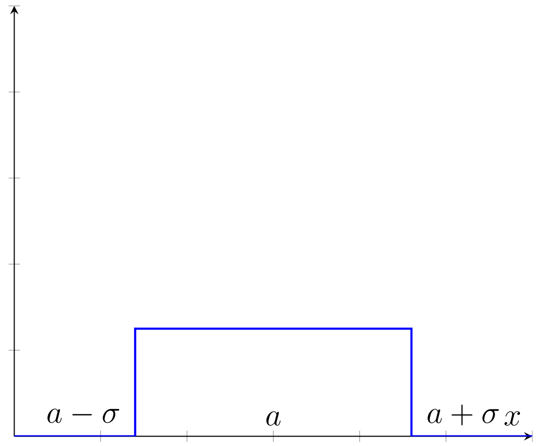

Figure 1: Rectangular representation of the Dirac delta function centered at $x = a$ with width 2σ and height $1/2\sigma$.

where the rectangle function can be expressed as:

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

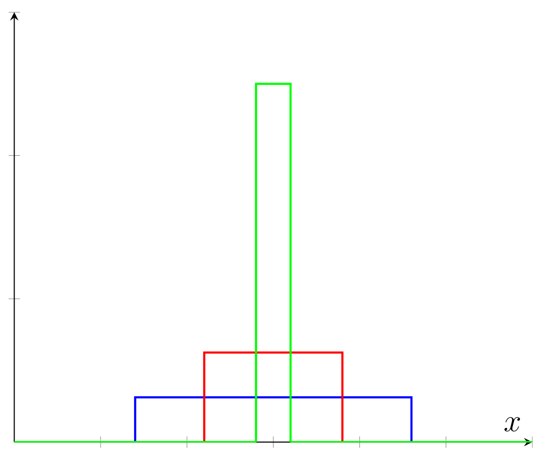

Figure 2: Blue is for $\sigma = 0.8$, red is for $\sigma = 0.4$ and green is for $\sigma = 0.1$

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:

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

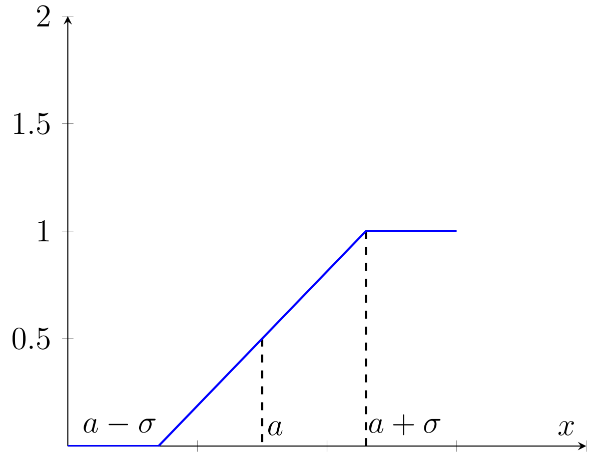

Figure 3: Ramp function

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 $x = a$:

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

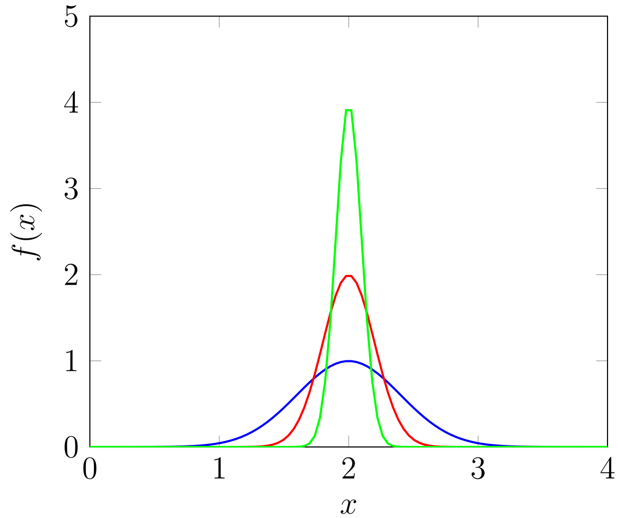

Figure 4: Gaussian function centered at $x = a = 2$ for $\sigma = 0.4$ (blue), $\sigma = 0.2$ (red) and $\sigma = 0.1$ (green)

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:

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

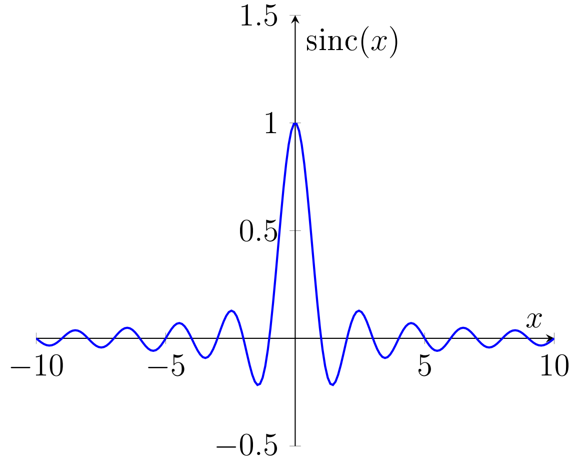

Figure 5: Plot of $sinc(x) = \frac{sin(\pi x)}{\pi x}$

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:

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

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:

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

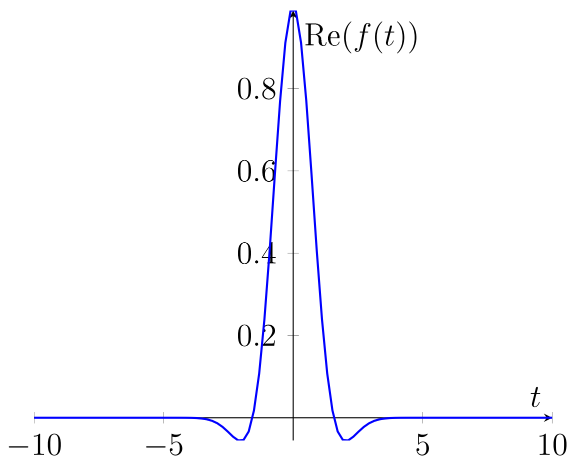

Figure 6: Plot of the real part of $f(t)$ for $\omega_0 = A = \tau = 1$

Now, using (45) we have:

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