The Quantum Mechanics of a Free Particle

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We know that the solution to the Time Dependent Schrödinger Equation, for a given Potential V

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi \tag{1}$$

can be obtained by first solving the Time Independent Schrödinger Equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \tag{2}$$

We can then state that, the solution to Time Dependent Schrödinger Equation is a linear combination of Wave Functions of the form:

$$\Psi(x,t) = \psi(x)e^{-\frac{iEt}{\hbar}} \tag{3}$$

for all allowed values of E. Note that the individual wave functions of the form above represent the stationary states of the particle, and have energy E.

Let us solve the Schrödinger Equation for a free particle moving in one dimension. A free particle does not interact with any other particles and hence has $V = 0$.

Let us now solve the Time Independent Schrödinger Equation (in one dimension) for a free particle.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \tag{4}$$

On rearranging terms, we get:

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \tag{5}$$

For $E > 0$, we get the solution

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{6}$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$. The corresponding $\Psi(x,t)$ for this solution would be:

$$\Psi(x,t) = Ae^{i(kx-\frac{Et}{\hbar})} + Be^{-i(kx+\frac{Et}{\hbar})} \tag{7}$$

Let us consider the functions $Ae^{i(kx-\frac{Et}{\hbar})}$ and $Be^{-i(kx+\frac{Et}{\hbar})}$ separately. Notice that both these functions are eigenfunctions of both Momentum and Energy.

$$\hat{p}\Psi = -i\hbar\frac{\partial\Psi}{\partial x} = \hbar k\Psi \tag{8}$$

Here the eigenvalue of $\hat{p}$ represents the momentum of the particle if it could exist in this state. Therefore,

$$p = \hbar k \tag{9}$$

Similarly, we find that

$$\hat{E}\Psi = i\hbar\frac{\partial\Psi}{\partial t} = E\Psi \tag{10}$$

And therefore, the particle has energy E.

We also notice that the Wave Function is of the form $F(x+ct)+G(x-ct)$. Hence this Wave Function represents a wave moving with velocity $v = \frac{E}{\hbar k} = \sqrt{\frac{E}{2m}}$. However, for a classical particle, $E = \frac{1}{2}mv^2$ and so $v = \sqrt{\frac{2E}{m}}$. Hence **the velocity we calculated is double the classical velocity of the particle!**

This discrepancy can be resolved by noting that, **the above Wave Functions are not normalizible and therefore they do not represent physically realizible states of the particle**.

This issue can be overcome by realizing that just because the solutions of the the Time Independent Schrödinger Equation are not normalizible, does not mean that their linear combination is not normalizible. Since the actual solution of the Time Dependent Schrödinger Equation is a linear combination of the obtained solutions, it can still be normalizible and therefore can represent a physically realizible state.

With this knowledge, let us calculate the speed of a Quantum Free Particle. We know that for solutions of the the Time Independent Schrödinger Equation with energy E and momentum p, $k = \sqrt{\frac{2mE}{\hbar^2}}$, i.e. $E = \frac{\hbar^2k^2}{2m}$ and $p = \hbar k$. The Wave Function of a Quantum Free particle would be of the form:

$$\Psi(x,t) = \int_{-\infty}^{\infty} f(k)e^{i(kx-\frac{\hbar k^2 t}{2m})}\,dk \tag{11}$$

Now the problem is to find $f(k)$. We can find it if we know $\Psi(x,0)$, i.e. the initial Wave Function of the particle.

$$\Psi(x,0) = \int_{-\infty}^{\infty} f(k)e^{ikx}\,dk \tag{12}$$

This means that $f(k)$ is the Fourier Transform of $\Psi(x,0)$. Therefore:

$$f(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\Psi(x,0)e^{-ikx}\,dx \tag{13}$$

Hence we have found the Wave Function of the Quantum Free Particle. This wave function is in the form of a Wave Packet. We know that a wave packet has a phase velocity $v_p = \frac{\omega}{k}$ and a group velocity $v_g = \frac{d\omega}{dk}$. The dispersion relation for a free particle is:

$$\omega = \frac{\hbar k^2}{2m} \tag{14}$$

So here the phase velocity is:

$$v_p = \frac{\omega}{k} = \frac{\hbar k}{2m} = \sqrt{\frac{E}{2m}} \tag{15}$$

This was the velocity that we calculated earlier! Since the actual velocity of a wave packet is its group velocity and not its phase velocity, this resolves the discrepancy that we faced earlier, where the calculated velocity was double the classical velocity. On calculating the group velocity:

$$v_g = \frac{d\omega}{dk} = \frac{\hbar k}{m} = \sqrt{\frac{2E}{m}} \tag{16}$$

we see that it is identical to the classical velocity of the particle ($v_{classical} = \sqrt{\frac{2E}{m}}$), as expected.