Quantum Physics Course Number: PHY 201 Instructor: Rajib Saha Assistant Professor Department of Physics IISER Bhopal

0.1 De Broglie's hypothesis (Wave-particle dualtiy)

Since we know that wave can have particle properties (e.g., Photoelectric effect, Compton effect) De Broglie proposed that particles also have wave properties and so they actually exhibit a dual nature of both particles and wave. Since he knew that the wavelength of a photon of momentum p is given by, $\lambda = h/p$ (e.g., see question 4 of assignment 1), drawing an analogy with it, he proposed that the wavelength of a particle with a momentum p is given by $\lambda = h/p$. Some years after he put forward this hypothesis, Davisson and Germer experimentally verified it by doing a diffraction experiment of electron from Nicol crystal. The wave nature of electron was also verified by the double slit interference experiment of electrons.

De Broglie's hypothesis is one of the two fundamental principles in quantum mechanics. The second fundamental principle in quantum mechanics is *uncertainty principle* proposed by Werner Heisenberg.

0.2 Uncertainty Principle

It is impossible to device any experiment which can simultaneously measure the position and momentum of a particle with infinite accuracy. The uncertainties, Δx , in the x component of position and Δp_x in the x component of momentum satisfy,

$$\Delta x \Delta p_x \ge \hbar/2 = h/(4\pi) \tag{1}$$

We have seen in the class that in a gamma ray microscope the product, $\Delta x \Delta p_x \sim h$, which is greater than $h/(4\pi)$. Thus uncertainty principle is satisfied there. Also, in case of single slit diffraction experiment (Question 3. assignment 2) we have seen that $\Delta y \Delta p_y \sim h$, which again satisfies uncertainty principle given by Eqn. 1 above.

0.3 Do De Broglie's hypothesis and uncertainty principle contradict each other?

De Broglie's hypothesis assigns a fixed momentum (and therefore a fixed wavelength) to any particle. We recall that the Davisson and Germer experiment assumes this property for the electrons and that assumption was verified by the experiment to be correct. On the other hand, uncertainty principle says that we can't *measure* the momentum and position *simultaneously* with infinite accuracies. Since, in case of Davisson and Germer experiment, we do not measure the position and momentum of the electrons simultaneously one can talk about a fixed momentum in this case and so uncertainty principle is not at all in contradiction with the Davisson and Germer experiment (or De Broglie hypothesis).

In fact, recall that when we gave example of the uncertainty principle in case of gamma ray microscope we assumed that the incident gamma ray has a wavelength λ . So according to De Broglie's hypothesis it has a fixed momentum p. However, by saying this, we did not violate the uncertainty principle since we did not try to measure the momentum of the gamma ray (neither the incident nor the scattered γ -ray). We tried to measure the position of the electron – and we saw that the position was uncertain by an amount Δx , such that $\Delta x \Delta p_x \sim h$ which is $\geq \hbar/2$, consistent with Eqn. 1 above.

0.4 Wave function

Since particles show wave properties (De Broglie's hypothesis) it is logical to assign a wave function to each particle to contain the wave nature. We denote a wave function by $\Psi(\vec{r}, t)$, like all wave we have learned in the first year physics course, the wave function, in general, is a function of the position coordinate \vec{r} and time t.

How do we interpret Ψ physically?

To answer this question, we recall that the intensity distribution of the Young's double slit interference pattern with light wave is actually (complex) square of the superimposed wave amplitude¹. We also recall that using electrons in this experiment we obtain an interference pattern exactly identical to the case with light wave. So we conclude that the intensity distribution of the electrons on the screen could be obtained by computing square of the associated wave! But wait a minute – what is intensity distribution of electrons at a point on the screen? Definitely, it is proportional to number of electrons incident per unit area near the concerned point on the screen. Now if you recall the video of electron interference experiment – there electrons are incident on the screen one by one at random location. At the end of the experiment, the probability of finding an electron in an unit area, around an arbitrary point P, on the screen is directly proportional to number of electrons incident per unit area near that point – which is nothing but the intensity of the interference pattern at P. Since intensity again directly proportional to the (complex) square of the electron wave we conclude that,

the probability of finding an electron on the screen is proportional to the complex square of its wave function.

This is how we arrive at the idea of the probabilistic interpretation of wave function squared. Max Born proposed this probabilistic interpretation of wave function squared. He was awarded nobel prize in physics in 1954. He said, the probability of finding a particle in an elementary volume element dv around a point \vec{r} in the space is given by $dp = \Psi \Psi^* dv$. The probability finding it in a volume area V is given by $p = \int_V \Psi \Psi^* dv$. Since the particle must be somewhere in the all space, if we had searched for it in the entire space we would have found it for sure. We say that probability of finding it in all space is unity. So, mathematically we

¹Recall that, there we had two waves $\Phi_1(x,t) = A_1 \sin(kx_1 - \omega t)$ and $\Phi_2(x,t) = A_2 \sin(kx_2 - \omega t)$ superimposing, so that the superposed wave $\Phi(x,t) = \Phi_1(x,t) + \Phi_2(x,t)$ and $I(x,t) = \Phi(x,t)\Phi(x,t) = \Phi(x,t)\Phi^*(x,t)$, since we assumed Φ was real.

write,

$$\int_{all \ space} \Psi \Psi^* dv = 1. \tag{2}$$

 $\Psi\Psi^*$ is called probability density function.

0.5 Wave packet

Let's now try to find out how one can write down a wave function of a particle. As it happens in most of the cases in quantum physical systems, although we may not know the exact position of a particle do know with confidence that its actual position lies somewhere in a range, say between coordinates x_1 and x_2 , on the x axis at a time t. Then the probability of finding the particle outside (x_1, x_2) at time t is zero, meaning the wave function of the particle is zero outside this interval. Can we write down a wave function which is non-zero for $x_1 \leq x \leq x_2$ and 0 otherwise?

There may be more than one possible answer to this question. In this section we shall consider one special type of wave function called *wave packet*.

How do we construct one such wave packet? We superpose many plane waves, $e^{i(kx-\omega t)}$, each with slightly different wave number k, with a modulating amplitude A(k),

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{i(kx-\omega t)} dk \,,$$

where, we introduce $1/\sqrt{2\pi}$, for convenience of mathematical calculation that would follow. The angular frequency, ω , of plane wave, $e^{i(kx-\omega t)}$, is given by, $\omega = 2\pi\nu = 2\pi\nu/\lambda = (2\pi/\lambda)v = kv$. Here v is the velocity of the plane wave. Using this in the above equation we obtain,

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ik(x-vt)} dk$$

We now need to know the form of A(k). We let,

$$A(k) = e^{-(k-k_0)^2/4}$$
(3)

How does this function looks like? We have shown this in the top left panel of the Fig. 1. This is called a *Gaussian function*. This is centered at $k = k_0$ and decays slowly on both sides of $k = k_0$. Using such form of A(k) is advantageous since it allows only a range of kvalues to contribute in the integral. You would learn later from the mathematics of Fourier analysis that a small spread in k values in the above integral actually ensures that $\Psi(x, t)$ is also spread only in a certain region in x, and 0 otherwise. Thus we are justified to assume a form of A(k) as given by Eqn. 3.

Before we proceed further let's see how the real and imaginary part of the integrand looks. The real and imaginary parts of the function $e^{ik(x-vt)}$ are respectively, $\cos(k(x-vt))$ and $\sin(k(x-vt))$. We have shown the imaginary part at t = 0 for k = 5 in blue color in right hand side of the Fig. 1. We have shown the product $A(k)\sin(k(x-vt))$ in green line in this figure. This is also shown in the bottom panel of this figure.



1 0.8 0.6 0.4 0.2 0 -0.2 -0.4 -0.6 -0.8 -1 10 k 12 6 8 14

Figure 1:

Let's carry out the integration now. Using Eqn. 3 in Eqn. 4 we obain,

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-(k-k_0)^2/4 + ik(x-vt)} dk$$

= $\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-(k-k_0)^2/4 + 2i(x-vt)(k-k_0)/2 + ik_0(x-vt)} dk$
= $\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-(k-k_0)^2/4 + 2i(x-vt)(k-k_0)/2 + (x-vt)^2 - (x-vt)^2 + ik_0(x-vt)} dk$
= $\frac{1}{\sqrt{2\pi}} \left(\int_{-\infty}^{\infty} e^{-((k-k_0)/2 - i(x-vt))^2} dk \right) e^{-(x-vt)^2 + ik_0(x-vt)}$

The integral in the bracket can be computed by using the method of complex integral. A standard formula involving integration of complex number says that,

$$\int_{-\infty}^{\infty} e^{-z_1(p+z_2)^2} dp = \sqrt{\frac{\pi}{z_1}}$$
(4)

where z_1 and z_2 are complex number and $Re(z_1) > 0$. In our case, $p = k/2, z_1 = 1$ and $z_2 = -k_0/2 - i(x - vt))^2$. Hence,

$$\Psi(x,t) = \sqrt{2}e^{-(x-vt)^2 + ik_0(x-vt)}$$
(5)

 $^{^{2}}$ We shall use this result as is. You would prove this relation within a year or two from now in a 'Mathematical Methods in physics' class.