Quantum Mechanics A

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Contents

1 The principles of classical mechanics

We first consider the classical mechanics of a single particle.

1.1 States

The state of a particle at any time t is specified by its position, $\vec{x}(t)$ and its momentum $\vec{p}(t)$. We assume that these quantities are mathematically described by three dimensional vectors. Thus the space is specified by six real numbers. We think of these six numbers, (x, y, z, p_x, p_y, p_z)as corresponding to a point in a six dimensional space, the **phase space**.

Physically, this amounts to the assumption that the position and the momentum of the particle can be measured to arbitrary accuracy.

1.2 Observables

All functions of the position and the momentum are known if the state is known. These are the mechanical properties of the particle which we will call the observables.
Examples:

$\frac{1}{2m}\vec{p}\cdot\vec{p}$	Kinetic energy of a particle with mass m
$\vec{x}\times\vec{p}$	Angular momentum
$\frac{q_1 q_2}{4\pi\epsilon_0}\frac{1}{\|\vec{x}-\vec{x}_0\|}$	Coulomb energy due on a particle of charge q_1 due to a charge q_2 located at $\vec{x}_0$

Observables are therefore functions on the phase space.

1.3 Dynamics

For a non-relativistic particle in a force field, Newtons laws of motion can be written as,

$$\frac{d\vec{x}}{dt} = \frac{1}{m}\vec{p} \tag{1}$$

$$\frac{d\vec{p}}{dt} = \vec{F}(\vec{x},\vec{p}) \tag{2}$$

where $\vec{x}$ is the position and $\vec{p}$ the momentum of the particle. m is its mass and $\vec{F}$ is the force applied to it.

If the force is conservative and velocity independent, it can be expressed as the gradient of a potential, $\vec{F} = -\vec{\nabla} V$. The equations of motion can then be written in Hamilton's form,

$$\begin{aligned} \frac{dx^i}{dt} &= \frac{\partial H}{\partial p_i} && (3) \\ \frac{dp_i}{dt} &= -\frac{\partial H}{\partial x^i} && (4) \\ H(\vec{x}, \vec{p}) &\equiv \frac{1}{2m} \vec{p} \cdot \vec{p} + V(\vec{x}) && (5) \end{aligned}$$

$H(\vec{x}, \vec{p})$ is called the hamiltonian. It is the observable corresponding to the total energy.

Hamilton's form of the equations of motion are quite general and hold even when the velocity is not proportional to the momentum. Eg. consider a particle in the presence of a magnetic field. We denote the magnetic field by $\vec{B}$ and the vector potential by $\vec{A}$, thus $\vec{B} = \vec{\nabla} \times \vec{A}$. The hamiltonian is,

$$H(\vec{x}, \vec{p}) = \frac{1}{2m} \left(\vec{p} - e\vec{A} \right) \cdot \left(\vec{p} - e\vec{A} \right) \tag{6}$$

The equations of motion are,

$$\begin{aligned} \frac{dx^i}{dt} &= \frac{1}{m} (p_i - eA_i) && (7) \\ \frac{dp_i}{dt} &= \frac{e}{m} (p_j - eA_j) \frac{\partial A_j}{\partial x^i} && (8) \end{aligned}$$

Thus the velocity is not proportional to to the momentum. In this context, $m\dot{\vec{x}}$ is often called the mechanical momentum and $\vec{p}$ the canonical momentum. We leave it as an exercise to show that the second equation is the same as Newtons equation with the force being the Lorentz force. i.e

$$m \frac{d^2 \vec{x}}{dt^2} = e \frac{d\vec{x}}{dt} \times \vec{B} \tag{9}$$

Another example is the relativistic particle with rest mass m_0. The hamiltonian is,

$$H(\vec{x}, \vec{p}) = \sqrt{c^2 \vec{p} \cdot \vec{p} + m_0 c^4} \tag{10}$$

where c is the speed of light. The equations of motion are,

$$\frac{d\vec{x}}{dt} = \frac{c^2\vec{p}}{\sqrt{c^2\vec{p}\cdot\vec{p} + m_0c^4}} \tag{11}$$

$$\frac{d\vec{p}}{dt} = 0 \tag{12}$$

Again the velocity is not proportional to the momentum. When the magnitude of the momentum goes to infinity, the speed goes to c, consistent with the principles of special relativity.

1.4 Summary

1. The state of a particle is represented by a point in phase space.
2. Observables are functions on the phase space.
3. The time evolution of the state of the particle is governed by the hamiltonian, which is the observable corresponding to the total energy.

2 The double slit experiment

The following questions are about the experiment reported in the paper

"Controlled double-slit electron diffraction",
Roger Bach, Damian Pope, Sy-Hwang Liou and Herman Batelaan,
New Journal of Physics 15 (2013) 033018 (7pp).
Online at http://www.njp.org/
doi:10.1088/1367-2630/15/3/033018
Published 13 March 2013

1. **What is the speed and De Broglie wavelength of** $600\ eV$ **electrons ?**

$$E = \frac{1}{2}m_e v^2 \tag{13}$$

$$\frac{v}{c} = \sqrt{\frac{2E}{m_e c^2}} \tag{14}$$

Electron mass, m_e, charge, e and the speed of light, c:

$$m_e = 9.11 \times 10^{-31}\ kg \tag{15}$$

$$e = -1.6 \times 10^{-19}\ C \tag{16}$$

$$c = 3.0 \times 10^{8} m/s \tag{17}$$

Electron rest mass energy:

$$m_e c^2 = 9.11 \times 9.0 \times 10^{-15}\ J \tag{18}$$

$$= \frac{8.2 \times 10^{-14}}{1.6 \times 10^{-19}}\ eV \tag{19}$$

$$= 0.51\ MeV \tag{20}$$

Hence

$$\frac{v}{c} = 0.048 \tag{21}$$

$$v = 1.45 \times 10^{7}\ m/s \tag{22}$$

The De'Broglie wavelength of an electron with speed $v = 1.45 \times 10^7\ m/s$ is,

$$\lambda = \frac{h}{p} = \frac{6.6 \times 10^{-34}}{9.1 \times 10^{-31} \times 1.45 \times 10^7}\ m = 50 \times 10^{-12}\ m \tag{23}$$

2. **If the electron obeyed the principles of classical mechanics, then what is the expected range of the spread in the y-direction at the detection plane ?**

   Time taken to travel from the collimation slit, 2 μ wide to the single slit 30.5 cm away,

$$t = 30.5/v = 2.1 \times 10^{-8}\ s \tag{24}$$

   We assume that the electrons can come out of the collimation slit at all angles but do not get scattered at the slit. In that case the uncertainty in the y component of the velocity of the electrons passing through the slit is the width of the collimation slit divided by the time taken travel from the collimation slit to the slit.

$$\Delta v_y = \frac{2 \times 10^{-6}}{2 \times 10^{-8}}\ m/s = 100\ m/s \tag{25}$$

   Time taken to travel from the slit to the detection slit 0.24 m away,

$$t = \frac{0.24}{v} = 1.65 \times 10^{-8}\ s \tag{26}$$

   So the expected uncertainty in the position

$$\Delta y = 100 \times 1.65 \times 10^{-8}\ m = 1.65\ \mu \tag{27}$$

3. **From the experimentally, observed spread in the y component of the positions, estimate the spread of the y component of the momentum at the slit.**

   The experiment detects most of the electrons in the range $-150\ \mu \leq y \leq 150\ \mu$ at the detection slit which is 0.24 m from the slit. Hence we infer an uncertainty in v_y,

$$\begin{aligned} \Delta v_y &= 150 \times 10^{-6}\ \frac{v}{0.24} && (28) \\ &= 9100\ m/s && (29) \end{aligned}$$

This implies an uncertainty in the y component of the momentum $\Delta p_y = m_e \Delta v_y$,

$$\Delta p = 9.1 \times 10^{-31} \times 9.1 \times 10^{3} = 8.3 \times 10^{-27}\ kg\ m/s \tag{30}$$

4. **Compute the product of the uncertainties of the momentum and position at the slit**

   Uncertainty of the y component of the position is about half the width of the slit,

$$\Delta y = 3.1 \times 10^{-8}\ m \tag{31}$$

   The product of these uncertainties is

$$\begin{aligned}
\Delta p_y \Delta y &= 8.28 \times 10^{-27} \times 3.1 \times 10^{-8} && (32)\\
&= 2.7 \times 10^{-34}\ Js && (33)\\
&= 2.5\ \hbar && (34)
\end{aligned}$$

5. **Consider a wave from two point sources,**

$$A(\vec{r}, t) = \frac{A_1}{r_1} \sin(\omega t + k r_1) + \frac{A_2}{r_2} \sin(\omega t + k r_2) \tag{35}$$

   where r_1 and r_2 are the distances of the two sources from the point $\vec{r}$.

   Compute the intensity of the wave at the $x = D$ line, where $D >> d$.

   The intensity of the wave is,

$$I(\vec{r}) = \frac{1}{T} \int_0^T dt\ A^2(\vec{r}, t) \tag{36}$$

   where T is the time period, $T = \frac{2\pi}{\omega}$.

   Using the fact that

$$\begin{aligned}
\frac{1}{T} \int_0^T dt\ \sin^2(\omega t + \phi) &= \tfrac{1}{2} = \frac{1}{T} \int_0^T dt\ \cos^2(\omega t + \phi) && (37)\\
\frac{1}{T} \int_0^T dt\ \sin(\omega t + \phi) &= 0 = \frac{1}{T} \int_0^T dt\ \cos(\omega t + \phi) && (38)
\end{aligned}$$

we get,

$$I(\vec{r}) = \frac{1}{2}\left(\frac{A_1^2}{r_1^2} + \frac{A_1^2}{r_1^2}\right) + \frac{A_1 A_2}{r_1 r_2}\cos k(r_1 - r_2) \tag{39}$$

Now we choose the coordinate system where the point sources are at $\mp\frac{d}{2}\hat{y}$ and consider the intensity along the line parallel to the y-axis, $x = D$, where $D >> d$. The path difference, $r_1 - r_2$ at the point $\vec{r} = D\hat{x} + y\hat{y}$, is

$$r_1 - r_2 = \sqrt{D^2 + \left(y + \frac{d}{2}\right)^2} - \sqrt{D^2 + \left(y - \frac{d}{2}\right)^2} \tag{40}$$

$$= \frac{yd}{D} + o\left(\frac{1}{D^2}\right) \tag{41}$$

From equation (39), we can see that the distance between two maxima of the intensity, Δy, will be approximately the distance between two maxima of $\cos k(r_1 - r_2)$. Thus,

$$\frac{k\Delta y d}{D} \approx 2\pi, \quad \frac{2\pi}{k} \approx \frac{\Delta y d}{D} \tag{42}$$

6. **If, as in the electron double slit experiment,**

$$d = 272 \times 10^{-9}\ m \tag{43}$$

$$D = .24\ m \tag{44}$$

$$\Delta y = 45 \times 10^{-6}\ m \tag{45}$$

Then compute the wavelength

$$\lambda \equiv \frac{2\pi}{k} \approx \frac{45 \times 10^{-6} \times 272 \times 10^{-9}}{.24}\ m \approx 50 \times 10^{-12}\ m \tag{46}$$

7. **Consider a Gaussian function,**

$$f(x) = \frac{1}{\pi^{\frac{1}{4}}\sqrt{a}} e^{-\frac{x^2}{2a^2}} \tag{47}$$

   (a) **Compute its Fourier transform,**

$$g(k) = \int_{-\infty}^{\infty} dx\ e^{-ikx} f(x) \tag{48}$$

(b) Compute the mean and standard deviation of $f^2(x)$

(c) Compute the mean and standard deviation of $g^2(k)$

$$
\begin{aligned}
g(k) &= \frac{1}{\pi^{\frac{1}{4}}\sqrt{a}}\int_{-\infty}^{\infty} dx\ e^{-ikx-\frac{x^2}{2a^2}} && (49)\\
&= \frac{1}{\pi^{\frac{1}{4}}\sqrt{a}}\int_{-\infty}^{\infty} dx\ e^{-\frac{1}{2a^2}\left((x+ika^2)^2+k^2a^4\right)} && (50)\\
&= \pi^{\frac{1}{4}}\sqrt{2a}e^{-\frac{k^2a^2}{2}} && (51)
\end{aligned}
$$

The means are both zero,

$$
\langle x\rangle = \int_{-\infty}^{\infty} dx\ xf^2(x) = 0 = \int_{-\infty}^{\infty} dk\ kg^2(k) = \langle k\rangle \qquad (52)
$$

The standard deviation of $f^2(x)$,

$$
\begin{aligned}
\langle x^2\rangle &= \frac{1}{\sqrt{\pi}a}\int_{-\infty}^{\infty} dx\ x^2e^{-\frac{x^2}{a^2}} && (53)\\
&= \frac{1}{\sqrt{\pi}a}\left(-\frac{d}{d\lambda}\int_{-\infty}^{\infty} dxe^{-\lambda x^2}\right)\Bigg|_{\lambda=1/a^2} && (54)\\
&= \frac{1}{a}\left(-\frac{d}{d\lambda}\frac{1}{\sqrt{\lambda}}\right)\Bigg|_{\lambda=1/a^2} && (55)\\
&= \frac{1}{2}a^2 && (56)
\end{aligned}
$$

The standard deviation of $g^2(k)$,

$$
\begin{aligned}
\langle k^2\rangle &= 2a\sqrt{\pi}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\ k^2e^{-k^2a^2} && (57)\\
&= 2a\sqrt{\pi}\left(-\frac{d}{d\lambda}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\ e^{-\lambda k^2}\right)\Bigg|_{\lambda=a^2} && (58)\\
&= \frac{1}{2a^2} && (59)
\end{aligned}
$$

Therefore, we have

$$
\sqrt{\langle x^2\rangle\langle k^2\rangle} = \frac{1}{2} \qquad (60)
$$

3 Quantum mechanics of a free particle

The double slit experiment shows that the the principles of Quantum mechanics significantly depart from those of classical mechanics:

1. In the quantum regime, the outcome of a single measurement is, in principle, unpredictable. The theory can only predict the probabilities of the various outcomes in an ensemble of experiments. In the double slit experiment, a single electron can be detected anywhere on the screen. Thus after a few electrons are detected, we only have a few random dots on the screen which contain almost no information about the way they are behaving. Only after a large number of electrons are detected (i.e a large number of observations) does the pattern emerge.

2. The uncertainties in the position and momentum are consistent with Heisenberg's uncertainty relation.

3. The observed probability distribution, was similar to the intensity of interfering waves, with the wavelength being the De Broglie wavelength.

3.1 Wave function, position and momentum

To take into account experimental observations of the kind mentioned above, the state of a quantum mechanical particle is specified by the wave function which is a complex valued function on the space of positions. Denoting the wave function by $\psi(\vec{x})$, its physical meaning is as follows:

1. The probability of finding the particle in a volume d^3x around $\vec{x}$ is $\psi^*(\vec{x})\psi(\vec{x})d^3x$. Thus the wave function is often referred to as the probability amplitude of finding a particle at $\vec{x}$. Since the particle has to be found somewhere, we must have,

$$\int d^3x\ \psi^*(\vec{x})\psi(\vec{x}) = 1 \tag{61}$$

2. The probability amplitude of finding the particle momentum in a volume $d^3p/(2\pi\hbar)^3$ around $\vec{p}$ is

$$\chi(\vec{p}) = \int d^3x\ e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{x}}\psi(\vec{x}) \tag{62}$$

Since the particle will have some momentum, we must have

$$\int \frac{d^3p}{(2\pi\hbar)^3}\; \chi^*(\vec{p})\chi(\vec{p}) = 1 \tag{63}$$

Thus given the wave function, we know the probability distribution functions of the position and momentum. From the general properties of Fourier transforms,it then follows that the standard deviations of these two probability distributions obeys the inequality,

$$\Delta x \Delta p \geq \frac{\hbar}{2} \tag{64}$$

This was illustrated in question 7 of the previous section for the gaussian function.

Thus the wave function hypothesis incorporates indeterminacy, the wave nature of particles and Heisenbergs uncertainty principle.

3.2 The Schrodinger equation

The time evolution of the free particle state is given by the Schrodinger equation,

$$i\hbar \frac{\partial \psi(\vec{x}, t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \psi(\vec{x}, t) \tag{65}$$

where m is the mass of the particle.

The equation is first order in time and hence given the initial condition,

$$\psi(\vec{x}, t_0) = \psi_{in}(\vec{x}) \tag{66}$$

the equation can be solved to obtain the state for all future times.

Specifically, the state at time $t = t_0 + \delta t$, for small enough δt, is given by

$$\psi(\vec{x}, t_0 + \delta t) = \psi(\vec{x}, t_0) + \frac{\delta t}{i\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2 \psi(\vec{x}, t_0)\right) \tag{67}$$

Repeating this step will yield $\psi(\vec{x}, t_0 + 2\delta t), \psi(\vec{x}, t_0 + 3\delta t), \psi(\vec{x}, t_0 + 4\delta t), \ldots$

De Broglie waves are solutions to the Schrodinger equation,

$$\psi(\vec{x}, t) = \frac{1}{\sqrt{V}} e^{\frac{i}{\hbar}(-E(\vec{p})t + \vec{p}\cdot\vec{x})} \tag{68}$$

where $E(\vec{p}) = \frac{1}{m}\vec{p}\cdot\vec{p}$ and V is the volume of the region the particle is present (which may be infinity).

3.3 The probability density and current

The conservation of probability requires that the condition in equation (61) be satisfied at all times. The condition was the mathematical statement of the fact that we considering physical sytems in which the particle is present somewhere in the space. So this condition must hold true at all times for any physical time evolution.

To see that the dynamics specified by the Schrodinger equation is consistent with this condition consider the equation and its complex conjugate,

$$i\hbar \frac{\partial \psi(\vec{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \psi(\vec{x},t) \tag{69}$$

$$-i\hbar \frac{\partial \psi^*(\vec{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \psi^*(\vec{x},t) \tag{70}$$

Multiply equation (69) by $\psi^*(\vec{x},t)$, equation (70) by $\psi(\vec{x},t)$ and add the two. After a little algabraic manipulation, the sum can be written in the form of a continuity equation,

$$\frac{\partial \rho(\vec{x},t)}{\partial t} + \vec{\nabla}\cdot\vec{J}(\vec{x},t) = 0 \tag{71}$$

$$\psi^*(\vec{x},t)\psi(\vec{x},t) \equiv \rho(\vec{x},t) \tag{72}$$

$$\frac{\hbar}{2mi}\left(\psi^*(\vec{x},t)\vec{\nabla}\psi(\vec{x},t) - \left(\vec{\nabla}\psi^*(\vec{x},t)\right)\psi(\vec{x},t)\right) \equiv \vec{J}(\vec{x},t) \tag{73}$$

If we integrate equation (71) over all space, we recover the condition in equation (61) for all times,

$$\frac{\partial}{\partial t}\left(\int d^3x\ \psi^*(\vec{x},t)\psi(\vec{x},t)\right) = -\int d^3x\ \vec{\nabla}\cdot\vec{J}(\vec{x},t) \tag{74}$$

$$= \int d\vec{S}\cdot\vec{J}(\vec{x},t) \tag{75}$$

where we have used the Gauss divergence theorem and the surface integral is over the surface at infinity. The wave functions must go to zero at infinity otherwise they will not be normalisable. Hence we have,

$$\frac{\partial}{\partial t}\left(\int d^3x\ \psi^*(\vec{x},t)\psi(\vec{x},t)\right) = 0 \tag{76}$$

Thus the Schrodinger dynamics does not change the normalisation of the wave function. Such a time evolution is called unitary.

The continuity equation (71) also tells us that the probability is locally conserved. Namely that the rate of loss (or gain) of the probability density at any point is carried away (or brought in) by the probability current to (from) the neighbouring regions.

It is instructive to express the probablity current in terms of the modulus and phase of the wavefunction,

$$\begin{aligned} \psi(\vec{x},t) &\equiv \sqrt{\rho(\vec{x},t)}e^{\frac{i}{\hbar}\Omega(\vec{x},t)} &(77)\\ \vec{J}(\vec{x},t) &= \frac{1}{m}\rho(\vec{x},t)\vec{\nabla}\Omega(\vec{x},t) &(78)\end{aligned}$$

Thus the probability current is proportional to the gradient of the phase of the wave function. For a De Broglie wave with momentum $\vec{p}$, in a region of volume V,

$$\begin{aligned} \psi(\vec{x},t) &= \frac{1}{\sqrt{V}}e^{\frac{i}{\hbar}(-E(\vec{p})t+\vec{p}\cdot\vec{x})} &(79)\\ \Omega(\vec{x},t) &= -E(\vec{p})t+\vec{p}\cdot\vec{x} &(80)\\ \vec{J}(\vec{x},t) &= \frac{1}{V}\frac{\vec{p}}{m} &(81)\end{aligned}$$

$1/V$ is the uniform probability density and $\vec{p}/m$ the velocity of the particle. In general, if we visualise the probability as a fluid, then ρ and $\frac{1}{m}\vec{\nabla}\Omega$ can be interpreted as its density and velocity fields respectively.

3.4 The general solution

As we mentioned previously, De Broglie waves given in equation (68) are solutions of the Schrodinger equation. The equation is linear, namely if ψ_1 and ψ_2 are solutions, then so is any linear combination, $\psi_3 = A_1\psi_1 + A_2\psi_2$, where $A_{1,2}$ are complex numbers. Thus a linear combination of De Broglie waves of the form,

$$\psi(\vec{x},t) = \int \frac{d^3k}{(2\pi)^3}\, A(\vec{k})e^{-\frac{i}{\hbar}(E(\vec{k})t-\hbar\vec{k}\cdot\vec{x})} \qquad (82)$$

is a solution of the Schrodinger equation where $E(\vec{k}) = \frac{\hbar^2}{2m}\vec{k}\cdot\vec{k}$ for all complex, square integrable functions $A(\vec{k})$

We now put in the requirement of the initial condition in equation (66). Without any loss of generality we can choose $t_0 = 0$,

$$\psi_{in}(\vec{x}) = \int \frac{d^3k}{(2\pi)^3}\; A(\vec{k}) e^{i k\cdot \vec{x}} \tag{83}$$

Thus $A(\vec{k})$ is uniquely fixed to be the Fourier transform of the initial wave function,

$$A(\vec{k}) = \int\; d^3x\; e^{-i\vec{k}\cdot\vec{x}}\; \psi_{in}(\vec{x}) \tag{84}$$

Equations (82) and (84) give the general solution of the Schrodinger equation satisfying the initial condition in equation (66).

3.5 Gaussian wave packets

We will now study a class of initial conditions for which the Schrodinger equation can be analytically solved, namely gaussian wave packets. For simplicity we restrict ourselves to one dimension and analyse the time evolution of the initial wave functions,

$$\psi_{in}(x) = \frac{1}{\pi^{\frac{1}{4}}\sqrt{a}} e^{-\frac{x^2}{2a^2} + i k_0 x} \tag{85}$$

The Fourier transform can be computed to be,

$$A(k) = \pi^{\frac{1}{4}}\sqrt{2a}\; e^{-\frac{(k-k_0)^2 a^2}{2}} \tag{86}$$

As seen earlier, this is a minimum uncertainty wave packet with $\Delta x = \frac{a}{\sqrt{2}}$ and $\Delta p = \frac{1}{a\sqrt{2}}$.

The solution for all times $t \geq 0$ is then,

$$\psi(x,t) = \pi^{\frac{1}{4}}\sqrt{2a}\; \int \frac{dk}{2\pi}\; e^{-\left(\frac{(k-k_0)^2 a^2}{2} + i\frac{\hbar k^2}{2m} t - ikx\right)} \tag{87}$$

We make the change of variable, $k' = k - k_0$, in the above integral. The term in the exponential can then be written as,

$$\frac{(k-k_0)^2 a^2}{2} + i\frac{\hbar k^2}{2m} t - ikx = i\frac{\hbar k_0^2}{2m} t - ik_0 x + \frac{1}{2}\left(a^2 + i\frac{\hbar t}{m}\right) k'^2 - ik'(x - \frac{\hbar k_0}{m} t) \tag{88}$$

We denote

$$\frac{\hbar^2 k_0^2}{2m} \equiv \frac{1}{\hbar} E_0 \qquad \frac{\hbar k_0}{m} \equiv v_0, \qquad a^2 + i\frac{\hbar t}{m} \equiv w(t) \tag{89}$$

The k' integral can be done to get,

$$\psi(x,t) = \frac{1}{\pi^{\frac{1}{4}}} \sqrt{\frac{a}{w^2(t)}} e^{-\frac{(x-v_0 t)^2}{2w^2(t)}} e^{-\frac{i}{\hbar}E_0 t + ik_0 x} \tag{90}$$

We will now express the wave function in terms of its modulus and phase. We first study the complex width $w^2(t)$,

$$\frac{w^2(t)}{a} = a + i\frac{\hbar t}{am} \tag{91}$$

We define $u = \hbar/ma$, the speed of a particle with wavevector equal to $1/a$. We then have,

$$\begin{aligned} \frac{1}{w^2} &= \frac{1}{a}\frac{1}{a+iut} && (92) \\ &= \frac{1}{a^2+(ut)^2} - i\frac{\frac{ut}{a}}{a^2+(ut)^2} && (93) \\ & && (94) \end{aligned}$$

We further denote,

$$\frac{w^2}{a} \equiv \alpha e^{\frac{i}{\hbar}\phi} \qquad \alpha = \sqrt{a^2+(ut)^2} \qquad \tan\frac{\phi}{\hbar} = \frac{ut}{a} \tag{95}$$

With the notation defined above we write the wave function in terms of its modulus and phase,

$$\begin{aligned} \psi(x,t) &= \sqrt{\rho(x,t)} e^{\frac{i}{\hbar}\Omega(x,t)} && (96) \\ \rho(x,t) &= \frac{1}{\sqrt{\pi}\alpha(t)} e^{-\frac{(x-v_0 t)^2}{a^2+(ut)^2}} && (97) \\ \Omega(x,t) &= \frac{-1}{2}\phi(t) - iE_0 t + ik_0 x - \frac{(x-v_0 t)^2 \tan\phi}{2(a^2+(ut)^2)} && (98) \end{aligned}$$

Note that the wave packet spreads of in space in time. The uncertainty in the position grows with time as $\sqrt{a^2+(ut)^2}$. This is a consequence of the fact the the speed of a De Broglie wave depends on its wavelength ($v = \hbar k/m$). Since the different waves in the packet travel at different speeds, the wave packet does not retain its shape under time evolution.

3.6 The classical regime

We can calculate the expectation values of $x(t)$ and $p(t)$ using the wave function in equation (90), it yields,

$$\langle x(t)\rangle = v_0 t, \qquad \langle p(t)\rangle = \hbar k_0 \tag{99}$$

Thus the expectation values satisfy the classical equations of motion. This illustrates the general result, Ehrenfest's theorem, which states that this will always be the case. The deviation from classical mechanics are therefore contained in the standard deviations, the uncertainties.

No measurement is without errors. Let us denote the errors in the measurement of the position and momentum by δx and δp respectively. As before, we denote the standard deviations of the position and momentum quantum probability distribution functions by Δx and Δp respectively.

In the quantum theory, the outcome of an single measurement of the position and the momentum at time t will lie between $\langle x(t)\rangle \pm 2\Delta x$ and $\langle p(t)\rangle \pm 2\Delta p$ with a probability of about 0.95. So if $\delta p >> \Delta p$ and $\delta x >> \Delta x$ for the full observation time, the probability of the result of a single observation of x and p to be between $\langle x\rangle \pm \delta x$ and $\langle p\rangle \pm \delta p$ respectively will be very close to 1. In such a situation, the observations will be well described by classical mechanics.

As an example, let us consider the case of the gaussian wave packet described in the previous section. Let us take $\delta x = 50\ nm$ and $a = 10\ nm$. The uncertainty in the position is thus much less than the measurement error at $t = 0$. After a time t the uncertainty is $\sqrt{a^2 + (ut)^2}$, where $u = \hbar/ma$. For an electron we have $u \approx 10^4\ m/s$. So within a few picoseconds, the uncertainty will exceed the measurement errors. Now consider the case of a nano-particle consisting of about 10^3 atoms and a mass about 10^8 times the electron mass. The position uncertainty will exceed the measurement accuracy after a few seconds. If it were a particle of mass 1 kg the time is $\sim 10^{18}\ s \sim 3 \times 10^{10}\ y$ which about the age of the universe.

Thus a general thumb rule is, the heavier the particle, the larger the regime of parameters where classical mechanics correctly predicts the results of measurements.

4 Approximate theory of the double experiment

In this section we will attempt to model the electron in the double slit experiment using gaussian wave packets. First we will consider the case of only one slit being open. We then know that at the time the electron passes through the slit, its wave function is localised in the y-direction to the extent of the slit width. We also know it average velocity in the x-direction. We will therefore hypothesize that at the time is passing through the slit, it is well described by a gaussian wave packet with suitably chosen parameters detailed in the following sections. We can then use the free particle time evolution and predict the probability of it being detected at different points on the screen. For the case of both the slips being open, we will hypothesize that the electron is in a superposition of two gaussian wave packets localised at the two slits and repeat the calculation.

4.1 The single slit theory

We choose the slit to be in the $x = 0$ plane and the detection slit to be in the $y = D = 0.24\ m$ plane. The slit is centered at $(x, y) = (0, 0)$ and extends upto $(x, y) = (0, \pm\frac{a}{2}) = (0, 31 \times 10^{-9}\ m)$.

We assume the initial wave function to be a gaussian wave packet of the form

$$\begin{aligned}
\psi(x, y, 0) &= \phi(y, 0)\chi(x, 0) && (100)\\
\chi(x, 0) &= \frac{1}{\pi^{\frac{1}{4}}\sqrt{a_x}} e^{-\frac{x^2}{2a_x^2}} e^{ik_0 x} && (101)\\
\phi(y, 0) &= \frac{1}{\pi^{\frac{1}{4}}\sqrt{a_y}} e^{-\frac{y^2}{2a_y^2}} && (102)
\end{aligned}$$

We choose a_y such that the probability of the particle being at $|y| > \frac{d}{2}$ is extremely small. If we take $a_y = \frac{d}{4}$, then the probability of the particle being at $|y| > \frac{d}{2}$ is $< e^{-4} = 0.018$. So we take $a_y = \frac{d}{4}$. k_0 is chosen to correspond to the known De Broglie wavelength of the particle, namely $\frac{2\pi}{k_0} = 50 \times 10^{-12}\ m$. We leave a_x unfixed for the moment.

From the calculations in the previous section, at time t the wave function is

$$\psi(x,y,t) = \phi(y,t)\chi(x,t) \tag{103}$$

$$\chi(x,0) = \sqrt{\rho_x(x,t)}e^{\frac{i}{\hbar}\Omega_x(x,t)} \tag{104}$$

$$\rho_x(x,t) = \frac{1}{\sqrt{\pi}\alpha_x(t)}e^{-\frac{(x-v_0t)^2}{a_x^2+(u_xt)^2}} \tag{105}$$

$$\Omega_x(x,t) = \frac{-1}{2}\phi_x(t) - iE_0t + ik_0x - \hbar\frac{(x-v_0t)^2\tan\phi_x}{2(a_x^2+(u_xt)^2)} \tag{106}$$

$$v_0 = \frac{\hbar k_0}{m} \qquad u_x = \frac{\hbar}{ma_x} \tag{107}$$

$$\alpha_x = \sqrt{a_x^2+(u_xt)^2} \qquad \tan\frac{\phi_x}{\hbar} = \frac{u_xt}{a_x} \tag{108}$$

$$\phi_(y,0) = \sqrt{\rho_y(x,t)}e^{\frac{i}{\hbar}\Omega_y(x,t)} \tag{109}$$

$$\rho_y(x,t) = \frac{1}{\sqrt{\pi}\alpha_y(t)}e^{-\frac{y^2}{a_y^2+(u_yt)^2}} \tag{110}$$

$$\Omega_y(x,t) = \frac{-1}{2}\phi_y(t) - iE_0t - \hbar\frac{y^2\tan\phi_y}{2(a_y^2+(u_yt)^2)} \tag{111}$$

$$u_y = \frac{\hbar}{ma_y} \tag{112}$$

$$\alpha_y = \sqrt{a_y^2+(u_yt)^2} \qquad \tan\frac{\phi_y}{\hbar} = \frac{u_yt}{a_y} \tag{113}$$

We are interested in the probability of detecting the particle at $(x,y) = (D,y)$ at any time. Denoting this probability by $P(y)$, we have,

$$P(y) = \frac{1}{T}\int_0^T dt\ |\psi(D,y,t)|^2 \tag{114}$$

From equation (105), we see that $|\psi(D,y,t)|^2$ will peak at $t = \frac{D}{v_0} \equiv t_0 = 1.65 \times 10^{-8}\ s$ so we approximately evaluate the probability to be,

$$P(y) \approx |\psi(D,y,\frac{D}{v_0})|^2 \tag{115}$$

$$= \rho_x(D,t_0)\rho_y(y,t_0) \tag{116}$$

$$= \frac{1}{\pi\alpha_x(t_0)\alpha_y(t_0)}e^{-\frac{y^2}{a_y^2+(u_yt_0)^2}} \tag{117}$$

$$\tag{118}$$

As we saw earlier, this gaussian probability distribution function will be almost zero at $|y| > 2\sqrt{a_y^2 + (u_y t_0)^2}$. We compute this distance,

$$
\begin{aligned}
u_y t_0 &= \frac{\hbar}{m a_y}\frac{Dm}{\hbar k_0} && (119)\\
&= \frac{D}{a_y k_0} && (120)\\
&= 0.24 \cdot \frac{4}{62 \times 10^{-9}} \cdot \frac{50 \times 10^{-12}}{2\pi}\ m && (121)\\
&= 123\ \mu && (122)
\end{aligned}
$$

This is approximately equal to the width of the spread of the electons detected in the data which is $\approx 150\ \mu$.

4.2 The Double Slit theory

For the case where both slits are open we hypothesize the wave function to be,

$$\psi_{DS}(x,y,t) = \frac{1}{\sqrt{2}}\left(\psi(x, y + \frac{d}{2}, t) + \psi(x, y - \frac{d}{2}, t)\right) \tag{123}$$

Where $\psi(x,y,t)$ is the wave funtion in equation (103). Just as in the previous section, the probability of detection of the particle at $(x,y) = (D,y)$ is approximated as,

$$
\begin{aligned}
P(y) &= |\psi_{DS}(D,y,t_0)|^2 && (124)\\
&= \rho_x(D,t_0)\left(\rho_y\left(y + \frac{d}{2}, t_0\right) + \rho_y\left(y - \frac{d}{2}, t_0\right)\right. && (125)\\
&\quad \left. +2\sqrt{\rho_y(y + \frac{d}{2}, t_0)\rho_y(y - \frac{d}{2}, t_0)}\cos\left(\frac{1}{\hbar}\Delta\Omega(y)\right)\right) && (126)\\
\Delta\Omega(y) &= \Omega_y\left(y + \frac{d}{2}, t_0\right) - \Omega_y\left(y - \frac{d}{2}, t_0\right) && (127)\\
&= \hbar\ 2yd\ \frac{u_y t_0}{a_y}\frac{1}{2(a_y^2 + (u_y t_0)^2)} && (128)
\end{aligned}
$$

In the previous section we had computed $u_y t_0 = D/(a_y k_0) = 123\ \mu >> a_y$. So we neglect a_y^2 with respect to $(u_y t_0)^2$ in the above equation to get,

$$\frac{1}{\hbar}\Delta\Omega(y) = \frac{2\pi dy}{D\lambda_0} \tag{129}$$

where $\lambda_0 \equiv 2\pi/k_0$. The distance between two peaks of the interference pattern, which we denote by Δy is given by,

$$\Delta y = \frac{D\lambda_0}{d} = 41\ \mu \tag{130}$$

The data shows 7 peaks over a range of 300 μ, thus the observed distance between two peaks is $\approx 43\ \mu$ which is in good agreement with our approximate theory.