Quantum Description of Electron Diffraction Through Single Slit

Abhinaba Pahari : Roll no. 23PH40001
Arnab Satpati : Roll no. 23PH40010
Sandipan Hazra : Roll no. 23PH40042

Indian Institute of Technology Kharagpur, Depertment of phyiscs

30/11/2023

Abstract

We have studied single slit diffraction of light waves and seen how consequtive bright and dark fringes are produced. But what happens when an electron beam faces a narrow slit is the topic of discussion of this term paper. Our approach is quite straightforward. We solved the Time Independent Schrodinger's equation for different regions of diffraction i.e. inside the slit and back of the slit by considering a plane wave falling on the slit from front. Firstly we solved the TISE using separation of variables and matching the wavefunction at the boundaries. Then we showed numerical results and plots of intensity distribution according to our theory of diffraction. The paper concludes with brief overview of significance of our work and comparison of our results with contemporary theoretical results.

1 Introduction

In Physics, many times we came across pheomenon where light or other waves encounter a narrow aperture and spread out into a pattern of alternating bright and dark regions. As we know this behavior occurs due to the interference of diffracted waves emerging from different points along the slit. This is the scenario for swarm of photons. Doing the exactly same experiment with classical particles (say, tennis balls) will not show anything special on the screen. Just a uniform distribution of the tennis balls is obtained on the area of the screen nearly equal to the width of the slit. But in the world of quantum mechanics, electrons exhibit a dual nature—simultaneously behaving as particles and waves. This paper focuses on unraveling the peculiarities of electron diffraction through a narrow single slit and wave particle duality of electrons.

2 Theory

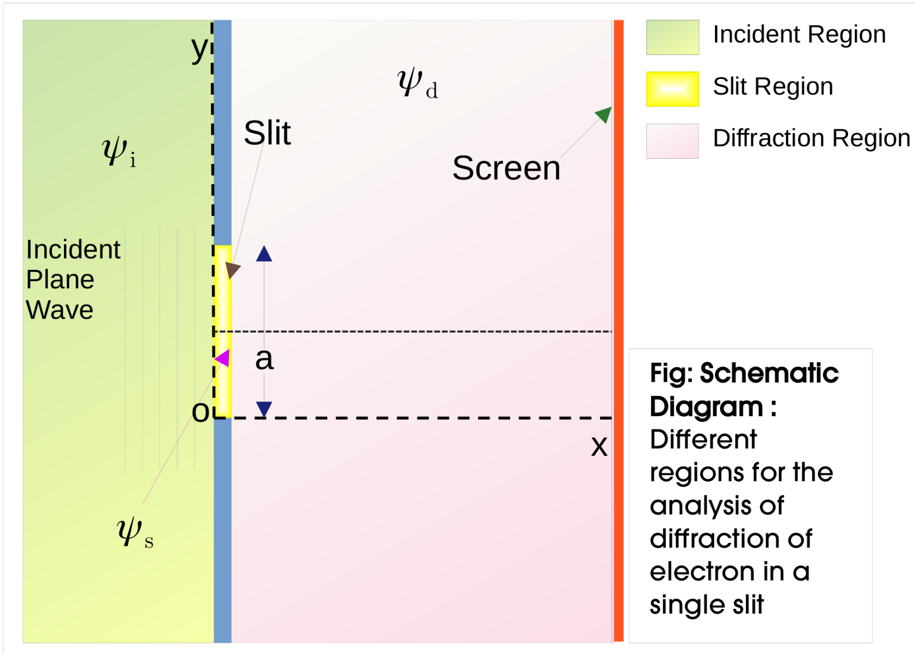
Although diffraction of electron is a relativistic phenomenon, we are confining our discussion in non-relativistic case. If the slit is rectangular and one of the dimension of the slit is considered much larger than the other, the problem can be resolved in two dimensions without any loss of generality. The potential due the slit is not changing with time. So we apply Time Independent Schrodinger Equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) + V(x,y,z)\psi = E\psi(x,y,z)$$

Let us consider the situation where the slit is placed perpendicular to x axis (at x=0). The slit opening is extended from y = 0 to y = a. The screen is parallel to the slit, at some finite distance along x-axis (As shown in figure).

Our work is organized follows. We divide the whole setup in 3 regions i.e. **incident region**, **slit region** and **diffraction region**. A plane wave corresponding to the wavefunction of incident electrons falls on the slit from Incident region. We apply Schrodinger's equation inside the slit with proper choice of slit potential and matching the wavefunction of incident beam(ψ_i) at left. This will give us the wavefunction inside the slit(ψ_s) associated with the electrons. In the diffraction region, applying TISE will similarly give us a wavefunction. The boundary condition on right is : wavefunction in the slit will be similar to wavefunction in diffraction region(ψ_d) for $x = 0$ and at range $0 < y < a$.

Procceding in this way, it should give us the wavefunction on the screen (ψ_{screen}) if we consider the wavefunction of diffraction area for a particular value of x . Doing its inner product with itself ($I \propto |\psi|^2 = \psi^*\psi$) would be the probablity density of position of electron on the screen i.e. the intensity pattern.



2.1 Wavefunction Inside the slit

Let the wavefunction corresponding to the electron beam incident on the slit be

$$\psi_i(x, y) = A_0 \exp(ikx) \tag{1}$$

where A_0 is a constant(Amplitude of incident wave).
The range of x for the slit is extemely small but finite. So lets keep the x-dependence of slit wavefunction(ψ_s). The potential in the slit area can be expressed as

$$V(x) = \begin{cases} 0 & \text{if } 0 < y < a \\ \infty & \text{otherwise} \end{cases}$$

Now the time independent schrodinger equation inside the slit becomes

$$\nabla^2 \psi_s = -\frac{2mE}{\hbar^2} \psi_s \tag{2}$$

Here m is the mass of electron, E is the energy and ψ_s is the wavefunction inside the slit. In two dimensions it reduces to

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \psi_s = -\frac{2mE}{\hbar^2} \psi_s \tag{3}$$

Doing separation of variables, $\psi_s = X(x)Y(y)$, from eqn (3)

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} = -\frac{2mE}{\hbar^2} \tag{4}$$

If we let the seperation constant be $(-l^2)$ then equation (4) is reduced to two equations. One of which will be:

$$\frac{1}{Y}\frac{d^2Y}{dy^2} = -l^2$$

which has general solution of form

$$Y(y) = Asin(ly) + Bcos(ly) \tag{5}$$

where A and B are arbitrary constants. Again Y(y)=0 at y=0 and y=a for the wavefunction inside the slit,as the Y(y) part of the wavefunction(ψ_s) vanishes at the boudaries of the slit . So

$$Y(y=0) = 0$$

$$\implies Asin(0) + Bcos(0) = 0$$

$$\implies B = 0$$

And

$$Y(y=a) = 0$$

$$\implies Asin(la) = 0$$

$$\implies l = \frac{n\pi}{a}$$

$$\implies Y(y) = Asin(\frac{n\pi y}{a}) \tag{6}$$

The another part of eqn(4) reads

$$\frac{1}{X}\frac{d^2X}{dx^2} = (-\frac{2mE}{\hbar^2} + l^2)X \tag{7}$$

$$\implies \frac{1}{X}\frac{d^2X}{dx^2} + (\frac{2mE}{\hbar^2} - l^2)X = 0$$

The general solution of this equation is

$$X(x) = Csin(\sqrt{\frac{2mE}{\hbar^2} - \frac{n^2\pi^2}{a^2}}x) + Dcos(\sqrt{\frac{2mE}{\hbar^2} - \frac{n^2\pi^2}{a^2}}x) \tag{8}$$

Since A,B,C are arbitary constants, the general solution i.e. the product of $X(x)$ and $Y(y)$ can be written summing over all integer values of n. Thus from eqn(6) and (8) ψ_s can be written summing over n as

$$\psi_s(x,y) = \sum_n A_n sin(\frac{n\pi y}{a}) \exp(i\sqrt{\frac{2mE}{\hbar^2} - \frac{n^2\pi^2}{a^2}}x) \tag{9}$$

$$\implies \psi_s(x=0,y) = \sum_n A_n sin(\frac{n\pi y}{a}) \tag{10}$$

On the left side of the slit where the incident wave just faces the slit, the boundary condition is :

$$\psi_i(x=0,y) = \psi_s(x=0,y)$$

$$\implies A_0 = \sum_n A_n sin(\frac{n\pi y}{a}) \quad \text{[From(1) and(10)]}$$

Using Fourier's trick , we can write

$$A_n = \frac{2}{a}\int_0^a A_0 sin(\frac{n\pi y}{a})dy$$

$$\implies A_n = \begin{cases} 0 & \text{if n is even} \\ \frac{4A_0}{n\pi} & \text{if n is odd} \end{cases}$$

So we can conclude

$$\psi_s(x=0,y) = \sum_{n=..-3,-1,1,3,..} \frac{4A_0}{n\pi} sin(\frac{n\pi y}{a}) \tag{11}$$

$$\implies \psi_s(x=0,y) = \sum_{n=1,3,..} \frac{8A_0}{n\pi} sin(\frac{n\pi y}{a})$$

$$\implies \psi_s(x=0,y) = \sum_{n=0}^{\infty} \frac{8A_0}{(2n+1)\pi} sin(\frac{(2n+1)\pi y}{a}) \tag{12}$$

This is the expression for the wavefunction inside the slit.

2.2 Wavefunction on the screen

The potential V(x,y) for all the points in the diffraction region is zero. So the time independent schrodinger equation becomes

$$\nabla^2\psi_d = -\frac{2mE}{\hbar^2}\psi_d \tag{13}$$

ψ_d is the wavefunction in diffraction region. In a similar fashion as before we proceed with separation of variables $\psi_d = X(x)Y(y)$ and obtain the following equations

$$\frac{1}{Y}\frac{d^2Y}{dy^2} = -{k_y}^2$$

And

$$\frac{1}{X}\frac{d^2X}{dx^2} + (\frac{2mE}{\hbar^2} - {k_y}^2)X = 0$$

which has the solutions of the form

$$X(x) \sim \exp(ix\sqrt{\frac{2mE}{\hbar^2} - k_y^2})$$

and

$$Y(y) \sim \exp(ik_y y)$$

Therefore, the general solution is

$$\psi_d(x,y) = \int_{-\infty}^{\infty} A(k_y) \exp(ix\sqrt{\frac{2mE}{\hbar^2} - k_y^2}) \exp(ik_y y) dk_y \tag{14}$$

Here k_y is a continuous variable because there is no restriction and integration is done on entire $k_y$beacuse $\psi_d$is superposed over all k_y.

As we considered before, the boundary condition on right (At x=0) reads

$$\psi_d(x=0,y) = \begin{cases} \psi_s(x=0,y) & \text{when } 0 < y < a \\ 0 & \text{otherwise} \end{cases}$$

$$\implies \psi_s(x=0,y) = \int_{-\infty}^{\infty} A(k_y) \exp(ik_y y) dk_y \tag{15}$$

Now denoting $k_y = r$ and considering the inverse fourier transform of equation (15), we get

$$A(r) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi_s(x=0,y) \exp(ik_y y) dk_y$$

$$\implies A(r) = \frac{1}{2\pi} \int_0^a \exp(-iry)[\sum_{n=0}^{\infty} \frac{8A_0}{(2n+1)\pi} sin(\frac{(2n+1)\pi y}{a})]dy \tag{16}$$

Since the boudary condition is valid for $0 < y < a$, the limit of the intagration is modified as 0 to a .

If we do the follwing integration for integer value of n it comes out as

$$\int_0^a \exp(-iry) sin(\frac{(2n+1)\pi y}{a})dy = \frac{a\pi(2n+1)(1+\exp(iar))\exp(-iar)}{(\pi(2n+1))^2 - a^2r^2}$$

So ultimately

$$A(r) = \frac{4aA_0}{\pi} \sum_{n=0}^{\infty} \frac{1+\exp(-iar)}{((2n+1)\pi)^2 - a^2r^2} \tag{17}$$

Thus from equation (14)

$$\psi_d(x,y) = \frac{4aA_0}{\pi} \int_{-\infty}^{\infty} \exp(ix\sqrt{\frac{2mE}{\hbar^2} - r^2}) e^{iry} \sum_{n=0}^{\infty} \frac{1+\exp(-iar)}{((2n+1)\pi)^2 - a^2r^2} dr \tag{18}$$

For a fixed value of x (say at x=b) the wavefunction $\psi_d(x,y)$ becomes the wavefunction at the screen. Therefore

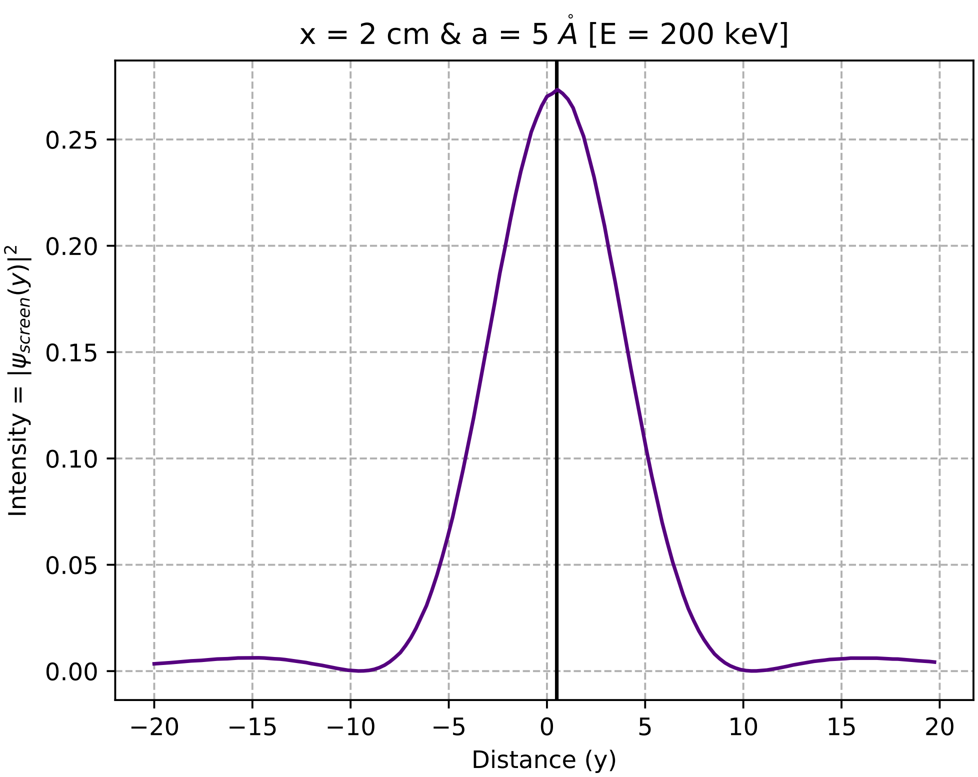
$$\psi_{screen}(y) = \frac{4aA_0}{\pi} \int_{-\infty}^{\infty} \exp(ib\sqrt{\frac{2mE}{\hbar^2} - r^2}) e^{iry} \sum_{n=0}^{\infty} \frac{1+\exp(-iar)}{((2n+1)\pi)^2 - a^2r^2} dr \tag{19}$$

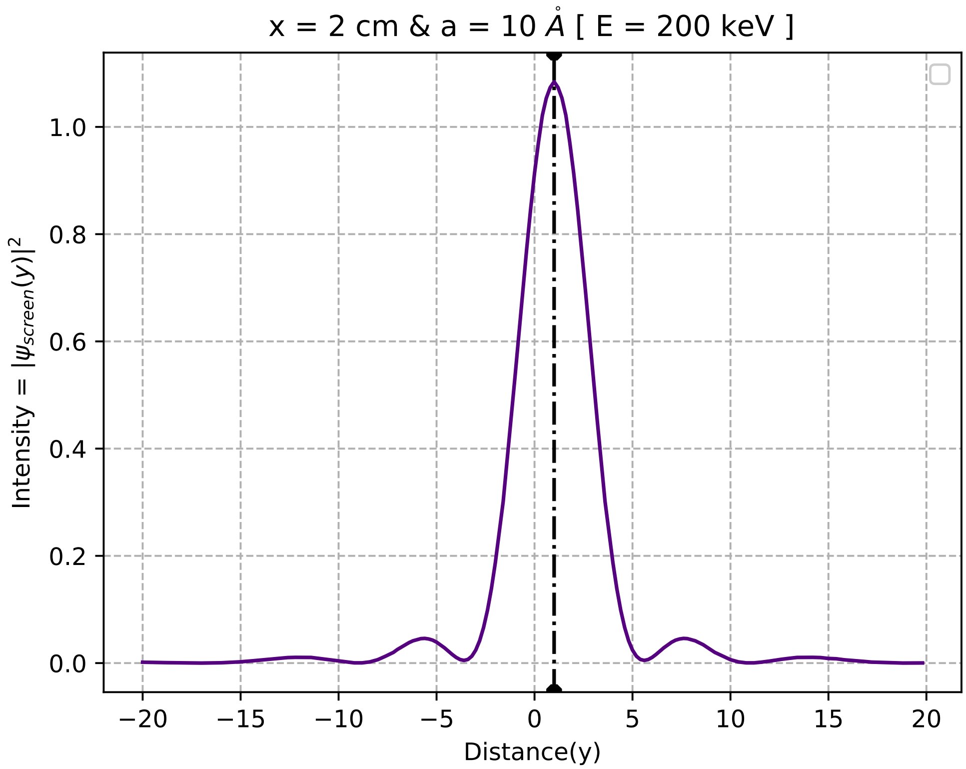
The integration of equation (19) is evaluated numerically to get the wavefunction and thus taking product with is complex conjugate, we have got the probablity density of electrons on the screen i.e. the intensity variation on the screen .

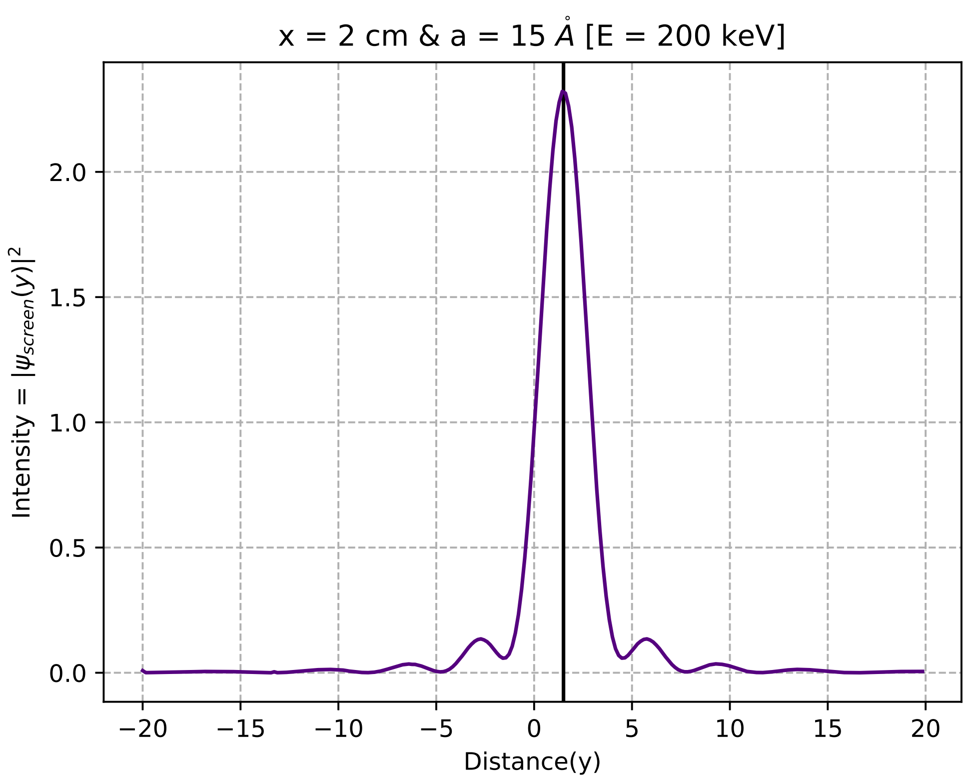
$$\text{Intensity on screen } (I) \propto \psi^*_{screen}\psi_{screen}$$

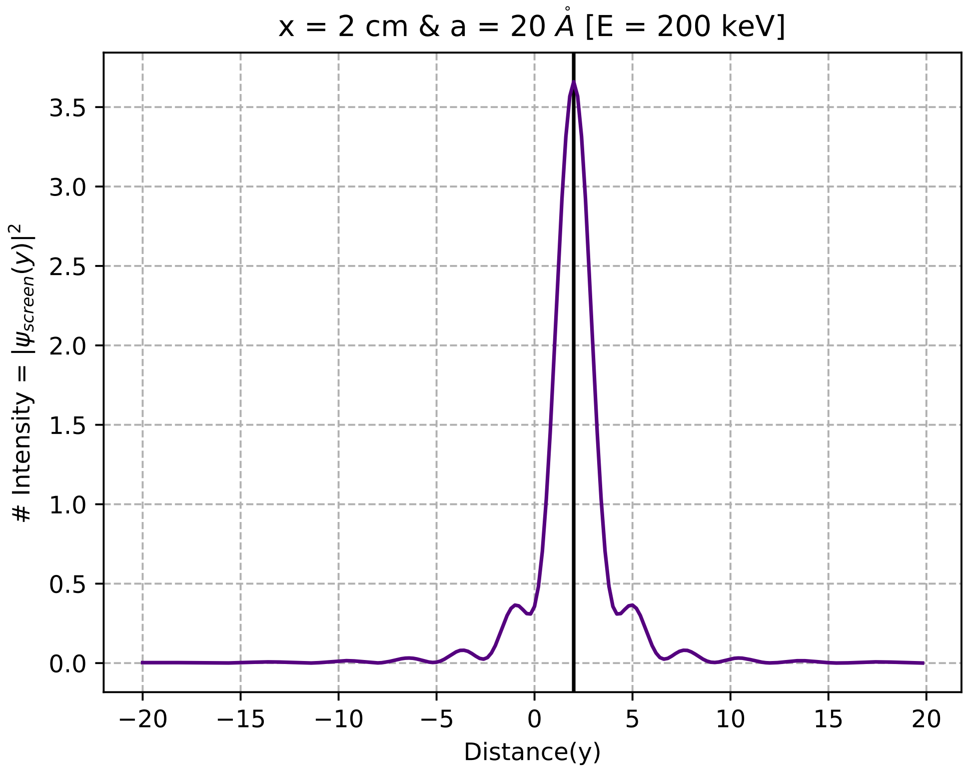
3 Numerical Results

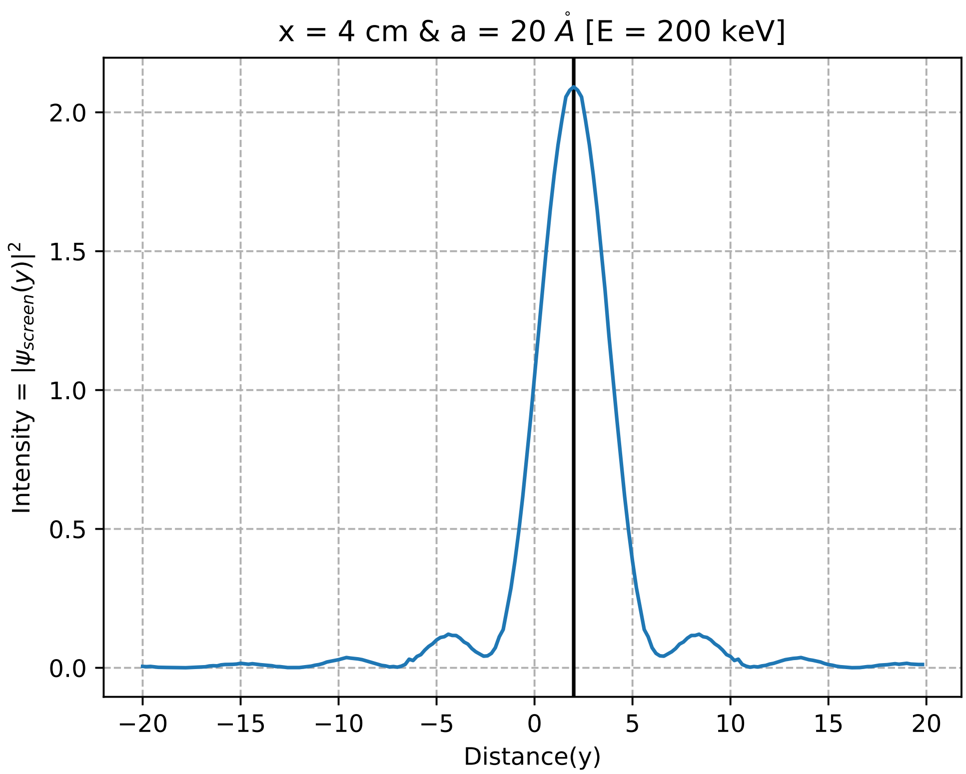
From equation (19) it is clear that evaluating the integral is not an easy task. Therefore, we write a Python code [Appendix A] to evaluate the integral of equation (19) and Plot the variation of Intensity with distance.
In the following figures, x denotes destance between screen and slit and a is the slit width. The electrons are considered monochromatic having energy of 200 keV (First 5 figures) and 400 keV (Last Figure).
The vertical black line in each plot shows the maxima of each intensity distribution.

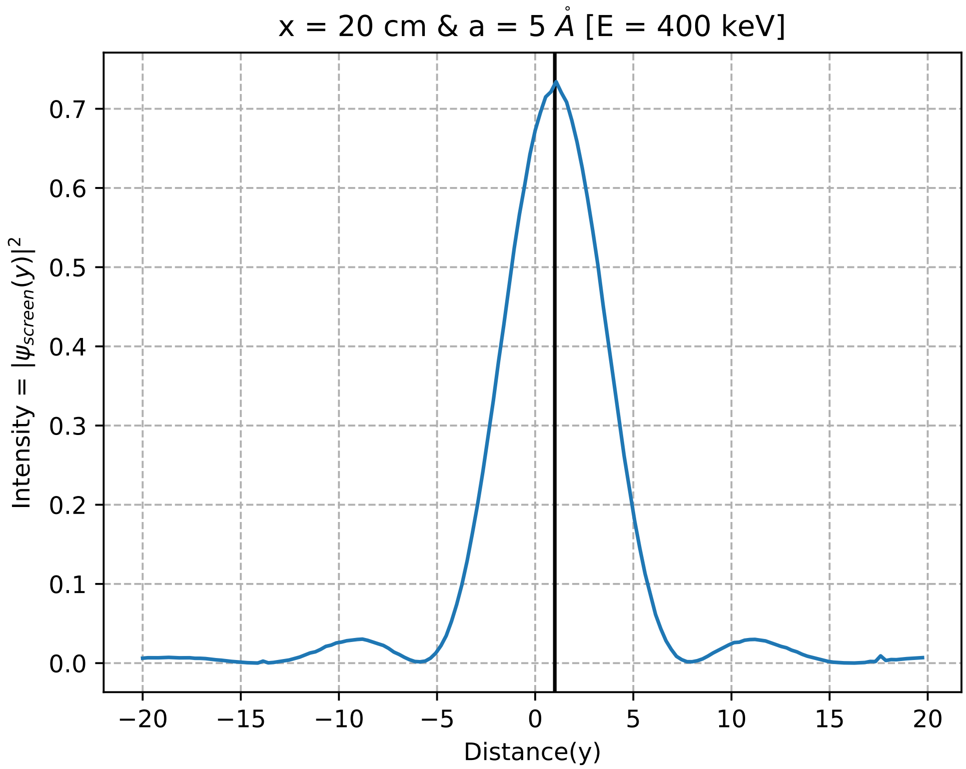



x = 2 cm & a = 10 $\mathring{A}$ [E = 200 keV]
Intensity = $|\psi_{screen}(y)|^2$
Distance(y)


x = 2 cm & a = 15 $\mathring{A}$ [E = 200 keV]
Intensity = $|\psi_{screen}(y)|^2$
Distance(y)


x = 2 cm & a = 20 $\AA$ [E = 200 keV]
# Intensity = $|\psi_{screen}(y)|^2$
Distance(y)


x = 4 cm & a = 20 $\AA$ [E = 200 keV]
Intensity = $|\psi_{screen}(y)|^2$
Distance(y)



We observe that the maxima of the intensity occurs at y = a/2 for each cases. Also the width of central maxima decreases with increase of the slit width. The intensity of central maxima increases if slit width is decreased. The central maxima is broadened if energy of electron is decreased. All of these are precisely the properties of electron diffracting through a single slit.This shows that our theory and calculations of single slit diffraction i.e. determination of wavefunction at screen as a boundary value problem is undoubtedly correct.

4 Conclusion

To study the diffraction we considered the electron to be non relativistic. However, the actual description requires relativistic treatment and we had to consider thr Relativistic Schrodinger's equation for that. However, the non-relativistic case, as we have seen gives us good result when energy value of electron is low. It can be drastically altered if energy of electrons would be higher ($\approx$ MeV). This study of electron diffraction through the single slit has provided valuable insights into the wave-particle duality of electrons and the principles of diffraction. By analyzing the patterns on the screen we can appreciate the wave nature of particle. This experiment not only reinforces the wave particle duality but also underscores the significance of diffraction phenomena in understanding the fundamental nature of matter.

5 References

- Quantum Mechanics : Concepts and Applications by Nouredine Zettili
- Quantum Theory of light diffraction by Yan Wang, Jing-Wu Li
- Quantum Mechanics by David J Griffiths
- Single-Slit Electron Diffraction with Aharonov-Bohm Phase : Feynman's Thought Experiment with Quantum Point Contacts by Pradip Khatua, Bhavtosh Bansal, Dan Shahar
- Fundamentals of Optics by Jenkins White

Appendix A

PYTHON PROGRAM FOR INTEGRATION OF EQUATION 19

```
import numpy as np
from cmath import *
import matplotlib.pyplot as plt
from scipy.integrate import quad
jj = 0 + 1j
width = 2   # width of slit
x = 30  # screen position
def summ(a,r):
    dof = 0
    for n in range(25):
        dof = dof + (1 + exp(-jj*r*a))/((2*n*pi+pi)**2 - a*a*r*r)
    return a*dof
def psi_real(r,x,y):
    answer = exp(jj*x*sqrt(200-r**2))*exp(jj*r*y)*summ(width,r)
    return answer.real

def psi_imag(r,x,y):
    answer = exp(jj*x*sqrt(200-r**2))*exp(jj*r*y)*summ(width,r)
    return answer.imag
yarr = [] ; varr = []
alpha = -20 ; beta = 20
h = (beta-alpha)/150
for ii in range(150):
    y = alpha + ii*h
    int_real = quad(psi_real,-15,15,args = (x,y))
    int_imag = quad(psi_imag,-15,15,args = (x,y))
    mval = int_real[0]**2 + int_imag[0]**2
    yarr.append(y)
    varr.append(mval)
plt.grid(True,linestyle="--")
plt.axvline(x=width/2,color='black')
plt.plot(yarr,varr)
plt.show()
```