Available online www.jsaer.com

***Journal of Scientific and Engineering Research*, 2016, 3(6):446-451**

Research Article

ISSN: 2394-2630
CODEN(USA): JSERBR

Computation of Differential Cross Section for Mercury at Varying Energies using Eikonal Approximation

Salisu I. Kunya[1*], Sadiq G. Abdu[2], Muhammad Y. Onimisi[3]

[1]Department of Science Laboratory Technology, Jigawa State Polytechnic, Dutse-Nigeria
[2]Department of Physics, Kaduna State University, Kaduna-Nigeria
[3]Department of Physics, Nigerian Defence Academy, Kaduna-Nigeria

Abstract A wide variety of approximation have been used to investigate scattering process, the eikonal method was used in this work which is valid at high incident energy. The work report the Differential cross section for elastic electron scattering from mercury atom, the incident electron energies considered are 80.0e V, 90.0eV and 100.0eV, the eikonal and NIST SRD 64 have good agreement, when compared with Born approximation, there is discrepancy from 9^0 to 70^0.

Keywords Differential cross section, Born, Eikonal, Electron, Mercury

1. Introduction

One of the most important examples of interaction at the microscopic scale is the phenomenon of scattering. For example, much of what has been learned about the structure of the nucleus, indeed even its discovery, was the result of scattering experiment. Similarly, the analysis of scattering has yield most of our present knowledge of elementary particle physics [1]. Rutherford and his collaborators, H. Geiger and E. Marsden performed an important quantum mechanical scattering experiment i.e., scattering of particle off Gold foil [2]. The research help Rutherford developed his theory that an atom consist of a nucleus with a positive charge and an electron shell with the negative electron moving in orbit about it [2].

To describe the probability of an interaction occurring, a cross section is defined. A cross section is a concept that plays a fundamental role in the study of atomic collision. It may be seen as the size of the area of an atom which the bombarding particle must hit in order that a particular reaction may take place [3]. In quantum mechanics, freely moving incident particles are described by wave functions usually having the form of plane waves. Due to the interaction between the incident and the target particle (scatterer) the wave function are modified, and beside the incident plane wave one must include another wave, identified as a scattered wave, propagating outward from the scatterer [4].

2. Scattering Theory

Consider a particle of mass m and energy

$$E = \frac{\hbar^2 K^2}{2m} \rangle\, 0 \qquad (1)$$

Described by a plane wave

$$\Psi_{in} = e^{ikz} \qquad (2)$$

Traveling in the Z- direction that satisfy Schrödinger wave equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi \qquad (3)$$

The free particle wave function becomes "distorted" in the presence of a potential $V(r)$. the distorted wave function is composed of an incident plane wave and a scattered wave.

$$\Psi_{sc} = e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \quad (4)$$

Equation (4) can be calculated by solving the Schrödinger wave equation. Where $f(\theta)$ *is* the complex scattering amplitude embodies the observable scattering properties and is the basic function we seek to determine.

Moreover, collisions are always characterized by the differential cross section (that is, measure of the probability distribution) given by:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \quad (5)$$

This has the simple interpretation of the probability of finding scattered particles within a given solid angle. The total cross section can be obtained by integrating the differential cross section on the whole sphere of observation (4π steradian).

$$\sigma = \int \frac{d\sigma}{d\Omega}\, d\Omega = \int_0^{2\pi} d\phi \int_o^{\pi} d\theta \sin\theta \frac{d\sigma}{d\Omega} \quad (6)$$

3. Eikonal approximation

For scattering problems where the potential V(x) is much smaller than the energy, one can make use of the Eikonal approximation in order to solve the problem. This approximation covers a situation in which the potential varies very little over distances of the order of Compton wavelength. This approximation is semi classical in nature; it is essence is that each ray of the incident plane wave suffers a phase shift as it passes through the potential on a straight line trajectory as shown in Fig. 1.were, $r= (b^2+z^2)^{1/2}$.

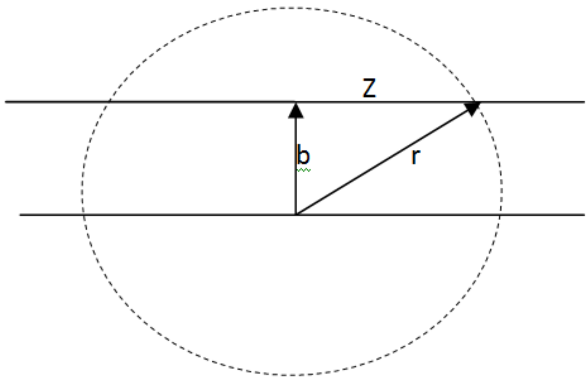

Figure 1: Geometry of Eikonal approximation

The approximation can be derived by using the semi classical wave function

$$\Psi(r) = \phi(r)e^{ik_i.r} \quad (7)$$

Where, ϕ(r) is a slowly-varying function, describing the distortion of the incident wave. The dynamic of the motion can be described by Schrödinger wave equation

$$\frac{-\hbar^2}{2m}\nabla^2\Psi(r) + V(r)\Psi(r) = E\Psi(r) \quad (8)$$

Putting equation (7) in equation (8) give

$$\frac{-\hbar^2}{2m}(2ik_i\nabla + \nabla^2)\phi(r) + V\phi(r) = 0 \quad (9)$$

If we now assume that ϕ(r) varies slowly enough so that the $\nabla^2\phi$ term can be ignored (i.e. k is very large), we have

$$\frac{ik\hbar^2}{m}\frac{\partial}{\partial z}\phi(b,z) = V(b,z)\phi(b,z) \quad (10)$$

Here, we have introduced the coordinate b in the plane transverse to the incident beam, so that;

$$V(b,z) = V(r) \quad (11)$$

From, Fig.1

$$r = (b^2 + z^{2)^{\frac{1}{2}}} \quad (12)$$

From symmetry considerations, we expect that Ψ will be azimuthally symmetric and so independent of b. equation (10) can be integrated immediately and using the boundary condition that $\Psi \rightarrow 1$ as $Z \rightarrow \infty$ since there is no distortion of the wave before the particle reaches the potential, we have

$$\phi(b,z) = e^{2i\chi(b,z)} \quad (13)$$

$$\chi(b,z) = -\frac{m}{2\hbar^2 k}\int_{-\infty}^{\infty} V(b,z')dz \quad (14)$$

Having obtained the eikonal approximation to the scattering wave function, we can now obtain the eikonal scattering amplitude $f(\theta)$, inserting equation (8) in to an exact integral expression for the scattering amplitude.

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\int e^{-ik_f.r}V(r)\Psi(r)d^3 r \quad (15)$$

We have,

$$f_e = \frac{-m}{2\pi\hbar^2}\int d^2 b \int_{-\infty}^{\infty} dz\, e^{-iq.r}V(b,z)\phi(b,z) \quad (16)$$

Using eqn. (9), we can relate V(r)ϕ(r) directly to $\frac{\partial\phi}{\partial z}$.

Furthermore, if we restrict our consideration to relatively small scattering angles, so that$q_z = 0$, then the Z integral in equation (17) can be done immediately and using eqn. (15) for φ(r), we obtain.

$$f_e = -\frac{ik}{2\pi}\int d^2\ be^{-iq.b} \quad (17)$$

With the profile function

$$\chi(b) = \chi(b, z=\infty) = -\frac{m}{2\hbar^2 k}\int_{-\infty}^{\infty} V(b,z)dz \quad (18)$$

Since χ is azimuthally symmetric, we can perform the azimuthally integration in equation (17) and obtain our final expression for the eikonal scattering amplitude.

$$f_e = -ik\int_0^{\infty} bdbJ_o(qb)\left(e^{2i\chi(b)} - 1\right) \quad (19)$$

In deriving this expression, we have used the identity of Bessel function.

$$J_o(qb) = \frac{1}{2\pi}\int_0^{2\pi} e^{-iqbcos\phi}\ d\phi \quad (20)$$

Hence, f_e depend upon both E (through K) and q.

An important property of the exact scattering amplitude is the optical theorem, which relates the total cross-section to the imaginary part of the forward scattering amplitude. After a bit of algebra, one can show that f_e satisfied this relation in the limit that the incident momentum becomes large compared to the length scale over which the potential varies.

$$\delta = \frac{4\pi}{k}Imf(q=0) = 8\pi\int_0^{\infty} bdbsin^2\chi(b) \quad (21)$$

4. Central Potential

A three dimensional physical systems have a central potential i.e. a potential energy that depends only on the distance r from the origin $V(r) = V(r)$. If we use spherical coordinates to parameterize our three dimensional space, a central potential does not depend on the angular variable θ and Φ. Therefore, in a scattering experiment it is easier to work in the Centre of mass frame, where a spherically symmetric potential has the form V(r) with $r = |\overrightarrow{x}|$, due to the quantum mechanical uncertainty (i.e. we can only predict the probability of scattering in a certain direction).

In Born and eikonal approximation calculations of the scattering of electrons from atoms, in general it is a complicated multi- channel scattering problem, since there are reactions leading to final states in which the atom is excited. However, as the reaction probabilities are small in comparison to elastic scattering, for many purposes the problem can be modeled by the scattering of an electron from a central potential [5]. This potential represents the combined influence of the attraction of the central nuclear charge (Z) and the screening of this attraction by the Z atomic electrons. For a target atom, the potential vanishes at large distances faster than r^{-1}. A very accurate approximation to this potential can be solved for the self-consistent Hartree Fock potential of the neutral atom. However a much simpler estimate can be obtained using an approximation to the Thomas Fermi model of the atom given by Lenz and Jensen (Blister and Hautala, 1979).

$$V = -\frac{ze^2}{r}e^{-x}(1 + x + b^2x^2 + b^3x^3 + b^4x^4) \quad (22)$$

With, e^2=14.409, b_2=0.3344, b_3=0.0485, b_4=2.647× 10^{-3}, and x=4.5397$Z^{1/6}$ $r^{1/2}$

The potential is singular at the origin, However, if the potential is regularized by taking it to be a constant within some small radius $r_{min,}$ (say the radius of the atom 1s shell), the calculated cross section will be unaffected except at momentum transfers large enough so that

$$Qr_{min} \gg 1 \quad (23)$$

The incident particle is assumed to have the mass of the electron and is appropriate for atomic systems; all lengths are measured in angstrom (Å) and all energies in electron volt (eV). The potential is assumed to vanish beyond 2Å. Furthermore, the r^{-1} singularity in the potential is cut off inside the radius of the 1s shell of the atom.

5. Methodology

The computation of Eikonal approximation to the total cross section of strontium for a given central potential at specified incident energy, a FORTAN program developed by Koonin and Meredith (1989) have been used. The program is made up of four categories of file: common utility program, physics source code, data files and include files [5].

The physics sources code is the main sources code which contains the routine for the actual computation. The data files contain data to be read into the main program at run-time and have the exertion. DAT. The first thing done was the successful installation of the FORTRAN codes in the computer. This requires familiarity with the linker, editor and the graphics package to be used in plotting. The program runs interactively. It begins with a title page describing the physical problem to be investigated and the output that will be produced; next, the menu is displayed, giving the choice of entering parameter values, examining parameter values, running the program or terminating the program. When the calculation is finished, all values are zeroed (except default parameter), and the main menu is redisplayed, giving us the opportunity to redo the calculation with a new set of parameters or to end execution. Data generated from the program were saved in a file which would be imported into the graphics software for plotting [6].

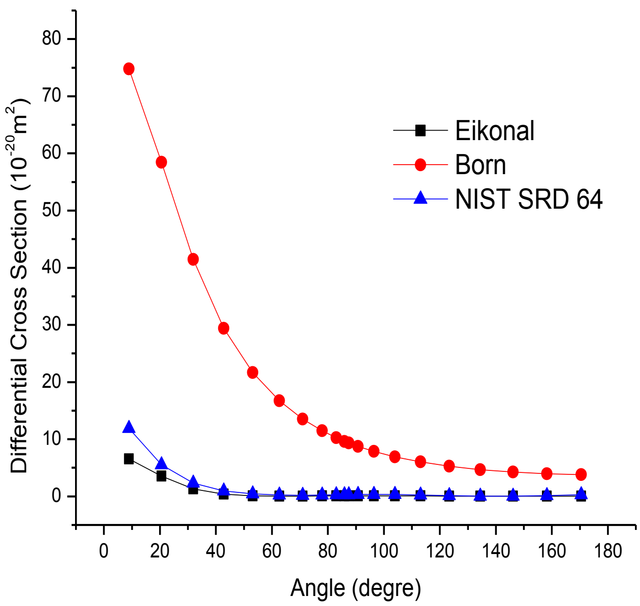

Figure 2: Graph of differential cross section using eikonal together with data obtained from born and NIST SRD 64 at incidence energy 80.0eV

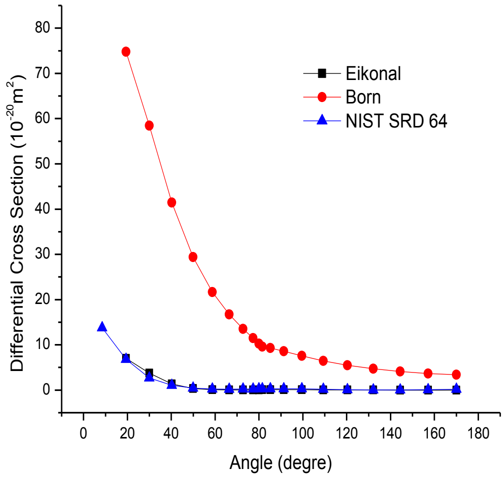

Figure 2: Graph of differential cross section using eikonal together with data obtained from born and NIST SRD 64 at incidence energy 90.0 eV

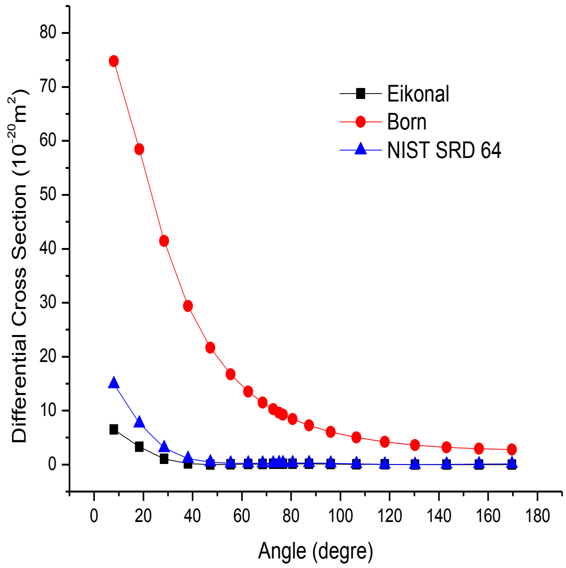

Figure 3: Graph of differential cross section using eikonal together with data obtained from born and NIST SRD 64 at incidence energy 100.0eV

6. Discussion

Figure 1 Shows the interpretation of differential cross section (DCS) at 80.0eV incident energy, the Born approximation curve are higher than the other curves and from 10.0^o to 110^o, DCS is in inverse proportion, there is no any overlap with two curves . Comparing eikonal and NIST SRD 64 there is little separation of lines from 10^o to 40^o, they also obey inverse relation but from 40^o to 170^o there is an agreement between the NIST SRD and eikonal.

The result of computed DCS at 90.0eV using eikonal approximation method were assessed with Born approximation and NIST SRD, and presented in Figure 2. The figure shows that, the present result and NIST SRD curves overlap, showing that they are in good accord, from 100^o to 170^o, the DCS is independent with

angles. Born approximation show a large difference, although there is a similarity at higher angles with eikonal, the discrepancy may be in Born approximation it is valid at higher incident energy.
The description of DCS at 100.0eV is given in figure 3. The Born approximation curve shows that as the incident angles increases, the curve declines from 120^o to above the curves appears to nearly converges with NIST SRD and eikonal, a good agreement is seen for NIST SRD and eikonal from 40^o to 170^o, therefore the Born approximation is generally valid at higher incident angle

7. Conclusion

A cross section is a concept that plays a fundamental role in the study of atomic collision, the eikonal method was used in this work which is valid at high incident energy, the incident electron energies considered in the work are 80.0e V, 90.0eV and 100.0eV, the eikonal and NIST SRD 64 have good agreement, when compared with Born approximation, there is discrepancy from 9^0 to 70^0.

Reference

[1]. Cox A. J., Deweerd A. J. and Linder J. (2002), an Experiment to Measure Mie and Rayleigh Total Scattering Cross Section, American Journal of Physics 70(6).

[2]. Kashimbila M. M. (2007), Electricity, Magnetism and Modern Physics, 2nd edition, The Publications and Documentation Division office of the Registrar Bayero University, Kano.

[3]. Ghoshal S. N. (2005), Nuclear Physics, S. Chand and Company L.T.D, Ram Nagar, New Delhi-110055.

[4]. Zakowicz W. (2003), Classical Properties of Quantum Scattering, Journal of Physics A: Mathematical and General 36.

[5]. Koonin S.E. and Meredith D.C. (1989), Computational Physics (FORTRAN version). Addison-Wesley, New York.

[6]. Abdu. S.G. (2011), Computation of Scattering Cross Sections for He, Ne, Ar, Kr, Xe and Rn. Science World Journal, Vol. 6, (No 2). Accessed, on 22/4/2016