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Computation of Total Cross Section for Lutetium Using Eikonal Approximation

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Abstract **– Eikonal approximation method is one of the theoretical frameworks of quantum mechanics to study scattering process; this approximation was applied to explain the total cross section for the interaction. Result shows that the total cross section for electron Lutetium collision is dependence on energy ranging from 1.0eV to 1000.0eV. This result is in agreement at these incident energies range when compared with NIST SRD 64.This result obtained were significant at higher energies.**

Keywords **– Total Cross Section, Born, Eikonal, Electron, Lutetium.**

I. Introduction

The interaction between photons, electrons, atoms and molecule are fundamental to the process of life, the universe and almost everything, the analysis of scattering has yield most of our present knowledge of elementary particle physics (Cox, Deweerd and Linder, 2002), Compton scattering of X-Rays by electron is often cited as experimental evidence for the particle nature of the photon (Cox, Deweerd and Linder, 2002).Rayleigh and Mie scattering are the theoretical framework of light scattering theory, these theoretical result explain the blue and red sunset.

Electron scattering from atom is usually divided in to elastic and inelastic scattering, in the former the electron exchanges momentum q with the atom and is deflected with no or very small energy loss. In the latter the scattered electron changes the electron configuration of the scattering atom without transferring momentum to the nucleus (Vos, 2010), a wide variety of approximation have been used to investigate scattering process, the theoretical study employed in this work is eikonal approximation to compute total cross section (TCS) i.e. a measure of the probability that an interaction occur (Abdu, Onimisi and Kunya, 2014). A cross section has dimension of area which is cm^2 or m^2, since the nuclear radii are of the order of 10^{-14}m to 10^{-15}m, thus cross section are normally measured in Barn (1barn=$10^{-28}m^2$)(Goshal, 2005), the atomic unit is also a common unit that can be used or amstrong square.

II. 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.

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

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:

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

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).

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

III. 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= $(b^2+z^2)^{1/2}$.

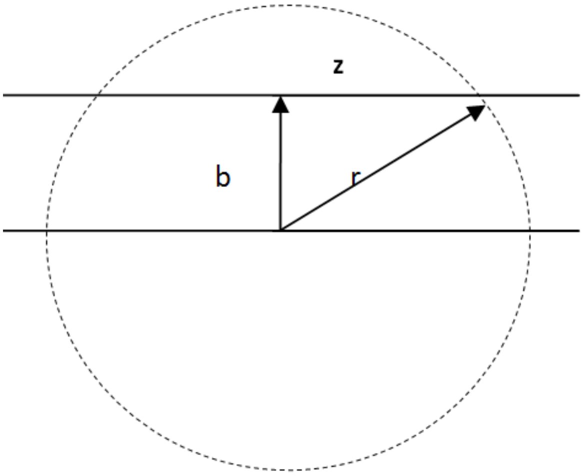

Fig. 1. Geometry of Eikonal approximation

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) we have

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

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 $\Psi \to 1$ as $Z \to \infty$ 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.

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

We have,

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

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.

$$f_e = -\frac{ik}{2\pi}\int d^2\, be^{-iq.b}\left(e^{2i\chi(b)} - 1\right) \quad (17)$$

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.

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

IV. 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 $r = |\vec{x}|$, 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 (Koonin and Meredith, 1989). 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.

V. Methodology

The computation of Eikonal approximation to the total cross section of Lutetium 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.

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 extension .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 (Abdu, 2011).

Table 1: Computed Total Cross Section For Electron-Lutetium Scattering Using Eikonal Approximation And Assessed In Comparisons With Born Approximation And NIST SRD 64

E(eV)	Approximation Method		
	Eikonal	Born	NIST SRD 64
1.0	1.793	860.0	
50.0	6.860	230.4	14.612
100.0	3.132	137.9	10.796
150.0	2.586	99.02	8.450
200.0	3.269	77.43	7.053
250.0	3.760	63.64	6.143
300.0	3.549	54.00	5.507
350.0	3.559	46.80	5.038
400.0	3.632	41.30	4.676
450.0	3.877	37.13	4.387
500.0	4.470	34.05	4.151
550.0	4.900	31.66	3.951
600.0	4.821	29.56	3.780
650.0	4.658	27.57	3.631
700.0	4.559	25.71	3.499
750.0	4.538	24.02	3.381
800.0	4.669	22.53	3.274
850.0	4.826	21.23	3.176
900.0	4.863	20.09	3.087
950.0	4.855	19.05	3.004
1000.0	4.935	18.13	2.928

Note: The minimum energy for NIST SRD 64 as provided by the code is 50.0eV

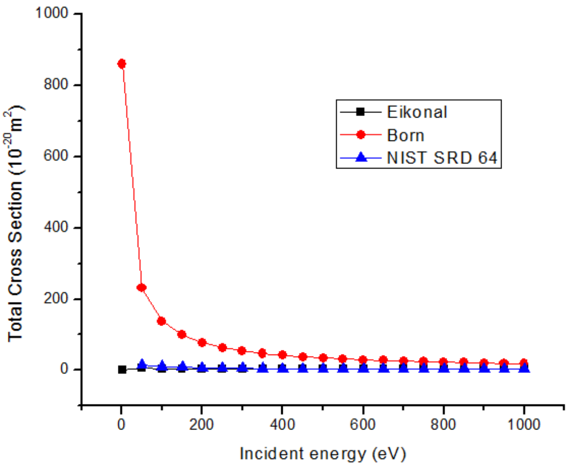

Fig. 2. Graph Of Computed Total Cross Section For Electron-Lutetium Scattering Using Eikonal Approximation And Assessed In Comparisons With Born Approximation And NIST SRD 64 Curves

VI. Discussion

Fig. 1 shows that, the present result and NIST SRD 64 data is much closer and converges at incidence energy above 400 e V, but in comparisms with the Born approximation, the total cross section is high at lower energy, this indication shows that it valid at higher energy. Furthermore, we observed that the curve for Born approximation is superior to the other curves. Hence the present result is in agreement to NIST SRD 64 and Born approximation at higher energies. This is because an eikonal approximation is valid at high energies and small scattering angles.

VII. Conclusion

The total cross section for electron- lutetium were presented, the eikonal approximation used for this work it is in agreement with the result of NIST SRD 64 and Born approximation.

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