

DIFFERENTIAL CROSS SECTIONS OF ELECTRON SILVER SCATTERING AT VARYING ENERGIES

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ABSTRACT

The differential scattering cross sections of electron - silver atom are calculated using the Eikonal approximation at incident energies of 50 eV, 60 eV and 70 eV, with the Lenz-Jensen potential. Results obtained are in good agreement with the NIST SRD 64 at scattering angles of about 80 to 180 degrees; and are in very good agreement with the Born approximation between 30 to 180 degrees.

Keywords: Differential cross section, Silver, Eikonal, Born approximation

INTRODUCTION

The dynamic of electron atom scattering can be explained by Schrödinger wave equation. It intensifies that the Schrödinger wave equation can be solved based on expansion of the function in power of \hbar , which, although of a semi convergent or asymptotic character, is also useful for the approximate solution of quantum mechanical problems in appropriate case. This known as Wentzel Krammers Brillouin (WKB) approximation (Schiff, 1968). It is applicable to situations in which the wave equation can be separated in to one or more total differential equation, each of which involved a single independent variable. The WKB approximation explains that the potential energy changes so slowly that the local momentum $\hbar k$ is sensibly constant over many wavelengths.

Hence, another approximation that is along the lines of the WKB approximation is the Eikonal approximation. The Eikonal (from the Greek word ELKOV or "Image") equation is traditionally encountered in the wave and geometric optics literature where the principal concern is the propagation of light rays in an inhomogeneous medium (Chartier, 2005). Its twin roots are in wave propagation theory and in geometric optics. In geometric optics it can be derived from Huygen's principle (Arnold, 1989), while in wave propagation theory it is obtained when the wave is approximated using the WKB approximation (Paris and Hurd, 1969).

The Eikonal approximation is useful in wave scattering equations which occur in quantum mechanics, quantum electrodynamics and partial wave expansion. The main advantage the Eikonal approximation offers is that the equations reduces to a differential equation in a single variable. This reduction to a single variable is the result of the straight line approximation or the Eikonal approximation which allows us to choose the straight line as a special direction.

In scattering theory, the probability of interaction depends on the properties of the beams and target particles, for instance, in a scattering problem 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. It is semi classical in nature; its 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

(Koonin and Meredith, 1989).

Furthermore electron-atom scattering are always characterized by the differential cross section (measure of the probability distribution) and total cross section , these can be calculated in various approximations – Born (Merzbacher, 1970), Eikonal (Innanen, 2010), partial wave method (Cox and Bonham, 1967), etc.

Literature Review

The differential cross section is the main observable in quantum scattering experiments. The notion was introduced first to describe the Rayleigh scattering of sunlight and the Rutherford scattering of alpha particles. In both scattering process, the differential cross section is well established in the framework of the correspondingly dynamical equations: The Maxwell equations in the case of Rayleigh scattering and the Newton's equations in the case of Rutherford scattering. On the other hand, a satisfactory justification of the quantum scattering cross section can be completely described by the framework of the Schrödinger wave equation, i.e.

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi = E\Psi \quad 1$$

Consider the particle beam been incident along the z- axis of mass m and energy

$$E = \frac{\hbar^2 k^2}{2m} > 0 \quad 2$$

approaches a target. Suppose the incident and scattered particle are described by a plane wave given below and satisfied the Schrödinger wave equation:

$$\Psi_{in} = e^{ikz} \quad 3$$

and

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

Equation (4) shows that the scattered wave is the super position, where the complex scattering amplitude $f(\theta)$ 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) to obtain

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

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; its 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.

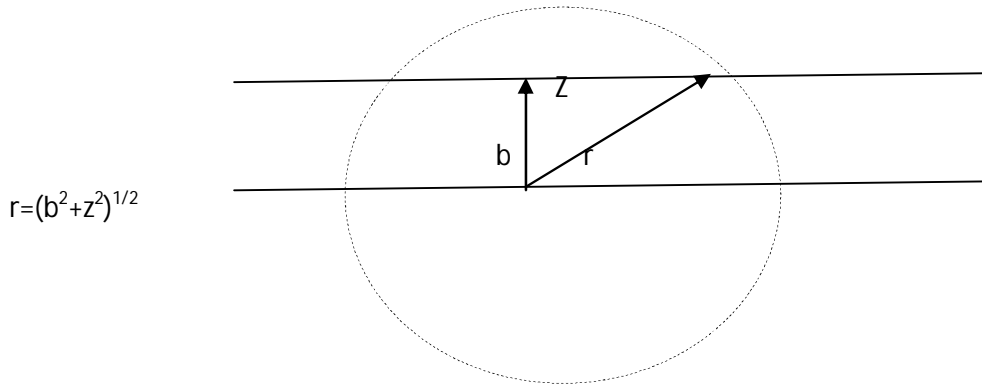


Fig.1: Geometry of Eikonal approximation.

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

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

where $\phi(r)$ 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 $\phi(r)$ 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

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

And, from Fig.1,

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

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_e , inserting equation (7) into an exact integral expression for the scattering amplitude we have

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

we have

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

Using equation (9), we can relate $V\phi(r)$ 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 (16) can be done immediately and using equation (14) for $\phi(r)$, we obtain

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

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 azimuthal integration in equation (6) and obtain our final expression for the eikonal scattering amplitude

$$f_e = -ik \int_0^{\infty} b db J_0(qb) (e^{2i\chi(b)} - 1) \quad 19$$

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

$$J_0(qb) = \frac{1}{2\pi} \int_0^{2\pi} e^{-iqb \cos \varphi} d\varphi \quad 20$$

Hence, f_e depends 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.

$$\delta = \frac{4\pi}{k} \text{Im}f(q=0) = 8\pi \int_0^{\infty} b db \sin^2 \chi(b) \quad 21$$

Central Potential

A three dimensional physical system have a central potential, that is, 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).

The Born and Eikonal approximation calculations of the scattering of electrons from atoms are, in general, complicated and multi-channel scattering problems, since there are reactions leading to final states in which the atoms are 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

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

With, $e^2 = 14.409$, $b_1 = 0.3344$, $b_2 = 0.0485$, $b_3 = 2.647 \times 10^{-3}$, and $x = 4.5397Z^{1/6} r^{1/2}$.

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's 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 and all energies in electron volt (eV). The potential is assumed to vanish beyond 2 angstrom. Furthermore, the r^{-1} singularity in the potential is cut off inside the radius of the 1s shell of the atom.

METHODOLOGY

The computations of total cross section of electron strontium atom using eikonal approximation were carryout using FORTRAN developed by Koonin and Meredith (1989). The FORTRAN code was first installed in the computer and this required the knowledge of computer and FORTRAN language. The program is made up of four categories: common utility program, physics source code, data file and include file. The physics sources code is the main source 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 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. The parameter value have default value displayed in bracket, to accept the default value, press "return" at the prompt, or a new value might be decided within the range of allowed values. . 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).

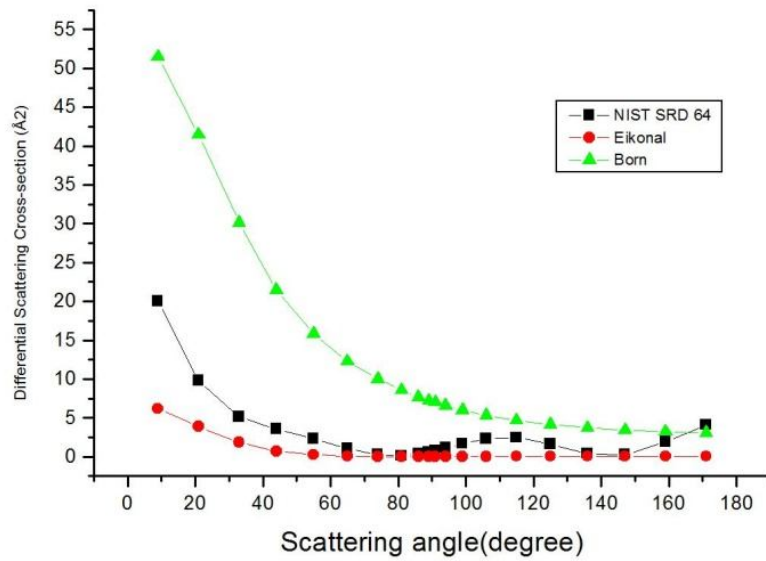


Fig.1: Graph of differential cross section as a function of scattering angle at incident energy of 50 eV.

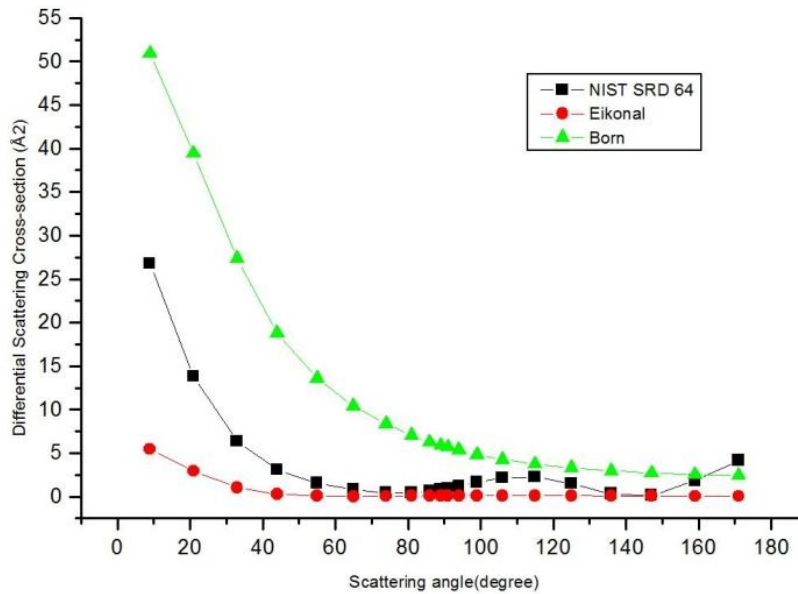


Fig. 2: Graph of differential cross section as a function of scattering angle at incident energy of 60 eV.

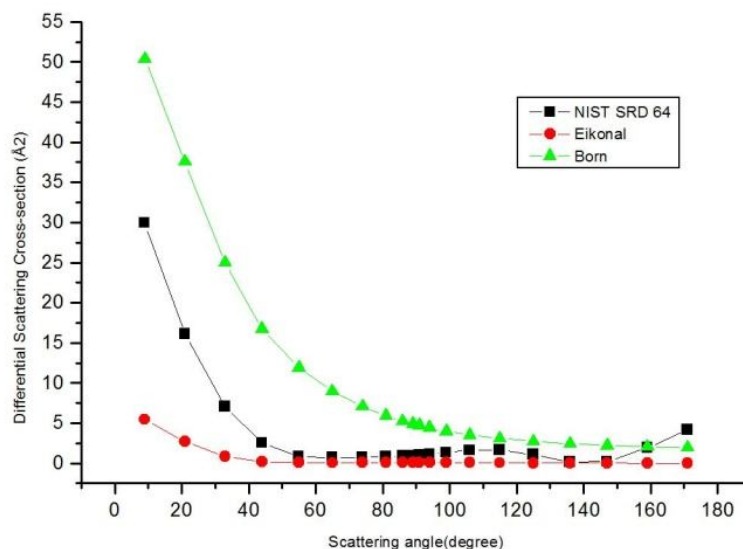


Fig. 3: Graph of differential cross section as a function of scattering angle at incident energy of 70 eV.

DISCUSSION

From Fig. 1, the calculated electron-silver scattering cross sections at 50 eV are in very good agreement with the ones obtained using the Born approximation between the angles of 20 to 180 degrees. Also, these calculated cross sections agree favourably with the data obtained from the National Institute of standards and Technology data base 64 (NIST SRD 64) of the USA between the angles of about 100 to 180 degrees.

From Fig. 2 at 60 eV, the computed cross sections are in very good agreement with the ones obtained using the Born approximation between the angles of 30 to 180 degrees; and also agree with the NIST SRD 64 between the angles of about 100 to 180 degrees.

As shown in Fig. 3, at 70 eV, the computed cross sections are in very good agreement with the ones obtained using the Born approximation between the angles of 40 to 180 degrees; and also agree with the NIST SRD 64 between the angles of about 100 to 180 degrees.

At lower scattering angles of between 0 to 20 degree, the computed cross sections disagree with those obtained using the Born approximation and those given by NIST SRD 64. Our calculated values are lower than those obtained using the Born approximation for all three incident energies considered. Also, values obtained from the NIST SRD 64 are much higher than those obtained using the Born approximation as well as our calculated values. This may be because both approximations are valid at high incident energies.

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