ENERGY DEPENDENCE OF ELECTRON-YTTERBIUM TOTAL CROSS-SECTIONS USING THE PARTIAL WAVE DECOMPOSITION METHOD: A COMPARISON WITH THE BORN AND EIKONAL APPROXIMATION METHODS AND NIST SRD 64.

*ABDU, S.G.[1] & BABAJI, G.[2]

[1]Department of Physics, Kaduna State University, Kaduna-Nigeria
[2]Department of Physics, Bayero University, Kano-Nigeria
*sgabdul@yahoo.com.

ABSTRACT
Computations of the Total Cross-Sections (TCS) of elastic electron-Ytterbium scattering were carried out using the partial wave decomposition method with the Lenz-Jensen potential at various incident energies. Results were compared with data obtained using the Born approximation method, Eikonal approximation method and the National Institute of Standard and Technology (NIST) Standard Reference Database (SRD) 64 of the U.S.A. There is good agreement between our results and the data from Eikonal approximation and NIST SRD 64. However, data from the Born approximation disagree with our results at lower incident energies. This disagreement is anticipated as the Born approximation is valid only at high electron incident energies.

Keywords: Elastic scattering, total cross sections, Ytterbium, partial wave method, Born approximation, Eikonal approximation.

INTRODUCTION
Elastic scattering of electrons by neutral atoms is a means of studying the dynamics of several particle systems. Much of what we know today about the forces and interactions in atoms and nuclei has been learned from scattering experiments, in which atoms in a target are bombarded with beams of particles (Achaver, 2003). Scattering studies are important because they reveal information about the nuclear forces as well as about the structure of the nuclei; provide information about the charge distribution in nuclei and within nucleons; provide data which can serve as input information for calculations of kinetic processes in gases where low energy collisions predominate; etc (Merzbacher, 1970).

Elastic scattering of electrons by an atom takes place if the final state of the atom after the collision coincides with the initial one (Winitzki, 2004). Total and differential cross-sections for such a process can be calculated using various approximation methods. These include the Born, Eikonal, optical theorem, partial wave decomposition, etc. In this work, the total cross-sections of Ytterbium were computed using the partial wave decomposition method.

MATERIALS AND METHODS
We used the FORTRAN code program developed by Koonin & Meredith, 1989) which takes the relativistic differential cross-section as a sum of squared modules of the real and imaginary scattering amplitudes. The amplitudes can be calculated through the phase shifts of spherical waves, which are obtained by integration of equations for radial wave functions. In these computations the analytical approximation for the atomic electrostatic potential given by Lenz and Jensen, called the Lenz-Jensen potential, based on the Thomas-Fermi model, is used.

Scattering Theory
For particles of mass m and energy

$$E = \frac{\hbar^2 k^2}{2m} > 0 \qquad \dots 1.0$$

scattering from a central potential, V(r) is described by a wave function, $\psi(r)$ that satisfies the Schrodinger Wave Equation (SWE)

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \qquad \dots 2.0$$

with the boundary condition at large distance

$$\psi_{r\to\infty} \to e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \qquad \dots 3.0$$

Equation (3) holds for a beam of electrons incident along z-axis, and the scattering angle, θ is the angle between r and $\hat{z}$ while f is the complex scattering amplitude, which is the basic function we seek to determine. The differential cross-section is given by:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \qquad \dots 4.0$$

The total cross-section is

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} = 2\pi \int_0^\pi d\theta \sin\theta |f(\theta)|^2 \qquad \dots 5.0$$

f is a function of both E and θ (Messiah, 1968).

Partial Wave Decomposition
The method of partial wave expansion is a special trick to simplify the calculation of the scattering amplitude, f (Schiff, 1968). The standard partial wave decomposition of the scattering wave function ψ is

$$\psi(r) = \sum_{l=0}^{\infty}(2l+1)i^l e^{i\sigma}\frac{R_l(r)}{kr}P_l(cos\theta) \qquad \dots 6.0$$

When equation (6) is substituted into the SWE (2) the radial wave functions, R_l are found to satisfy the radial differential equations:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E\right]R_l(r) = 0 \qquad \dots 7.0$$

This is the same equation as that satisfied by a bound state wave function but the boundary conditions are different. In particular, R vanishes at the origin, but it has the large-r asymptotic behaviour

$$R_l \to kr[cos\delta_l j_l(kr) - sin\delta_l n_l(kr)] \qquad \dots 8.0$$

Where j_l and n_l are the regular and irregular spherical Bessel functions of order l.

The scattering amplitude is related to the phase shifts δ_l by (Messiah, 1968):

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}sin\delta_l P_l(cos\theta) \qquad \dots 9.0$$

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From equations (5) and (9) the total cross-section is given by

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) sin^2 \delta_l \qquad \ldots 10.0$$

Although the sums in equations (9) and (10) extend over all l, they are in practice limited to only a finite number of partial waves. This is because for large l, the repulsive centrifugal potential in equation (7) is effective in keeping the particle outside the range of the potential and so the phase shift is very small (Koonin & Meredith, 1989).

If the potential is negligible beyond a radius r_{max}, an estimate of the highest partial wave that is important is had by setting the turning point at this radius:

$$\frac{l_{max}(l_{max}+1)\hbar^2}{2mr_{max}^2} = E \qquad \ldots 11.0$$

$$\Rightarrow \qquad l_{max} \approx kr_{max} \qquad \ldots 12.0$$

This estimate is usually slightly low since the penetration of the centrifugal barrier leads to non-vanishing phase shifts in partial waves somewhat higher than this (Niksic, 2003).

The Phase shifts

To find the phase shift in a given partial wave, we must solve the radial equation (7). The equation is linear, so that the boundary condition at large r can be satisfied simply by appropriately normalizing the solution.

If we put $R_l(r=0) = 0$ and take the value at the next lattice point, $R_l(r=h)$, to be any convenient small number we then use

$$f'' \approx \frac{f_1 - 2f_0 + f_{-1}}{h^2} \qquad \ldots 13.0$$

for $R_l''(h)$, along with the known values $R_l(0)$, $R_l(h)$, and $k(h)$ to find $R_l(2h)$.

Now we can integrate outward in r to a radius $r^{(1)} > r_{max}$. Here, V vanishes and R must be a linear combination of the free solutions, $krj_l(kr)$ and $krn_l(kr)$:

$$R_l^{(1)} = Akr^{(1)}\left[cos\delta_l j_l(kr^{(1)}) - sin\delta_l n_l(kr^{(1)})\right] \ldots 14.0$$

Although the constant, A above, depends on the value chosen for $R(r=h)$, it is largely irrelevant for our purposes; however, it must be kept small enough so that overflows are avoided (Koonin & Meredith, 1989). Now we continue integrating to a larger radius $r^{(2)} > r^{(1)}$:

$$R_l^{(2)} = Akr^{(2)}\left[cos\delta_l j_l(kr^{(2)}) - sin\delta_l n_l(kr^{(2)})\right] \ldots 15.0$$

Equations 14.0 and 15.0 can then be solved for δ_l to obtain

$$tan\delta_l = \frac{G j_l^{(1)} - j_l^{(2)}}{G n_l^{(1)} - n_l^{(2)}}; \ G = \frac{r^{(1)} R_l^{(2)}}{r^{(2)} R_l^{(1)}} \qquad \ldots 16.0$$

where $j_l^{(1)} = j_l(kr^{(1)}$ etc. Equation (16) determines δ_l only within a multiple of π but this does not affect the physical observables [see equations (9) and (10)]. The correct multiple of π's at a given energy can be determined by comparing the number of nodes in R and in the free solution, krj_l which occur for $r < r_{max}$. The phase shift in each partial wave vanishes at high energies and approaches $N_l\pi$ at zero energy, where N_l is the number of bound states in the potential in the l'th partial wave (Gianturco, 1989).

The Lenz-Jensen Potential

One practical application of the theory discussed above is the calculation of the scattering of electrons from neutral atoms. In general this is a complicated multi-channel scattering problem since there can be 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 (Hochstadt, 1971). 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 neutral target atom, the potential vanishes at large distances faster than r^{-1}. A very accurate approximation to this potential can be had by solving 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.

$$V = -\frac{Ze^2}{r} e^{-x}(1 + x + b_2 x^2 + b_3 x^3 + b_4 x^4); \qquad \ldots 17.0$$

with

$$e^2 = 14.409; \ b_2 = 0.3344; \ b_3 = 0.0485; \ b_4 = 2.647 \times 10^{-3}; \qquad \ldots 18.0$$

and

$$x = 4.5397 Z^{\frac{1}{6}} r^{\frac{1}{2}} \qquad \ldots 19.0$$

This potential is singular at the origin. 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), then the calculated cross-section will be unaffected except at momentum transfers large enough so that $qr_{min} \gg 1$.

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

Procedure

The first thing done was the successful installation of the FORTRAN codes in the computer. This requires familiarity with the computer's operating system, the FORTRAN compiler, linker, editor, and the graphics package to be used in plotting. Data generated from the program were saved in files which were later imported into the graphics software Origin 5.0 for plotting.

Compilation

To prepare the codes for compilation is a matter of simple but tedious editing. In general, the procedure of preparing the codes for compilation is as follows:

(i) First, if the FORTRAN compiler does not support the INCLUDE statement, each of the Physics and utility programs must be edited to include the common block files. The include file names must be exactly the same in the program and in the directory. The compiler used for this work supports the INCLUDE statement, thus this step was not executed.

(ii) If the compiler does not accept the '!' comment delimiter then we must compile, link and run the program STRIP to change all of the files (this includes utility codes, Physics codes, and common blocks, but not data files). The compiler used also accepts the '!' comment delimiter, hence this step was also not done.

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(iii) The next step is to edit the subroutine SETUP in the file SETUP.FOR. You must edit in constant values for variables that control I/O. For example, you will need to know how many lines there are on your terminal (24 in this case), unit numbers for I/O to the screen (these are *5* and *6*), unit numbers for output files, and your own preference for default output (screen, file or printer).

(iv)This last step is optional, and involves the three other routines in SETUP.FOR that are also hardware dependent. These routines come with all the lines commented out, except SUBROUTINE, RETURN, and END. Subroutine CLEAR clears the screen by sending escape characters to the terminal. This routine simply keeps the screen from looking too clustered: it is not essential. The last two routines (GMODE and TMODE) switch the terminal between graphics and text mode and vice versa.

With these changes completed, we can now compile the Physics program, UTIL.FOR, SETUP.FOR, and GRAPHIT.BLK; link them together; and execute.

Execution
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 parameters), and the main menu is re-displayed, giving us the opportunity to redo the calculation with a new set of parameters or to end execution.

RESULTS
Results were generated for several electron incident energies and the graphics software Origin 5.0 used to plot graphs. The results obtained were compared with data obtained from National Institute of Standards and Technology (NIST) Standard Reference Database 64 (Jablonski *et al.,* 2003) and data generated using the Born and Eikonal approximation methods.

TABLE 1. COMPUTED TOTAL CROSS-SECTIONS FOR ELECTRON-YTTERBIUM ELASTIC SCATTERING USING THE PARTIAL WAVE (PW), NIST SRD 64, BORN AND EIKONAL APPROXIMATION METHODS FOR VARIOUS INCIDENT ENERGIES.

E(eV)	Approximation Method			
	PW	NIST	Born	Eikonal
10	18.730		539.500	5.398
20	9.428		394.400	3.860
40	5.497		262.900	4.900
60	6.106	13.160	199.100	3.374
80	5.728	11.340	160.900	3.387
100	2.721	9.940	135.200	3.385
200	1.950	6.521	75.850	2.979
400	2.478	4.465	40.670	2.449
600	2.344	3.644	27.830	2.288
800	2.149	3.163	21.170	1.953
1,000	1.980	2.831	17.080	1.783
2,000		1.981	8.718	1.970
4,000		1.368	4.492	2.326
6,000		1.094	3.024	2.128
8,000		0.663	2.369	2.102
10,000		0.817	1.894	1.948
20,000		0.279	0.995	1.846

Note: The maximum energy for PW as provided by the code is 1000 eV while the minimum energy for NIST SRD 64 is 60 eV.
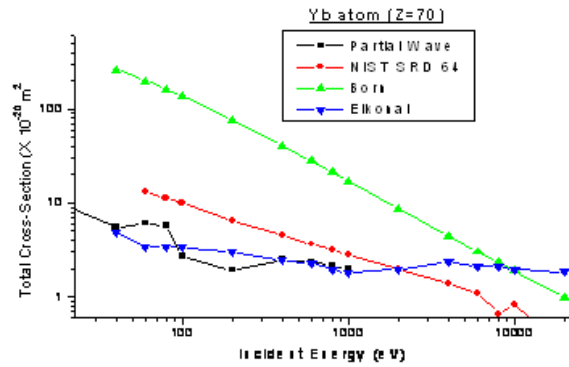

FIG 1: COMPARISONS OF THE ENERGY DEPENDENCE OF THE TOTAL CROSS-SECTIONS FOR THE PARTIAL WAVE METHOD WITH DATA OBTAINED FROM THE BORN, EIKONAL AND NIST SRD 64 FOR NEUTRAL YTTERBIUM ATOM (Z=70).

DISCUSSION
The total cross-sections computed using the partial wave decomposition method have inverse relationships with the electron incident energies as seen in Table 1 and Fig. 1. Total cross-section data obtained using the partial wave method are in good agreement with data from National Institute of Standards and Technology (NIST) Standard Reference Database 64 (Jablonski *et al.,* 2003). Data from Eikonal approximation method are in good agreement with present work but lower.

However, data from the Born approximation method disagree widely with present work, Eikonal and NIST SRD 64 data at low incident energies as seen in Fig. 1. These disagreements were anticipated as the Born approximation method is valid only at high electron incident energies (Winitzki, 2004). However, there is good agreement between the Born and other approximation methods at high incident energies as expected.

Quantitative agreements are seen in comparisons with other approximation methods at low and intermediate electron incident energies as seen in Fig 1.

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