CRITICAL MINIMUM IN ELASTIC ELECTRON-ARGON SCATTERING USING THE PARTIAL WAVE DECOMPOSITION METHOD.

*ABDU, S. G.¹ & BABAJI, G.²

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

ABSTRACT

Computations of critical minimum in the differential cross sections of electron-argon elastic scattering using the partial wave decomposition method are presented. The theoretical approach is based on the Dirac–Hartree–Fock method. The position of our computed critical minimum is at 115 degrees. This is in good agreement with experimental and calculated theoretical values.

Keywords: Critical minimum, differential cross-sections, Argon, elastic scattering, Partial wave method.

INTRODUCTION

Electron-atom collisions provide the means of investigating the dynamics of several particle systems at a fundamental level. In fact much of what is known 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 (Anchaver, 2003). Examples of the importance of scattering in studying internal structure of atoms and nuclei and the interactions which govern systems of elementary particles include: nucleons scattered from nuclei at various energies reveal information about the nuclear forces as well as about the structure of the nucleon; electrons of high energy, hence short wavelength, reveal information about the charge distribution in nuclei, and indeed within nucleons; electrons and heavier projectiles of low energy are scattered from atoms to obtain data which can serve as input information for calculations of kinetic processes in gases where low energy collisions predominate; etc. (Menzbacher, 1970).

Elastic electron-atom scattering takes place if the final state of an atom after the interaction coincides with the initial one (Wintzki, 2004). Total and differential cross-sections for such a process can be calculated in various approximations — Born, Eikonal, optical theorem, partial wave decomposition, etc. In this work, the differential cross-sections of electron-Argon elastic scattering were computed using the partial wave decomposition method.

MATERIALS AND METHODS

We used the FORTRAN code program developed by Koonin & Meredith (Koonin et al., 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

\[ E = \frac{k^2}{2m} > 0 \]

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

\[ -\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) = E\psi \]

with the boundary condition at large distance

\[ \psi_{\text{free}} \rightarrow e^{ikr} + f(\theta) \frac{e^{ikr}}{r} \]

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

\[ \frac{d\sigma}{d\Omega} = \left| f(\theta) \right|^2 \]

The total cross-section is

\[ \sigma = \int d\Omega \frac{d\sigma}{d\Omega} = 2\pi \int_0^\pi d\theta |f(\theta)|^2 \]

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

Critical Minimum

The critical minimum is defined by the points on the plane constituted by the scattering angle and incident energy axes where differential cross-section (DCS) attains its smallest value (Marinkovic et al., 2004). These minima appeared to be the most sensitive test for both experimental procedures and theoretical models, and for comparisons of experimental and theoretical results as well (Milosavjevic, 2004).

Another significance of critical minima lies in the fact that their positions indicate the highest values of spin polarization of scattered electrons (Sienkiewicz et al., 2001). The degree of spin polarization is given by \( P = \frac{\sigma^+ - \sigma^-}{\sigma^+ + \sigma^-} \), where \( \sigma^+ \) and \( \sigma^- \) are the cross sections of scattered electrons with spin momentum pointing ‘up’ and ‘down’ with respect to the scattering plane. The biggest difference between the \( \sigma^+ \) and \( \sigma^- \) cross section occurs in the angle region, where the differential cross section is minimal (Schwar et al., 1982).

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 \( \psi \) is

\[ \psi(r) = \sum_{l=0}^{\infty} (2l + 1) i^l \frac{R_l(r)}{kr} P_l(\cos \theta) \]

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

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

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.
where \( j_{l}(1) = j_{l}(k r^{1}) \) etc. Equation (16) determines \( \delta_{l} \) only within a multiple of \( \pi \) but this does not affect the physical observables [see equations (9) and (10)]. The correct multiple of \( \pi \)'s at a given energy can be determined by comparing the number of nodes in \( R \) and in the free solution, \( k r_{l1} \) which occur for \( r < r_{\text{max}} \). 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.

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 potential 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

\[ V = -\frac{Ze^{2}}{r} e^{-x}(1 + x + b_{2}x^{2} + b_{3}x^{3} + b_{4}x^{4}); \quad 17.0 \]

with

\[ e^{2} = 14.409; \quad b_{2} = 0.3344; \quad b_{3} = 0.0485; \quad b_{4} = 2.647 \times 10^{-3}; \quad 18.0 \]

and

\[ x = 4.53972\frac{Z^{1/3}}{r^{1/3}}; \quad 19.0 \]

This potential is singular at the origin. If the potential is regularized by taking it to be a constant within some small radius \( r_{\text{min}} \) (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 \( q r_{\text{min}} \gg 1 \).

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 (\( \text{Å} \)) and all energies in electronvolt (eV). The potential is assumed to vanish beyond 2A. Furthermore, the \( r^{-1} \) singularity in the potential is cutoff inside the radius of the 1s shell of the target atom.

Research Methodology

A FORTRAN program developed by Koonin and Meredith was the main program used for all the computations. The program is made up of four categories of files: common utility programs, physics source code, data files and include files.

The physics source code is the main source code which contains the routine for the actual computations. 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 computer's operating system, the FORTRAN compiler, 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 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. Data generated from the program were saved in files which were later imported into the graphics software Origin 5.0 for plotting.

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 experimental data obtained by Milosavjevic (2004) and theoretical data of Marinkovic et al., (2004).

TABLE 1. COMPUTED ANGLE DEPENDENT DIFFERENTIAL CROSS SECTIONS (Å²) FOR ELASTIC ELECTRON-ARGON SCATTERING IN THE VICINITY OF THE HIGH-ENERGY (100-150 eV) CRITICAL MINIMUM USING THE PARTIAL WAVE METHOD WITH LENZ-JENSEN POTENTIAL.

<table>
<thead>
<tr>
<th>E(eV)</th>
<th>100</th>
<th>105</th>
<th>110</th>
<th>115</th>
<th>120</th>
<th>125</th>
<th>130</th>
<th>135</th>
<th>140</th>
<th>145</th>
<th>150</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>3.076</td>
<td>2.916</td>
<td>2.783</td>
<td>2.674</td>
<td>2.563</td>
<td>2.508</td>
<td>2.446</td>
<td>2.396</td>
<td>2.247</td>
<td>2.197</td>
<td>2.154</td>
</tr>
<tr>
<td>60</td>
<td>0.797</td>
<td>0.846</td>
<td>0.900</td>
<td>0.929</td>
<td>0.961</td>
<td>0.987</td>
<td>1.008</td>
<td>1.023</td>
<td>1.040</td>
<td>1.085</td>
<td>1.012</td>
</tr>
<tr>
<td>80</td>
<td>1.850</td>
<td>1.746</td>
<td>1.648</td>
<td>1.556</td>
<td>1.471</td>
<td>1.391</td>
<td>1.316</td>
<td>1.246</td>
<td>1.182</td>
<td>1.120</td>
<td>1.083</td>
</tr>
<tr>
<td>100</td>
<td>1.177</td>
<td>1.029</td>
<td>0.899</td>
<td>0.784</td>
<td>0.684</td>
<td>0.597</td>
<td>0.521</td>
<td>0.455</td>
<td>0.404</td>
<td>0.355</td>
<td>0.314</td>
</tr>
<tr>
<td>110</td>
<td>0.470</td>
<td>0.373</td>
<td>0.293</td>
<td>0.226</td>
<td>0.172</td>
<td>0.129</td>
<td>0.095</td>
<td>0.068</td>
<td>0.058</td>
<td>0.045</td>
<td>0.037</td>
</tr>
<tr>
<td>115</td>
<td>0.216</td>
<td>0.155</td>
<td>0.106</td>
<td>0.069</td>
<td>0.042</td>
<td>0.022</td>
<td>0.0096</td>
<td>0.0025</td>
<td>0.000018</td>
<td>0.0014</td>
<td>0.006</td>
</tr>
<tr>
<td>120</td>
<td>0.097</td>
<td>0.070</td>
<td>0.052</td>
<td>0.040</td>
<td>0.035</td>
<td>0.034</td>
<td>0.038</td>
<td>0.046</td>
<td>0.066</td>
<td>0.070</td>
<td>0.092</td>
</tr>
<tr>
<td>140</td>
<td>1.570</td>
<td>1.629</td>
<td>1.674</td>
<td>1.709</td>
<td>1.736</td>
<td>1.757</td>
<td>1.773</td>
<td>1.784</td>
<td>1.679</td>
<td>0.070</td>
<td>1.655</td>
</tr>
</tbody>
</table>

FIG 1. ANGLE DEPENDENT DIFFERENTIAL CROSS-SECTIONS (DCS) FOR ELASTIC ELECTRON-ARGON SCATTERING IN THE VICINITY OF THE HIGH-ENERGY CRITICAL MINIMUM (PARTIAL WAVE METHOD).

DISCUSSION
From Fig. 1, our computed critical minimum was obtained at 115 degrees. This is in good agreement with the 119.4 ± 0.5 degrees experimental value obtained by Milosavjevic (2004) and the theoretical value of 118.9 ± 0.3 degrees calculated by Marinkovic et al., (2004). The value of the critical minimum obtained is 0.000018 at an incidence angle of 115 degrees and an incidence energy of 140 eV (Table 1).

REFERENCES


