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

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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 nuclei; 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; e.t.c. (Merzbacher, 1970).

Elastic electron-atom scattering takes place if the final state of an atom after the interaction coincides with the initial one (Winitzki, 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

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

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

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

with the boundary condition at large distance

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

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:

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

The total cross-section is

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

f is a function of both E and θ (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 (Sienkewicz *et al.*, 2001). The degree of spin polarization is given by $P = (\sigma\uparrow - \sigma\downarrow)/(\sigma\uparrow + \sigma\downarrow)$, where $\sigma\uparrow$ and $\sigma\downarrow$ 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 $\sigma\uparrow$ and $\sigma\downarrow$ 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 ψ is

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

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

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

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

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

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):

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

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

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

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:

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

$$\Rightarrow \qquad l_{max} \approx kr_{max} \quad ...12.0$$

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

$$f^{"} \approx \frac{f_1 - 2f_0 + f_{-1}}{h^2} \quad ...13.0$$

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 $krn_l(kr)$:

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

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 $r^{(2)} > r^{(1)}$:

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

Equations (14) and (15) can then be solved for δ_l to obtain

$$tan\delta_l = \frac{Gj_l^{(1)} - j_l^{(2)}}{Gn_l^{(1)} - n_l^{(2)}};\ G = \frac{r^{(1)}R_l^{(2)}}{r^{(2)}R_l^{(1)}} \quad ...16.0$$

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.

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

$$V = -\frac{Ze^2}{r}e^{-x}(1 + x + b_2x^2 + b_3x^3 + b_4x^4); \quad ... 17.0$$

with

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

and

$$x = 4.5397Z^{\frac{1}{6}}r^{\frac{1}{2}} \quad ...19.0$$

This potential is singular at the origin. If the potential is regularized by taking it to be a constant within some small radius r_{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.

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 ($Å^2$) 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.

E(eV) θ $(Deg.)$	100	105	110	115	120	125	130	135	140	145	150
20	28.560	27.400	26.360	25.420	24.560	23.780	23.070	22.400	21.460	20.860	20.310
40	3.076	2.916	2.783	2.674	2.583	2.508	2.446	2.396	2.247	2.197	2.154
60	0.797	0.846	0.890	0.929	0.961	0.987	1.008	1.023	1.840	1.095	1.102
80	1.850	1.746	1.648	1.556	1.471	1.391	1.316	1.246	1.182	1.120	1.063
100	1.177	1.029	0.899	0.784	0.684	0.597	0.521	0.455	0.404	0.355	0.314
110	0.470	0.373	0.293	0.226	0.172	0.129	0.095	0.068	0.058	0.045	0.037
115	0.216	0.155	0.106	0.069	0.042	0.022	0.0096	0.0025	0.000018	0.0014	0.006
120	0.097	0.070	0.052	0.040	0.035	0.034	0.038	0.046	0.066	0.079	0.092
140	1.570	1.629	1.674	1.709	1.736	1.757	1.773	1.784	1.679	0.079	1.655

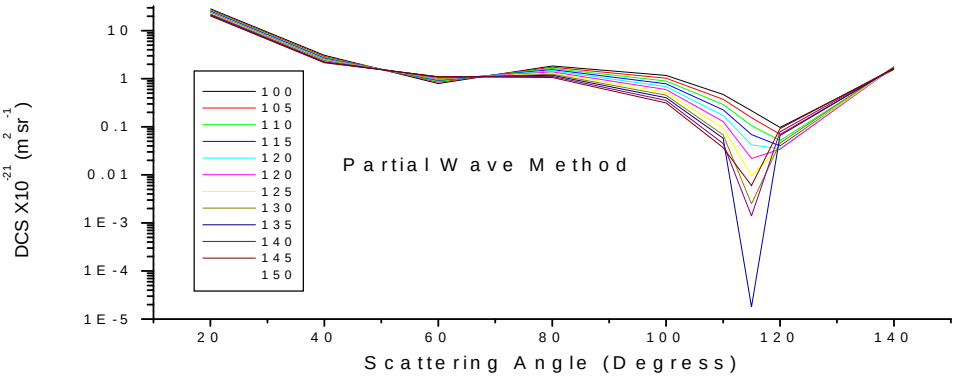

FIG 1. ANGLE DEPENDENT DIFFERENTIAL CROSS-SECTIONS (DCS) FOR ELASTIC ELECTRON-ARGON SCATTERING IN THE VICINITY OF THE HIGH-ENERGY CRITICAL MINIMUM (PARTIAL WAVE METHOD).

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).

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