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DCS and spin polarization parameter of argon by electron impact

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Abstract
In present paper, differential scattering cross section (DCS) and spin polarization parameter (S) of the elastic scattering of slow electrons from argon are reported and comparison is made with different available theoretical and experimental data. The present calculation is done with R-matrix theory. We have chosen a complex type potential, a part of which is directly calculated from the target charge density and other part is taken from Baluja and Jain [1]. The present work yields a satisfactory result for differential cross section and spin polarization parameter while previously large discrepancies were found in theoretical and experimental data.

Keywords: R-matrix, Complex Potential, Electron

INTRODUCTION

Due to its applications in various gaseous electronics, rare gases have gained a lot of attention in recent years. In so many applications, there is great demand for accurate low energy cross sections of these rare gases. In gas laser systems, where amplifier cells are pumped by a high energetic electron beam, high energy cross sections are required for atoms used as a buffer gas. Thus there is requirement of cross sectional data over a wide range of projectile energies. Electron interactions with atoms and molecule provide important facts into atomic and molecular structure and reaction mechanisms. These facts are wealth for both realization and potential applications in technology, biomedical science and environment.

The choice of noble gas is important as these are easy target for experimentalists as well as theoreticians and provide an excellent testing ground for the different experiments and theoretical models; even their electron excitation cross sections are having several useful applications. Moreover, experimentalist as well as theoreticians of the field of scattering has focused their attention on electron impact excitation of inert atoms because of use of excitation cross-section data in plasma modeling. The basic parameters of plasma such as electron temperature and electronic density *etc* can be obtained by collisional radiative models [2]. As a target, argon is of particular interest as it is the most ubiquitous noble gas of earth's atmosphere and has applications in variety of areas of lasers, incandescent lighting and in welding etc. Argon is also used in multi-species actionometry to study the dissociation fraction of a molecule such as nitrogen by comparing the emission lines from these gases. In case of optical emission spectroscopy of discharge plasma with known concentration of inert gases, argon can be used to determine the concentration of reactive species such as atomic fluorine. The present work demonstrates DCS and spin polarization parameter for elastic scattering of electron by argon atom.

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Mondal *et al* [3] have given their calculations of differential cross section data for excitation of $3p^5$ 4s state in argon by electron impact using time of flight (TOF) technique. Madison *et al* [4] have calculated integral cross section of ground state of argon to twelve state ($3p^5$ 3d) using R-matrix theory in which results are found to be very sensitive to the choice of atomic wave functions. Gangwar *et al* [5] have used relativistic distorted wave approximation (RDW) to calculate the cross sections for electron excitations from ground state of argon. They found that cross sections have expected behavior as the function of total angular momentum of excited levels. They have also fitted the total cross-section with an analytic formula to enable the determination of cross-section at arbitrary energies. McEachran and Stauffer [6] presented results of a complex ab initio optical potential calculation of elastic scattering of electron as well as positron from argon atom investigating critical minima occurring in DCS. Kretinin *et al* [7] devolved new method of calculation of cross section of electron molecule scattering that requires only ground state wave function and mean excitation energy of the target.

THEORY

In this paper the dynamics of electron argon scattering are calculated under R-Matrix formalism. Throughout we shall use atomic units in which $h = m_e = e = 1$.Denoting the position vector of i^{th} electron relative to atomic nucleus the Hamiltonian H for this system may be written as

$$H = -\frac{1}{4}\nabla_R^2 + H_A(\bar{r}_1, \ldots\ldots \bar{r}_N) + V(r_p, r_0; r_1 \;\ldots . r_N) \quad \text{.... (1)}$$

Where $\bar{t} = \bar{r}_p - \bar{r}_i, \;\; i = 0,1,2, \ldots\ldots N$

The ground state of argon is given by

$$\varphi_a = (n\bar{p}^2 np^4)_{J_a=0} \quad \text{.... (2)}$$

The radial wave functions for the different orbital and corresponding configuration mixing co-efficient are obtained using relativistic multiconfiguration Dirac-Fock (MCDF) programme of Grant *et al* [8].

The potential is chosen as a complex type and given by

$$V(r) = V_{st}(r) + V_p(r) + iV_{abs}(r) \quad .... (3)$$

The static potential is the average over the ground state atomic charge distribution of the electrostatic interaction of the electron and atom. The static potential V_{st}between the incoming electrons and fix charge distribution in atom is attractive. The static potential is calculated from

$$V_{st} = \frac{Z}{r} - \int \frac{\rho_0(r')d^3r'}{|r-r'|} \quad .... (4)$$

Where $\rho_0(r)$ is the target unperturbed charge density.

The polarization effect arises from the distortion of the target electronic wave due to the incident charged particle. For the elastic scattering, the polarization-correlation contribution accounts for all virtual transitions to the excited states. The polarization potential is always attractive but different forms in non similar cases. We have used a parameter-free polarization potential *(V_p)*, which is based on the correlation energy of the target atom [9]. It has two components, the short range *[V_{SR} (r)]* [and the long range *[V_{LR} (r)]* parts, and is given by

$$V_p(r) = \left.\begin{matrix} V_{SR}(r), & r < r_c \\ V_{LR}(r), & r \geq r_c \end{matrix}\right\} \quad .... (5)$$

Here r_c is the point where two forms cross each other for the first time. The corresponding point for argon atom occurs at 2.90 a.u. The short range form for the electron scattering with atomic systems is given by

$$V_{SR}(r) = \left.\begin{matrix} 0.0622\ln r_s + 0.018\, r_s \ln r_s - 0.02\, r_s - 0.096, & r_s \leq 0.7 \\ 0.03796\ln r_s - 0.1231, & 0.7 \leq r_s \leq 10.0 \\ -0.876\, r_s^{-1} + 2.65\, r_s^{-3/2} - 2.8\, r_s^{-2} - 0.3 r_s^{-5/2} & 10.0 \geq r_s \end{matrix}\right\} \quad .... (6)$$

The long-range form of polarization is taken as following well known asymptotic form

$$V_{LR}(r) = -\frac{\alpha_d}{2r^4}, \quad r > r_c \quad .... (7)$$

Where α_d is the dipole polarizability of target atom. For the present calculations, its value is taken as 11.08 a.u. for the argon atom [10]. In the usual potential scattering problem, the following Schrodinger equation is solved for scattered particle at energy K^2 *i.e.*

$$\left[\frac{d^2}{dr^2} + K^2 - \frac{l(l+1)}{r^2} - V(r)\right] f_l(Kr) = 0 \quad .... (8)$$

The scattering amplitude is obtained from the phase shift by

$$f(\theta) = \frac{1}{2iK}\sum_{l=0}^{l_{max}}(2l+1)[\exp(2i\delta_l) - 1]P_l(\cos\theta) + f_4(\theta) \quad .... (9)$$

The function f_4 is the higher l contribution from the Born phase shifts for the dipole (~ $1/r^4$) part of the polarization potential. For this function, the closed form expression is

$$f_4(\theta) = -\pi k \alpha_d \left(\frac{\sin(\theta/2)}{2} + \sum_{l=0}^{l_{max}} \frac{P_l(\cos\theta)}{(2l+3)(2l-1)}\right) \quad .... (10)$$

And spin flip amplitude $g(\theta)$, according to Kessler [11].

$$g(\theta) = \frac{1}{2iK}\sum_l [exp(2i\delta_l^{+})] P_l^1(\cos\theta) \quad .... (11)$$

Where θ is the scattering angle, $P_l(\cos\theta)$ and $P_l^1(\cos\theta)$ are the Legendre polynomial and Legendre associated function respectively. The $\delta_l^{\pm}$ are relativistic phase shifts, where the index '+' refers the solution with $k = -l - 1$ and $-$ ' refers to the solution with $k = l$.

Having the scattering amplitudes, the differential cross section is given by

$$\sigma(\theta) = \frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2, \quad .... (12)$$

And spin polarization parameters

$$S(\theta) = \frac{i(f(\theta)g(\theta)^* - f(\theta)^* g(\theta))}{\sigma(\theta)} \quad .... (13)$$

$$T(\theta) = \frac{|f(\theta)|^2 - |g(\theta)|^2}{\sigma(\theta)} \quad .... (14)$$

$$U(\theta) = \frac{f(\theta)g(\theta)^* + f(\theta)^* g(\theta)}{\sigma(\theta)} \quad .... (15)$$

These parameters are not independent, since $S + T + U = 1$.However in present work, we have calculated and presented only spin polarization parameter $S(\theta)$ given by equation (13).

RESULTS AND DISCUSSION

Using equations (12) and (13), we have calculated differential cross sections and spin polarization parameters (S) respectively for elastic scattering of electrons from argon atom using R-matrix theory at energy ranges from 2eV to 10eV.

DCS: We have plotted DCS in figures 1(a) to 1(d) for elastic scattering of argon by electron impact at energies 2, 3, 7.5 and 10eV respectively. In these figures, we have also plotted available experimental data of Gibson *et al* [12].

In figure 1(a) we observe that present results are in good agreement with available experimental data. In the range of angle 50^0-90^0, our theoretical results are slightly greater than that of experimental values. For the angle greater than 130^0, no experimental data is available to verify present result.

In figure 1(b), at incident energy 3eV, our results are slightly different (somewhere higher and somewhere lower) in the range 10^0-

80^0 and thereafter present result shows better agreement with data upto125^0. After 135^0 since no experimental data is available, so it is better not to comment anymore.

In figure 1(c) theoretical and experimental results are in good agreement in the range 10^0-80^0 and after that a little discrepancy is observed up to 130^0. In this figure we also observe same position of dip in DCS, both theoretical as well as experimental.

Figure 1(d) shows same feature as that of previous results. As usual the present results show dip, however prominent feature cannot be observed by experimentalist.

SPIN POLARIZATION PARAMETER (S)

Figure 2(a) shows the variation of spin polarization parameter (S) with scattering angle at incident energy 2eV. At this particular energy neither experimental data nor theoretical calculations are available for comparison purpose. In this figure we observe that up to 110^0, the variation of spin parameter is very small. But suddenly with the increase of scattering angle, the parameter shows a dip by obtaining its value in negative.

In figure 2(b), at 3eV, we have compared our results with other theoretical results of Nahar and Wadehra [13]. Both results are in good agreement only with the difference in the depth of minima centered at 130^0. Also, in small angular range ($40^0 < \theta < 30^0$), a dip also appears.

In figure 2(c), we have plotted present results at 7.5eV. Here, a peak can be observed at an angle 110^0.

In figure 2(d), the spin polarization at incident energy 10 eV, we have plotted the experimental result of Beerlarge *et al* [14] with our present result. In this figure, the experimental data shows much variation in spin parameter; however present results give almost same feature as that in previous figures *i.e.* a smooth increase showing a peak at about 115^0 and immediate after a dip at 120^0.

In general, we may conclude that with the increase of energy, the angular variation in spin polarization parameter remains same in higher range while it shows different behavior in small angular regions.

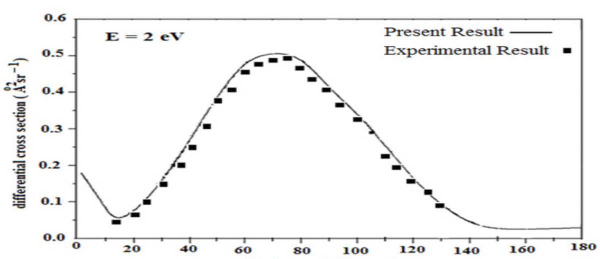

Fig 1 (a)

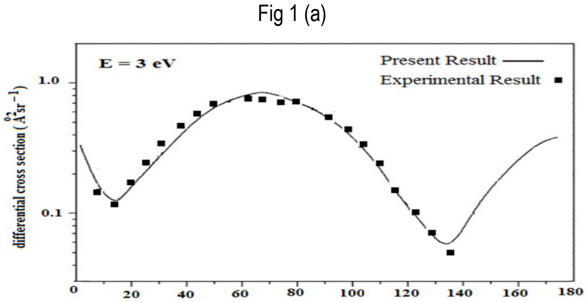

Fig 1 (b)

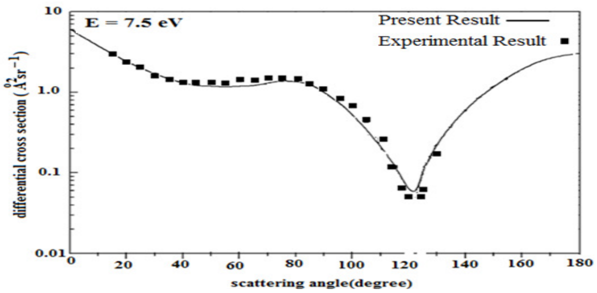

Fig 1 (c)

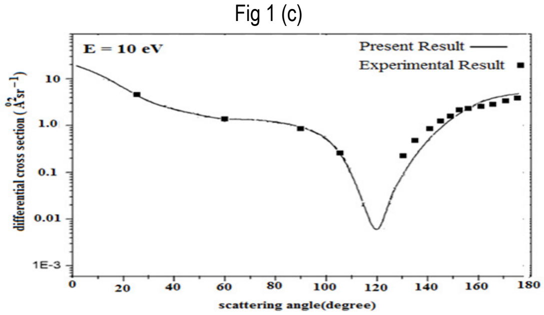

Fig 1 (d)

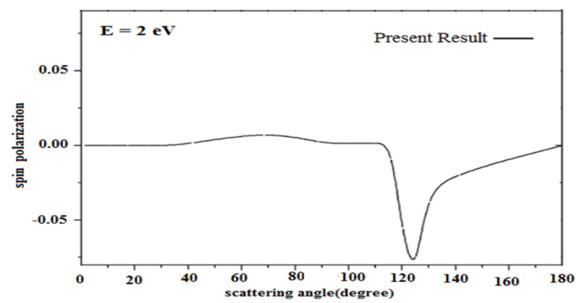

Fig 2 (a)

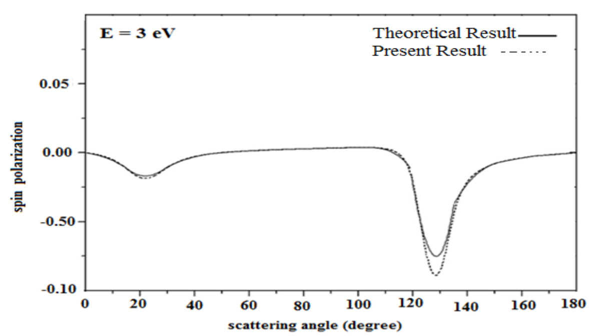

Fig 2 (b)

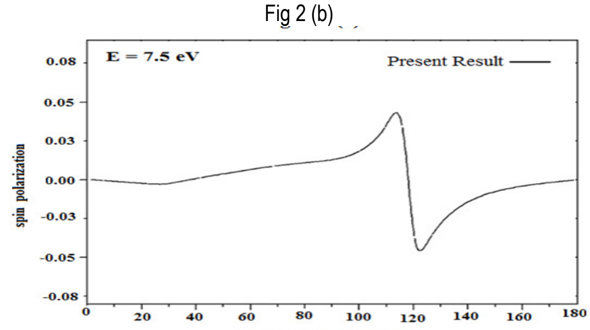

Fig 2 (c)

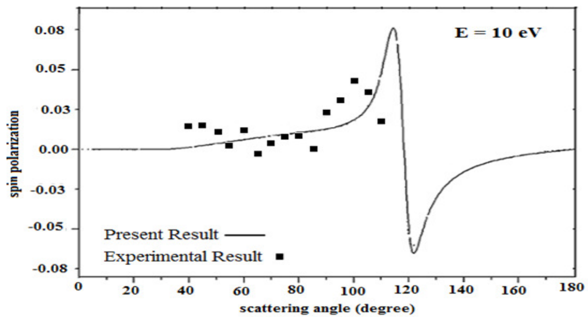

Fig 2 (d)

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