

The Elastic Scattering of Electrons from Cadmium Atom with the use of Model-Potential Approach

A. A. Khalf

Physics Department, College of Science, University of Basrah, Basrah, Iraq.

Abstract

Calculations of low-intermediate energies of electrons scattering from the ground state of cadmium atom are performed using the optical model approach. The differential cross sections (DCS's) are calculated with the semi-empirical polarization potential added to the Hartree-fock potential of the fixed core. The agreement between our calculated (DCS's) and the available theoretical results and experimental data was good for the electron scattering.

1.Introduction

In the present investigation we have determined the differential cross sections for the elastic electron scattering from cadmium atom in the energy region (2-75)eV. The method of partial wave along with optical model potential formalism has been employed. For electrons scattering, the spherical symmetric optical potential comprises of the static field, polarization and exchange interactions.

The only other investigations on elastic ($e^- - Cd$) scattering is that of Pangantiwar and Srivastava (1989), to our knowledge. Since the differential cross section provide more rigorous testing for theories and experiments, as compared to

the total cross section (TCS), it maybe of great interest to present the calculated (DCS) of the electron from cadmium.

The optical model potential approach (OMPA) has proved to be quite successful and attracted considerable interest in the past few years to study electron-atom elastic scattering [K.Bartschat et.al (1988,1990), A.Jain 1990, B.H.Brandsdent et al.1985, and P.Khan et.al.1984]. In general, for short-range interactions between projectile and target only a finite number of partial waves make contributions to the scattering amplitude, and the number of contributing partial waves increases with the increase in impact energy. If the projectile-target interaction has a long-range tail, then in principle, an infinite number of partial waves will contribute to the scattering amplitude.

2. Theory

In the optical potential approach the basic idea is to analyze the elastic scattering of a particle from a complex target by replacing complicated interactions between the projectile and the target particles by an optical potential or a pseudopotential in which the incident particle moves. Thus once the optical potential is determine, the many-body problem is reduced to an equivalent one-body problem. The differential equation for the scattering electron, in atomic units ($e = m = \hbar = 1.0$) is given by

$$(\nabla^2 + k^2 - V_{opt}(r))\Psi(r) = 0 \quad (1)$$

Where (k) is the incident wave vector of the projectile. However, the equivalent optical potential, in general, is a complex, non-local, non-spherically symmetric and energy-dependent potential and it is exact determination is non-possible at present. One is required to take $V_{opt}(r)$ in an approximation form. In this investigation $V_{opt}(r)$ is represented by a localized, real, and energy-dependent potential which is spherically symmetric, so that equation (1) can be solved using the partial wave method. We have performed $V_{opt}(r)$ in equation (1) by static field-polarization-exchange approximation, and expressed as

$$V_{opt}(r) = V_{00}(r) + V_{ex}(r) + V_{pol}(r) \quad (2)$$

Where the static field

$$V_{00}(r) = \langle \Phi_0 / V(r_1, r_2, \dots, r_Z, r) / \Phi_0 \rangle \quad (3)$$

Where $\Phi_0(r_1, r_2, \dots, r_Z, r)$ is the ground state wave function of the target atom having (Z) electrons (Z=54 for Cd) and $V(r_1, r_2, \dots, r_Z, r)$ is the interaction potential due to the target and the incident particle given as

$$V(r_1, r_2, \dots, r_Z, r) = \frac{NQ}{r} - Q \sum_{j=1}^N \frac{1}{|r - r_j|} \quad (4)$$

Where (Q=-1) for electron.

$V_{pol}(r)$ is the polarization potential and $V_{ex}(r)$ is the electron exchange term. The non-local exchange term is converted into an equivalent local exchange potential following Truhlar (1981), expressed as

$$V_{ex}(r) = -\frac{2}{3} \left[\frac{3}{\pi} \rho(r) \right]^{1/3} \quad (5)$$

Where $\rho(r)$ is the spherical one electron charge of the cadmium atom.

Hartree-Fock wavefunction for the ground state of (Cd) atom as given by Clementi and Roetti (1974), have been employed to evaluate $V_{00}(r)$ and $\rho(r)$. The semi-empirical formula of polarization potential proposed by Norcross and Seaton (1976), given as

$$V_{pol}(r) = -\frac{\alpha_d g^2(r)}{2r^4} \quad (6)$$

Where

$$g^2(r) = 1 - \exp\left(-\frac{r}{\rho}\right)^6 \quad (7)$$

The factor (α_d) is the static dipole polarizability, and it's value is $(43.7 a_o^3)$ for (Cd), where (a_o) is Bohr radius.

$(g^2(r))$ is the cut-off function designed to make the polarization potential finite at the origin, (ρ) is the cut-off parameter, and equal (2.5805) for (Cd).

After defining suitable choice for $V_{opt}(r)$, as given by equation (2), we substitute it in to equation (1) and using the standard partial wave expansion for $\Psi(r)$, then we get

$$(\nabla^2 + k^2 - 2V_{opt}(r) - \frac{\ell(\ell+1)}{r^2})u_\ell(r) = 0 \quad (8)$$

Where $u_\ell(r)$ is the radial scattering asymptotic wave function given as

$$u_\ell(r) \underset{r \rightarrow \infty}{\approx} \frac{1}{k} \sin(kr - \frac{\ell\pi}{2} + \delta_\ell) \quad (9)$$

Where (δ_ℓ) is the phase shift corresponding to the ℓ th partial waves.

The scattering amplitude is obtained using the following expression:

$$f(\theta) = \frac{1}{2ik} \sum (2\ell+1)[e^{2i\delta_\ell} - 1]p_\ell(\cos\theta) \quad (10)$$

The differential and total cross sections are obtained in the conventional manner from $f(\theta)$.

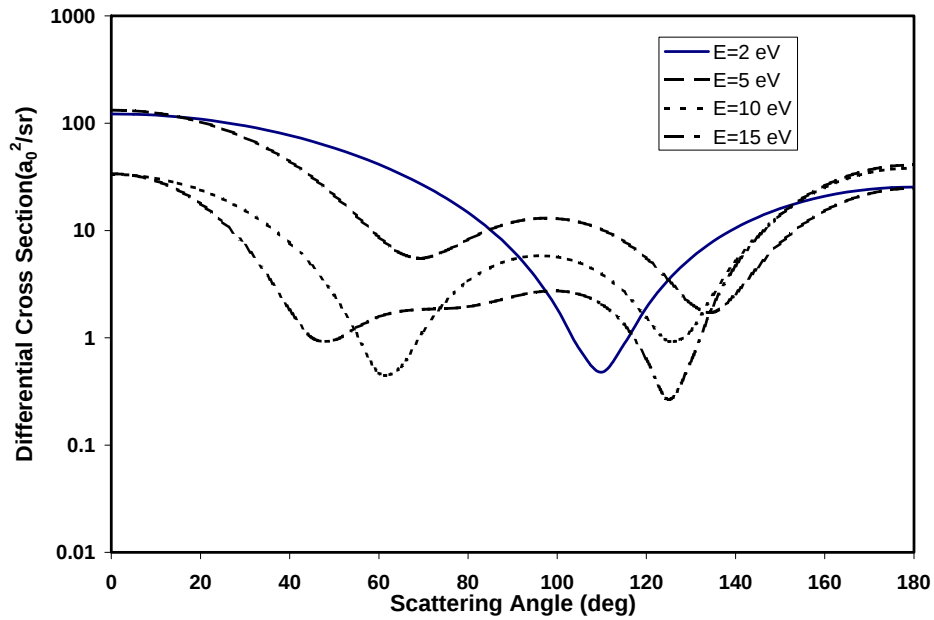
3.Results and Discussion

We present in Table(1) and figures (1,2) our various calculated results, where figures present a comparison with the available theoretical and experimental results.

Table(1): The elastic scattering phase shifts in (rad) for three partial waves (s,p,d) different values of (E).

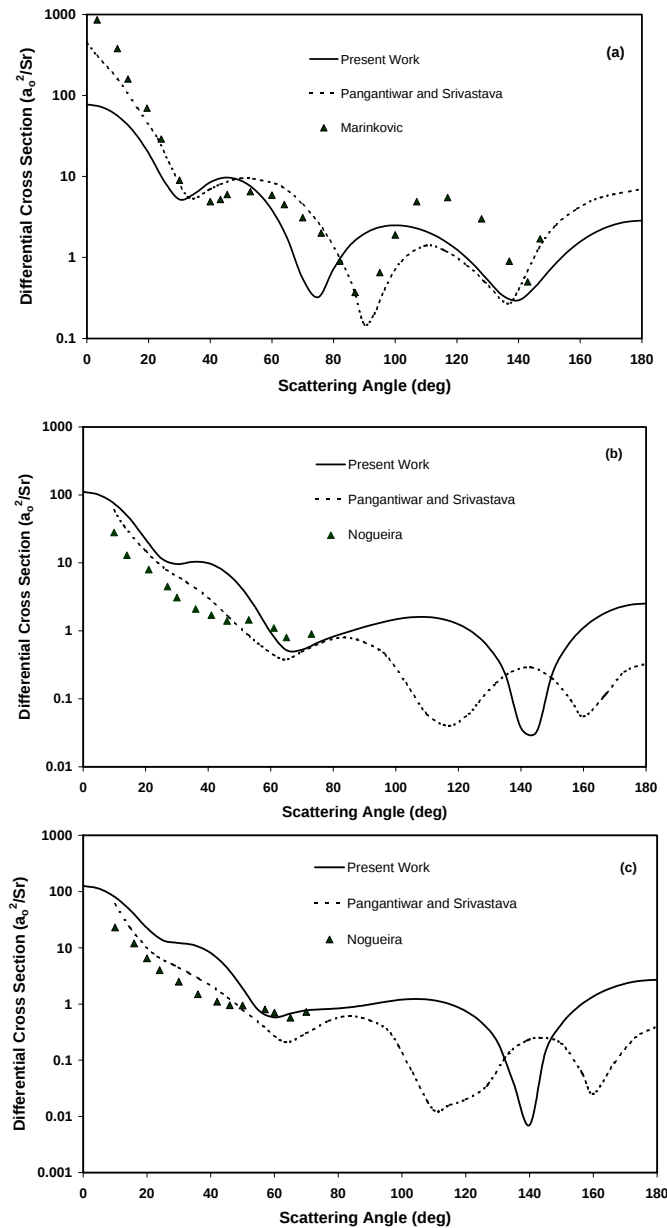
E(eV)	Electron Phase Shift		
	δ_0	δ_1	δ_2
2	-1.6583	1.4691	0.1537
5	-2.3607	1.2931	2.1117
10	-2.9801	0.8536	2.3095
15	-3.3508	0.5239	2.4438
20	-3.6031	0.2808	2.6359
25	-3.7936	0.0995	2.7458
30	-3.9530	-0.0403	2.7704
35	-4.0960	-0.1551	2.7551
40	-4.2295	-0.2572	2.7287
45	-4.3545	-0.3527	2.7032
50	-4.4708	-0.4442	2.6812
55	-4.5781	-0.5320	2.6610
60	-4.6761	-0.6153	2.6400
65	-1.6240	-0.6935	2.6165
70	1.4363	-0.7660	2.5899
75	4.5036	-0.8326	2.5607

In figure(1) we present the differential cross sections for the scattering of electrons from cadmium atom at the impact energies (2,5,10 and 15)eV. So far, there is no theoretical calculations or experimental measurements are available to compare it with our results at these energies to our knowledge.



Figure(1): The Differential Cross Section for electron at incident Energies (2,5,10 & 15eV).

In figure (2a) our (DCS) for elastic scattering of electrons from cadmium atom at (40)eV are compared with the experimental data of Marinkovic et al.(1987) and the calculations of Pangantiwar and Srivastava (1989). In figures (2b&2c) our (DCS) for ($e^- - Cd$) elastic scattering at the incident energies (60 & 75)eV respectively, are compared with the corresponding absolute (DCS) measurements of Nogueira et al.(1987), which are available only up to scattering angles of (70°) and the calculations of Pangantiwar and Srivastava (1989). Our results at these energies also show similar structures as shown by the experimental and theoretical and our results at (40)eV impact energy. Also our results show minima at a nearly the same scattering angles as predicted by experiment. In the angular region (60° - 76°) and (107° - 143°) our results are found to be lower than the experimental data in Fig.(2a).



Figure(2):The differential cross section for electron scattering by Cadmium at incident energies (a)40 eV (b)60 eV (c)75 eV.

4.Conclusions

We apply the partial wave method along with the optical model potential to calculate phase shifts and differential cross sections for the scattering of electrons from cadmium atom.

For electrons scattering, our results were in a good agreement with the calculations and experimental measurements that we had made a comparison with it.

The difference between our results and the calculations of Pangantiwar and Srivastava (1989), maybe attribute to the following reasons.

The formula of polarization potential and the scattering amplitude of them quite differ of us. We think that the neglecting of the inelastic channels like ionization, absorption channels effect in the behavior of (DCS) curves, where we notice the increasing of minima in (DCS) as the energy increases. In return this has come in getting on results corresponding with the researchers calculations.

References

- [1].A.Jain, Phys.Rev.A **41**,2437(1990).
- [2].A.W.Pangantiwar and R.Srivastava,Phys.Rev.A **40**,2346(1898).
- [3].B.H.Bransdent, I.E.McCarthy and A.T.Stelbovics, J.Phys.B: At.Mol. Opt. Phys.**18**,823 (1985).
- [4].B.Marinkovic, V.Pejcev,Dfillipovic and L.Vuskouic, in Abstract of Contributed, Proceedings of the Fifteenth International Conference on the Physics of Electronic and Atomic Collision, Brighton, 1987, edited by J.Geddes, M.B.Gillbody, A.E.Kingston, and C.J.Latimar(Queen's University, Belfast,1987),P186.
- [5].D.G.Truhlar, in "Chemical Application of atomic and Molecular Electrostatic Potentials",New York,P123,1981).
- [6].D.R.Norcross and M.J.Seaton, J.Phys.B:At.Mol.Opt.Phys.**9**,2983(1976).
- [7].E.Clementi and C.Roetti, At.Data.Nucl.Data Table **14**,177(1974).
- [8].J.C.Nogueira, W.R.Newell and W.M.Johnstone, J.Phys.B:At.Mol. Opt.Phys.**20**,L537(1987).
- [9].K.Bartschat, R.P.McEachran, and A.D.Stauffer,J.Phys.B:At.Mol. Opt.Phys.**23**,2349(1990).
- [10].K.Bartschat, R.P.McEachran, and A.D.Stauffer,J.Phys.B:At.Mol. Opt.Phys.**21**,2349(1988).
- [11].P.Khan, S.K.Datta,D.Bhattacharyya and A.S.Ghosh,Phys.Rev.A **29**,3129 (1984).