Elastic scattering of electrons and positrons by the cadmium atom

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Elastic scattering of electrons and positrons by the cadmium atom is studied. A real optical potential is used to calculate the phase shifts of the first few partial waves. Then the differential cross sections (DCS's) are calculated from the formula given by Nesbet [Phys. Rev. A **20**, 58 (1979)] using the calculated phase shifts of the first few partial waves. The calculations are performed at incident projectile energies of 40, 60, 75, 85, 100, and 150 eV, where the experimental DCS measurements for electron scattering are available. The agreement between our calculated DCS and the available experimental DCS is reasonable at lower energies and very good at higher energies. Total cross sections are also obtained, but no other results, theoretical or experimental, are available for comparison with them.

I. INTRODUCTION

Recently Nogueira *et al.*[1] reported the first absolute elastic differential cross sections (DCS) for electron-cadmium scattering at incident energies of 60, 75, 85, 100, and 150 eV. Relative DCS measurements for elastic electron scattering by the cadmium atom have also been reported by Marinkovic *et al.*[2] for 40-eV impact energy. These DCS results show interesting structures, but so far there is no theoretical calculation in the literature to confirm or compare these experimental predictions, to our knowledge. Since the differential cross sections provide more rigorous testing for theories and experiments, as compared to the total cross section (TCS), it may be of great interest to present the calculated DCS of electrons from cadmium. Recent various efforts to generate intense positron beams have led to many exciting developments in positron-scattering experiments, particularly from atoms and molecules. As a result, direct measurements for the DCS of positrons elastically scattered from heavy atoms are now becoming available.[3] Therefore it is also desirable to present the calculated DCS for positrons scattered 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 (or positron)-atom elastic scattering.[4-7] 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 an 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. Some recent works[8-10] use methods that include the contributions of higher partial waves to the elastic scattering amplitude for long-range interactions.

In this paper we aim to present calculations for the elastic scattering of electrons and positrons by the cadmium atom through the OMPA. The phase shifts δ_l of the first few partial waves (say, x) depending upon the incident projectile energy have been calculated exactly and the phase shifts of the higher partial waves (say from $x+1$ to infinity) are estimated using the closed-form expression obtained by Thompson[11] for the $1/r^4$ potential. Thus the DCS's are calculated from the formula given by Nesbet[12] using the partial-wave phase shifts δ_l up to $l=x$. The results are obtained at incident projectile energies of 40, 60, 75, 85, 100, and 150 eV in order to explore the suitability of the present method by comparing these results with the available DCS measurements. The TCS's are also obtained at these energies but no other results, theoretical or experimental, are available for comparison to our knowledge.

II. THEORY

In OMPA the basic idea is to analyze the elastic scattering of a particle from a complex target by replacing the complicated interactions between the beam and target particles by an equivalent suitable model potential in which the incident particle moves. Thus once the optical model potential is defined, the original many-body elastic scattering problem reduces to a one-body problem. Then the differential equation for the scattering of projectile electron (positron) can be given by (atomic units are adopted throughout)

$$[\nabla^2+k^2-2V_{\rm opt}(r)]\psi(\mathbf{r})=0\ . \tag{1}$$

Here, $\mathbf{k}$ is the incident wave vector of the projectile. $V_{\rm opt}(r)$ is the optical potential of the system which we have chosen for the present calculation as

$$V_{\rm opt}(r)=V_{\rm st}(r)+V_{\rm ex}(r)+V_{\rm pol}(r)\ , \tag{2}$$

where $V_{\rm st}(r)$ is the static potential given as usual by $\langle i|V|i\rangle$, with i representing the ground state of the cadmium atom and V is the Coulomb interaction potential between projectile and target. $V_{\rm ex}(r)$ refers to the exchange potential and is absent for positron scattering. In general exchange potential is nonlocal but it is converted into an equivalent local exchange potential following Vanderpoorten[13] as

$$V_{\mathrm{ex}}(r)=\tfrac{1}{2}([\tfrac{1}{2}k^2-V_{\mathrm{st}}(r)] -\{[\tfrac{1}{2}k^2-V_{\mathrm{st}}(r)]^2+8\pi\rho(r)\}^{1/2}) . \quad (3)$$

Here $\rho(r)$ is the spherical one electron charge density of the cadmium atom. For the evaluation of $V_{\mathrm{st}}(r)$ and $V_{\mathrm{ex}}(r)$, we have used multi-ζ Hartree-Fock wave functions of the ground state of the cadmium atom compiled by Clementi and Roetti.[14]

Also, to include the polarization effect from the target atom, $V_{\mathrm{pol}}(r)$ is the polarization potential used previously by Madison and Shelton[15] and Srivastava and Williamson, Jr.[16] having the functional form

$$V_{\mathrm{pol}}(r)=-\frac{\alpha_d}{2r^4}\left\{1-\exp\left[-\left[\frac{r}{r_c g}\right]^8\right]\right\} . \quad (4)$$

Here α_d is the dipole polarizability of the cadmium atom and its value (43.7) is taken from the literature.[17] r_c (=2.006) is the cutoff parameter determined by the position of the last maximum of the absolute value of the outermost wave function. g is an energy-dependent adjustable parameter determined by fitting our calculated DCS for the elastic scattering of electrons by the cadmium atom with the available experimental values of the same at a particular energy. (In the present calculations the value of g varies from 3.9 to 3.0 and it decreases with increasing energy.)

After defining a suitable choice for $V_{\mathrm{opt}}(r)$, as given by Eq. (2), we substitute it into Eq. (1) and using the standard partial wave expansion for $\psi(\mathbf{r})$ we get

$$\left[\frac{d^2}{dr^2}+k^2-2V_{\mathrm{opt}}(r)-\frac{l(l+1)}{r^2}\right]u_l(r)=0 , \quad (5)$$

where $u_l(r)$ is solved so that it represents the radially scattered asymptotic wave function expressed as

$$u_l(r)\underset{r\to\infty}{\sim}\frac{1}{k}\sin\left[kr-\frac{l\pi}{2}+\delta_l\right] , \quad (6)$$

where δ_l is the phase shift corresponding to the lth partial wave. The scattering amplitude is obtained using the following expression given by Nesbet:[12]

$$f(\theta)=\frac{1}{k}\sum_{l=0}^{x}(2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\theta) +\pi\alpha_d k\left[\tfrac{1}{3}-\tfrac{1}{2}\sin\frac{\theta}{2}-\sum_{l=1}^{x}\frac{P_l(\cos\theta)}{(2l+3)(2l-1)}\right] , \quad (7)$$

where the value of x is 2 for 40-eV; 5 for 60-, 75-, and 85-eV; and 6 for 100- and 150-eV projectile impact energies, respectively. This different choice of x for calculations at different energies in the present work is consistent with the earlier statement that for short-range interactions the number of contributing partial waves increases with the increase in impact energy. The DCS and TCS are obtained in the conventional manner from $f(\theta)$.

III. RESULTS AND DISCUSSION

We present in Figs. 1–6 and Table I our various calculated results. Figures 1–6 also compare our results with the available experimental results.

In Fig. 1 our DCS for the elastic scattering of electrons by cadmium atom at 40 eV are compared with the available relative DCS of Marinkovic *et al.*,[2] which we have normalized to our results at $\theta=35°$ for purpose of comparison. It is found that our results are in good agreement with the experimental data up to a scattering angle of 85°. Also our results show minima at nearly the same scattering angles as predicted by experiment. In the angular region 85°–145° our results are found to be lower than the experimental data.

In Figs. 2–6 our DCS for the elastic scattering of electrons by the cadmium atom at energies of 60, 75, 85, 100, and 150 eV, respectively, are compared with the corresponding absolute DCS measurements of Nogueira *et al.*,[1] which are available only up to scattering angles of 70°. Our results at these energies also show similar structures as shown by the experiment and our results at a 40-eV impact energy. Only at higher energies of 100 and 150 eV we see that the second and/or third minimum changes into more dips. At all energies our results show the first minimum nearly at the same scattering angle as predicted by experiment. At 60-, 75-, and 85-eV impact energies our results are found to be in good agreement with the experimental data up to scattering angles of 45°

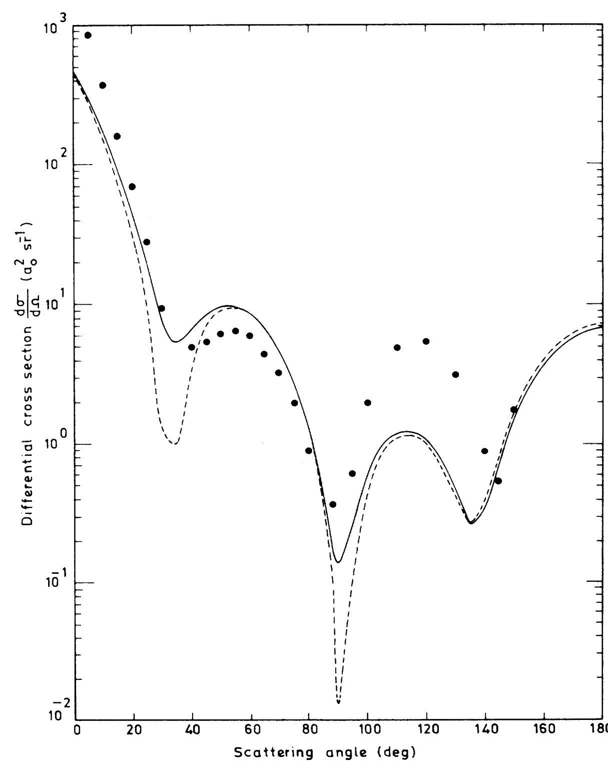

FIG. 1. Differential elastic cross sections (in a_0^2 sr^{-1}) at 40 eV. ——, present results (for electron scattering); — — —, present results (for positron scattering); ●, normalized experimental results of Ref. 2.

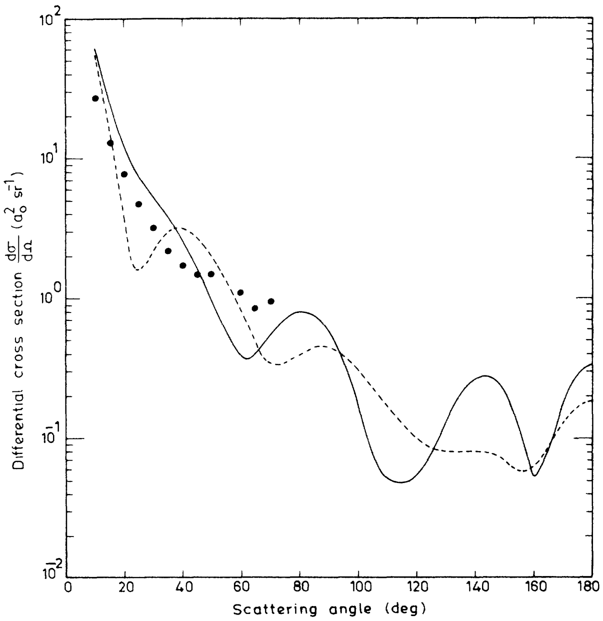

FIG. 2. Differential elastic cross sections (in a_0^2 sr^{-1}) at 60 eV. ●, Experimental results (Ref. 1). The curves are the same as in Fig. 1.

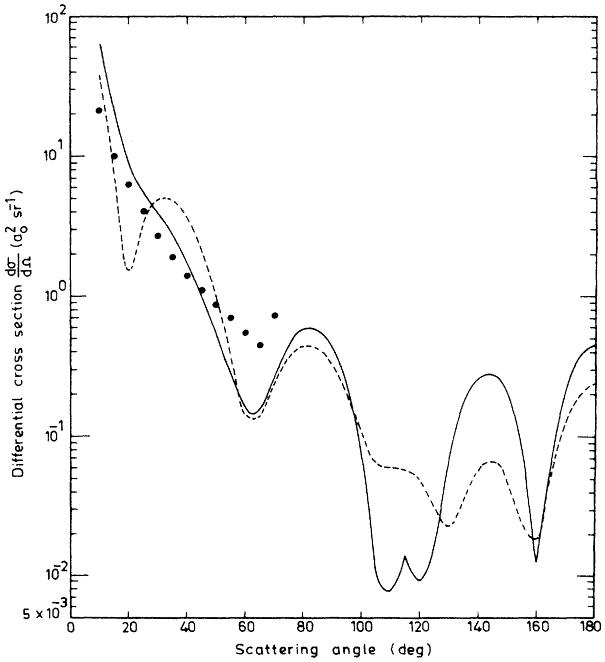

FIG. 4. Differential elastic cross sections (in a_0^2 sr^{-1}) at 85 eV, same as in Fig. 2.

and above 45° our results are lower than the experiment. But this difference between our results and experimental data above scattering angles of 45° is found to decrease with the increase in impact energy. Also, at 100 and 150 eV the agreement between our results and experiment is very good. The maximum error in our computed forward differential cross section (scattering angles ranging from 0°–85°) for the elastic scattering of electrons by cadmium atom, due to uncertainty (50%) in the value of the atomic polarizability ranges from 1.58% at 40 eV up to 8.09% at 150 eV. The maximum change noticed in the present computed forward DCS for electron impact due to reasonable variation (we considered it here up to 25%) in the assumed parameters r_c and g is estimated to range

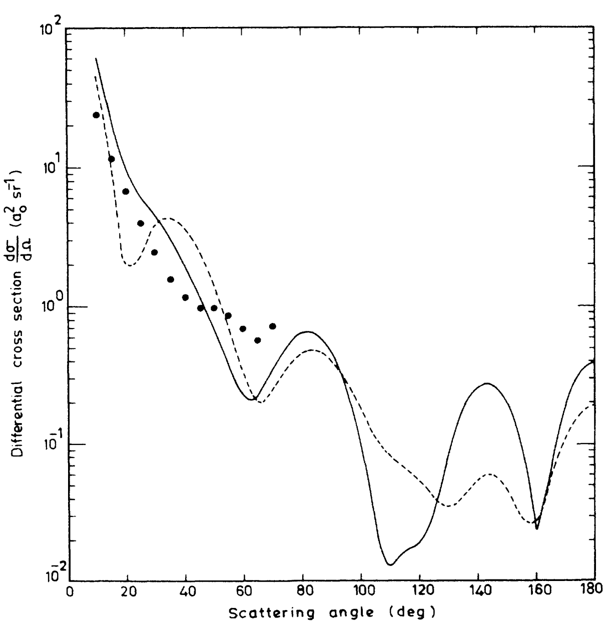

FIG. 3. Differential elastic cross sections (in a_0^2 sr^{-1}) at 75 eV, same as in Fig. 2.

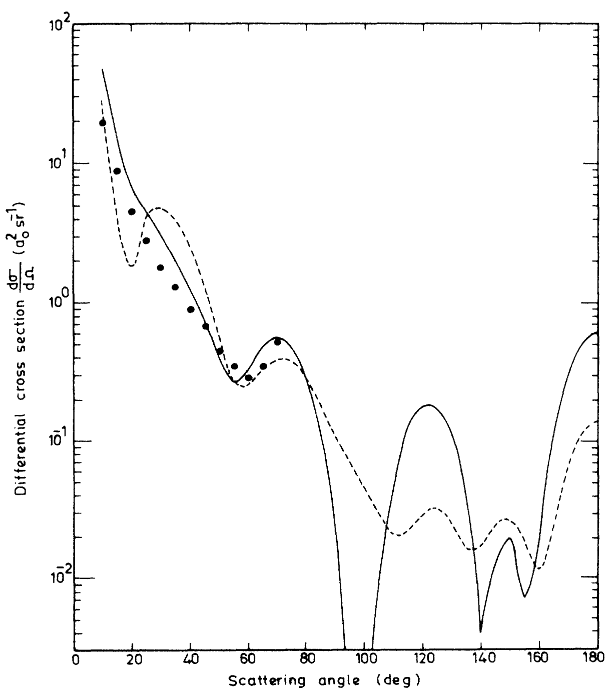

FIG. 5. Differential elastic cross sections (in a_0^2 sr^{-1}) at 100 eV, same as in Fig. 2.

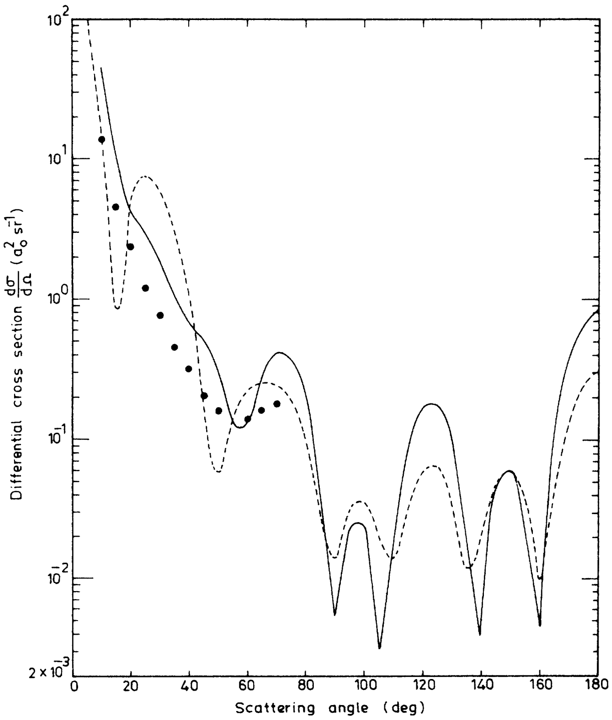

FIG. 6. Differential elastic cross sections (in a_0^2 sr^{-1}) at 150 eV, same as in Fig. 2.

from 4.52% at 40 eV up to 15.33% at 150 eV.

We have used the same static and polarization potentials and the values of r_c and g as in the case of electron-cadmium scattering to calculate the DCS for the positron-cadmium scattering, but the results were found unsatisfactory with two many oscillations. Basu *et al.*[18] also found out from their recent investigations for positron-krypton elastic scattering and using almost similar type of polarization potential that the potential $V_{\rm pol}$ with a single cutoff parameter is not suitable both for electron and positron scattering in the case of heavy atoms. So by changing the cutoff parameter only by choosing $g=1$ at all energies, we have calculated DCS for positron-cadmium scattering at 40, 60, 75, 85, 100, and 150 eV, and these results are displayed in Figs. 1–6 along with our electron scattering results. This choice of g in expression (4) for $V_{\rm pol}$ is found to produce satisfactory TCS results for positron-cadmium scattering (see proceeding discussion).

TABLE I. Total cross sections (in units of πa_0^2) for elastic scattering of electrons and positrons by cadmium atoms at various energies.

Energy (eV)	Electron results	Positron results
40	30.25	25.1
60	9.24	7.73
75	8.59	6.77
85	8.31	6.36
100	6.64	5.14
150	6.05	4.35

Finally, in Table I, our total elastic cross sections for the scattering of electrons and positrons are shown. No other results, theoretical or experimental, are available for comparison. Our positron TCS are found to be lower than our electron TCS at all energies. Even at 150 eV, there is a difference of 1.70 a.u. between the positron and electron TCS. The similar variation of total cross sections (TCS) have also been noticed by Khare *et al.*[4] in their calculations for elastic scattering of electrons and positrons by calcium atom.

In the present calculations, we have not included the absorption effect since the inclusion of absorption effect is expected to increase the DCS in the forward direction as noticed by Khare *et al.*[19]

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