

Elastic scattering of electrons by neon and argon atoms and hydrogen molecules

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Received 4 September 1973

Abstract. Elastic scattering of electrons by neon and argon atoms and hydrogen molecules are considered in the plane wave approximation. Comparison of the present results with the available experimental data indicates that the polarization potential is of importance even up to incident energies as high as 800 eV.

1. Introduction

Recently Khare and Shobha have employed the plane wave approximation to investigate elastic scattering of electrons by hydrogen (Khare and Shobha 1971a) and helium atoms (Khare and Shobha 1970, 1971b) and the hydrogen molecule (Khare and Shobha 1972). In the present investigation the approach has been extended to heavier inert gases, namely neon and argon, and scattering by the hydrogen molecule has been re-examined by employing a better wavefunction. It may be noted, however, that in the present approach the free electron is always represented by plane waves; hence for heavier targets the plane wave approximation is expected to yield reliable results at relatively higher impact energies. For the target hydrogen molecule, it may be pointed out that the two one-centre wavefunctions employed by Khare and Shobha (1972) yield poor values of the quadrupole moment. To correct for this discrepancy a semi-empirical potential was added. In the present investigation we have employed the one-centre wavefunction of Joy and Parr (1958) which yields a much better value of the quadrupole moment and has been successfully employed by Lane and Henry (1968) to discuss rotational and vibrational excitations.

2. Theory

In the plane wave approximation the differential cross section for the elastic scattering of electrons by an atom, including exchange and correct to the third order in the interaction potential, is given by (Khare and Shobha 1971b)

$$I(\theta) = |f_{B1} - g|^2 \left(1 + \frac{2f_{dp}}{|f_{B1} - g|} \right) \quad (1)$$

where θ is the angle of scattering, f_{B1} and g are first Born and first order exchange scattering amplitudes respectively. f_{dp} is the second order scattering amplitude due to

the dynamic polarization potential $V_{dp}(r)$. For molecular targets (1) is averaged over all possible orientations of the molecular axis.

In order to calculate f_{B1} and g we require suitable wavefunctions of the targets. For Ne and Ar we have used the wavefunctions employed by Sheorey (1969). For an N electron atom the wavefunction is given by

$$\Psi(r_1, r_2, \dots, r_N) = \phi_{1s}(r_1)\phi_{1s}(r_2)\phi_{2s}(r_3) \dots \phi_{nl}(r_N) \quad (2)$$

where

$$\phi_{nl}(r) = \mathcal{R}_{nl}(r)Y_{lm}(\hat{r}). \quad (3)$$

$Y_{lm}(\hat{r})$ are the normalized spherical harmonics and $\mathcal{R}_{nl}(r)$ are the normalized orthogonal radial wavefunctions. Since for a many electron atom the hydrogenic radial function $R_{nl}(r)$ is not orthogonal, the functions $\mathcal{R}_{nl}(r)$ are taken to be the linear combinations of $R_{nl}(r)$. For example

$$\mathcal{R}_{2s}(r) = C_{2s-2s}R_{2s}(r) + C_{2s-1s}R_{1s}(r) \quad (4)$$

with

$$R_{nl}(r) = N_{nl}r^{n-1} \exp(-\alpha_{nl}r). \quad (5)$$

The values of the various orthogonalizing coefficients and the variational parameters α_{nl} are given by Sheorey (1969) and need not be repeated here.

Carrying out the elementary algebra we obtain

$$f_{B1}(\text{Ne}) = \frac{20}{K^2} - \frac{4}{K^2}X \quad (6)$$

$$f_{B1}(\text{Ar}) = \frac{36}{K^2} - \frac{4}{K^2}(X + Y) \quad (7)$$

where K is the change in the momentum vector and X and Y are given by

$$X = \frac{1}{K} \int_0^\infty r \sin Kr (\mathcal{R}_{1s}^2(r) + \mathcal{R}_{2s}^2(r) + 3\mathcal{R}_{2p}^2(r)) dr \quad (8)$$

and

$$Y = \frac{1}{K} \int_0^\infty r \sin Kr (\mathcal{R}_{3s}^2(r) + 3\mathcal{R}_{3p}^2(r)) dr. \quad (9)$$

Both X and Y have been analytically evaluated (Shobha 1972).

In the Ochkur approximation the exchange scattering amplitude g is given by

$$g(\text{Ne}) = -\frac{2}{k_0^2}X \quad (10)$$

$$g(\text{Ar}) = -\frac{2}{k_0^2}(X + Y) \quad (11)$$

where k_0^2 is the energy of the incident electron.

For hydrogen molecule we have employed one-centre wavefunction of Joy and Parr (1958) given by

$$\Psi(r_2, r_3) = \sum_{i=1}^7 c_i \Phi_{2i-1} \Phi_{2i} \quad (12)$$

where

$$\Phi_i \Phi_j = [2(1 + \delta_{i,l_i} \delta_{m_i m_j} S_{ij}^2)]^{-1/2} (\phi(r_2 | n_i l_i m_i) \phi(r_3 | n_j l_j m_j) + \phi(r_3 | n_i l_i m_i) \phi(r_2 | n_j l_j m_j)) \quad (13)$$

and

$$S_{ij} = \int \phi^*(r | n_i l_i m_i) \phi(r | n_j l_j m_j) dr \quad (14)$$

$$\phi(r | n_i l_i m_i) = N(n_i, z_i) r^{n_i-1} \exp(-z_i r) Y_{l_i m_i}(\hat{r}). \quad (15)$$

It may be noted that the values of n_i are not integers but are defined in terms of gamma functions. The values of c_i , n_i , z_i , l_i and m_i are given by Joy and Parr and need not be repeated here.

Following the usual procedure we obtain

$$f_{B1} = \frac{4}{K^2} [\cos(\frac{1}{2} \mathbf{K} \cdot \mathbf{R}) - J] \quad (16)$$

where

$$J = \int \exp(i \mathbf{K} \cdot \mathbf{r}^2) |\Psi(r_2, r_3)|^2 dr_2 dr_3 \quad (17)$$

and R is the equilibrium internuclear distance which we have taken to be 1.4. Defining

$$M = \int |\Psi(r_2, r_3)|^2 dr_3 \quad (18)$$

and putting (15) in (12) we find that M is a 7×7 matrix. It can easily be shown that all its diagonal elements are non-zeros. However, the off diagonal elements M_{ij} survive only if $i \leq 4$ and $j \leq 4$. The two exceptions being M_{57} and M_{75} elements. Thus in all we obtain 21 elements. Putting

$$\exp(i \mathbf{K} \cdot \mathbf{r}) = 4\pi \sum_{lm} (i)^l j_l(Kr) Y_{lm}(\hat{r}) Y_{lm}(\hat{K}) \quad (19)$$

in (17), where $j_l(r)$ are spherical Bessel functions, and carrying out the integration we obtain analytic expression for J_{ij} . The expressions are quite lengthy and have been given by Shobha (1972), hence, they need not be reproduced here. As usual the exchange scattering amplitude is given by

$$g = -\frac{2}{k_0^2} J. \quad (20)$$

To calculate f_{dp} we have taken (Khare and Shobha 1972)

$$V_{dp}(r) = -\frac{\alpha_d r^2}{(r^2 + r_d^2)^3} - \frac{\alpha'_d r^2 P_2(\cos \theta)}{(r^2 + r_d^2)^3} - \frac{(\alpha_q - 6\beta_1) r^2}{(r^2 + r_d^2)^4} \quad (21)$$

where $P_l(\cos \theta)$ are the Legendre polynomials and r_d is a cut-off parameter. α_d and α'_d are mean dipole polarizability and a measure of the anisotropy of the polarizability, respectively. α_q is the mean quadrupole polarizability and β_1 is a parameter which corrects the adiabatic polarization potential due to finite velocity of the incident electron. The values of the various parameters for the hydrogen molecule are taken to be exactly the same as given by Khare and Shobha (1972) (with $\alpha_q = 17.27$). For the inert gases $\alpha'_d = 0$ and $\alpha_d(\text{Ne}) = 2.69$, $\alpha_d(\text{Ar}) = 11.0$ (Kaneko 1959); $\alpha_q(\text{Ne}) = 6.368$, $\alpha_q(\text{Ar}) = 46.5$

(Lahiri and Mukerjee 1967a, b); $\beta_1(\text{Ne}) = 1.27$, $\beta_1(\text{Ar}) = 8.28$ (Dalgarno *et al* 1968). The value of the cut-off parameter r_d for argon is taken to be equal to 2.5, which is the mean value of r for the bound 3s state and has been employed by Kivel (1959) to fit his calculations, to low energy scattering data. To obtain r_d for Ne the following relation, proposed by Hammerling *et al* (1957), is employed :

$$r_d^2(\text{Ne}) = \left(\frac{\alpha_d(\text{Ne})}{\alpha_d(\text{Ar})} \frac{N(\text{Ar})}{N(\text{Ne})} \right)^{1/2} r_d^2(\text{Ar}) \quad (22)$$

where N is the number of electrons in the target. The above relation gives $r_d(\text{Ne}) = 1.66$.

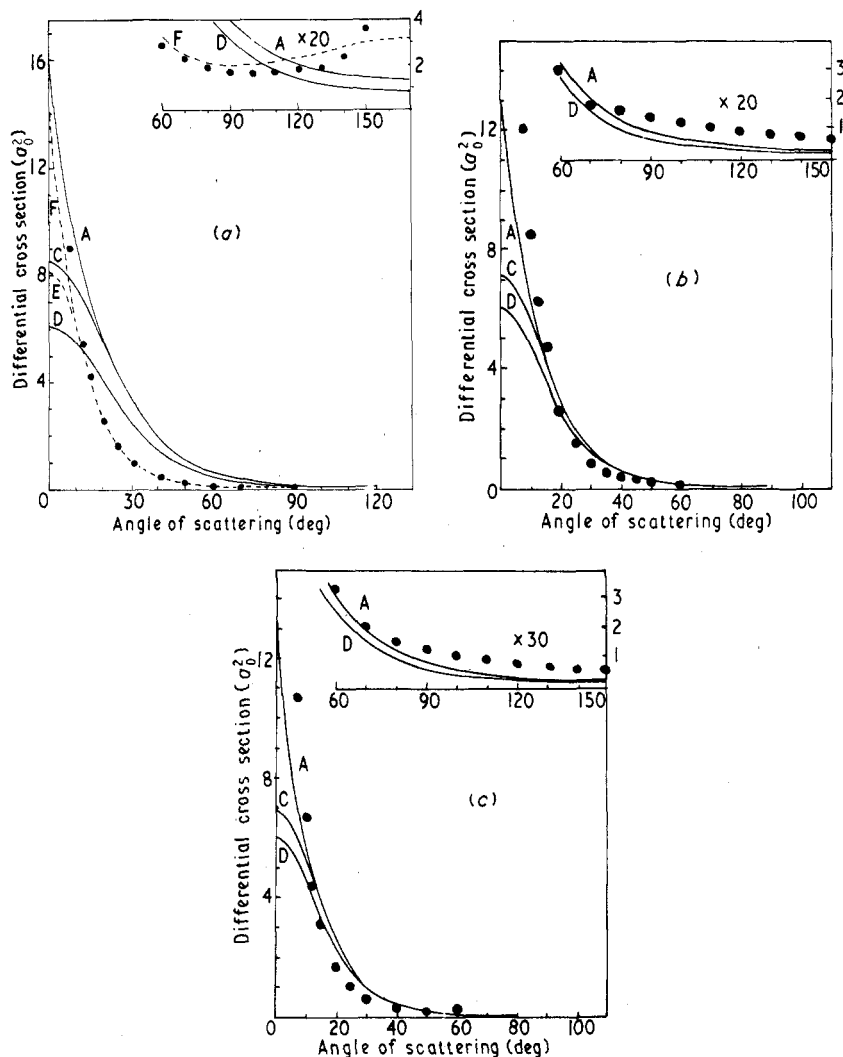


Figure 1. Differential cross sections $I(\theta)$ for (a) 300 eV, (b) 625 eV, (c) 800 eV electrons elastically scattered by the neon atoms. Curves D, C and A denote the present values of $I(\theta)$ obtained in first Born, Ochkur and plane wave approximations respectively. Curve E denotes $I(\theta)$ in exchange-adiabatic approximation employing only the first nine partial waves (Thompson, private communication) whereas in Curve F all partial waves are included through (24). ● are the normalized experimental data of Hughes and McMillen (1933).

Putting (21) in the expression for f_{dp} and carrying out the integration we obtain

$$f_{dp} = \frac{\pi e^{-Kr_d}}{16} \left[\alpha_d \left(\frac{3}{r_d} - K \right) + \frac{(\alpha_q - 6\beta_1)}{6r_d} \left(\frac{3}{r_d^2} + \frac{3K}{r_d} - K^2 \right) - K\alpha'_d \left(\frac{4\pi}{5} \right)^{1/2} Y_{20}^*(\hat{K}) \right]. \quad (23)$$

It may be noted that the most accurate calculations for the elastic scattering of electrons by neon and argon have so far been carried out by Thompson (1966) in the dipole-exchange approximation. Recently he has extended his calculations to higher energies (up to 288 eV for Ne and 207 for Ar, private communication). However, only the first nine partial waves are obtained. Since for the above energies the higher partial waves are also expected to contribute we have extended the calculations to include all the partial waves. It is legitimate to assume that for $l \geq 9$ the electron is scattered only by the long range potential which can be replaced by its asymptotic form $-\alpha_d/r^4$ and the contribution of exchange is negligible. Under these assumptions we have

$$f(\theta) = \frac{1}{2ik_0} \sum_{l=0}^8 (2l+1)(e^{2i\eta_l} - 1)P_l(\cos \theta) + \pi\alpha_d \left(\frac{k_0}{3} - \frac{K}{4} \right) - \pi\alpha_d k_0 \sum_{l=1}^8 \frac{P_l(\cos \theta)}{(2l+3)(2l-1)}. \quad (24)$$

3. Results and discussions

In figure 1 we have represented by curve E the differential cross section obtained by Thomson's first nine partial waves for the elastic scattering of 288 eV electrons by neon atoms. For comparison the results obtained from (24) and those obtained from (1) (shown by curves F and A, respectively) are also plotted. The relative data of Hughes and McMillen (1933) at 300 eV normalized to curve E for the best visual fit are also shown. First Born cross sections with and without exchange are shown by the curves

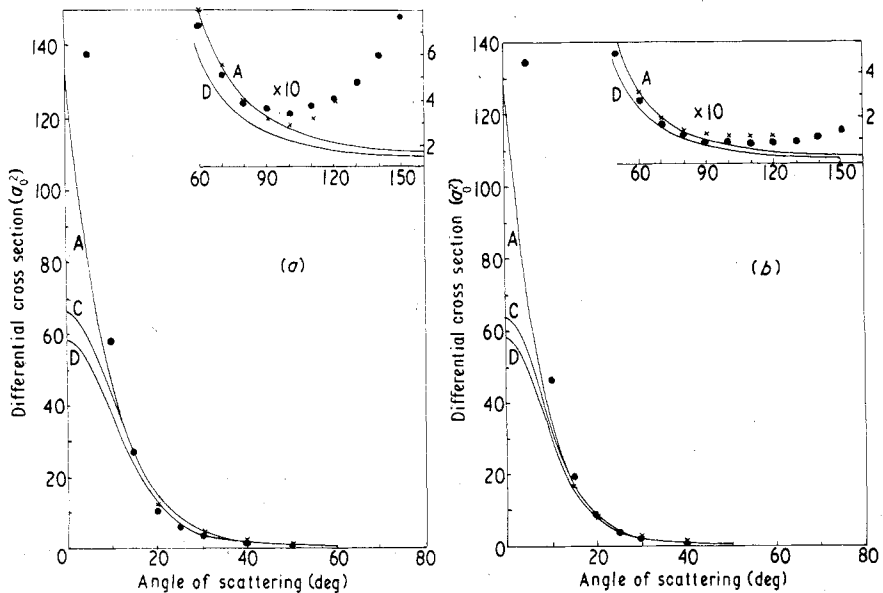


Figure 2. Differential cross sections for (a) 510 eV, (b) 780 eV electrons elastically scattered by the argon atoms. ● and × are the normalized experimental data of Webb (1935a) and Arnot (1931) respectively. For the details of the curves see the caption of the figure 1.

C and D, respectively. It is evident from the figure that the curve E is in good agreement with the experimental data and the agreement improves, especially for low angles, if higher partial waves are included (curve F). On the other hand the curves A, C, and D exhibit poor agreement with the experimental data. An examination of the phase shifts given by Thomson (private communication) shows that even at 288 eV the phase shifts are fairly large hence the plane wave approximation is not expected to yield good results.

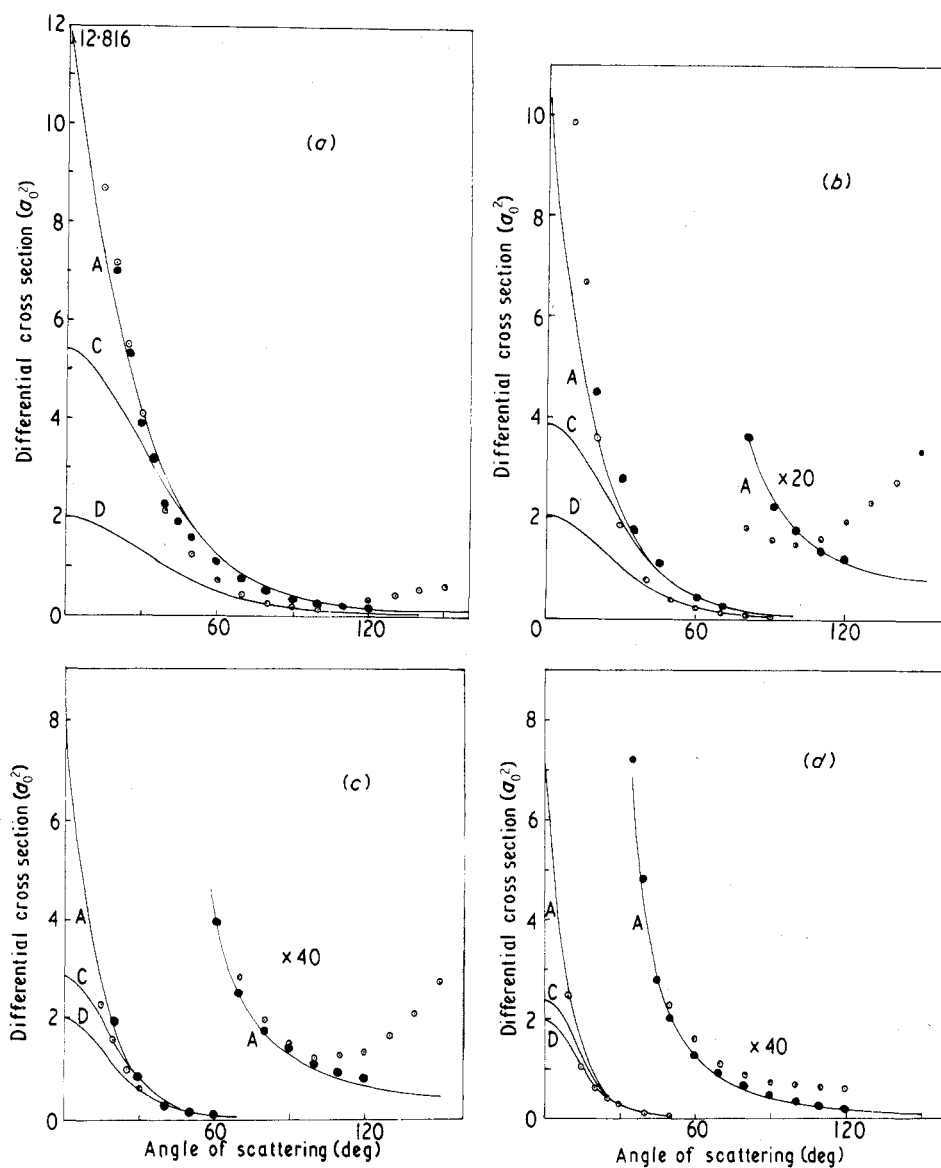


Figure 3. Differential cross section for (a) 30 eV, (b) 50 eV, (c) 100 eV, (d) 200 eV electrons elastically scattered by hydrogen molecules. ● and ○ are the normalized experimental data of Williams (1969) and Webb (1935b) respectively. For the details of the curves see the caption of the figure 1.

The figures 1(b), 1(c) and 2 show the results at relatively higher energies (> 500 eV). The experimental data are again normalized for the best visual fit with the theoretical curves. It is evident from the figure that even in the 500–800 eV range the first Born approximation fails to explain the shape of the experimental data and the agreement between the theory and the experiment considerably improves by including the polarization effects. It may be noted that both for neon and argon α_a is very nearly equal to $6\beta_1$ hence the contribution of the long range potential which falls off asymptotically as r^{-6} is always very small.

In figure 3 the present differential cross sections for e-H₂ scattering are compared with the relative experimental data of Williams (1969) and of Webb (1935b). The agreement is satisfactory and is of the same type as obtained by Khare and Shobha (1972). This supports our earlier conclusion that the cross sections are not very sensitive to the ground state wavefunctions. The results at higher energies (up to 912 eV) are given by Shobha (1972).

Finally in table 1 we compare the present total cross sections with those obtained by Khare and Shobha (1972) in plane wave approximation and Truhlar and Rice (1970) in the BP/D(5) approximation (see the above reference for the details of the BP/D(5) approximation). We notice that the present values are lower than those obtained by Khare and Shobha, however, the difference is not large. On the other hand the cross sections obtained by Truhlar and Rice are about 30 to 60% higher than the present values.

Table 1. Total cross section for the elastic scattering of electrons by the hydrogen molecule

$E(\text{eV})$	$Q(a_0^2)$		
	Khare and Shobha (1972)	Present values	Truhlar and Rice (1970)
30	15.0	14.2	—
50	7.15	6.65	—
100	2.99	2.72	3.64
200	1.37	1.23	1.84
350	0.75	0.67	1.06
650	0.44	0.38	0.618
912	0.29	0.25	0.406

Acknowledgments

The authors are thankful to Dr Thompson for supplying the numerical values of the phase shifts for e-Ne scattering.

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