

Elastic scattering of electrons by hydrogen molecules

B L JHANWAR, S P KHARE and M K SHARMA*

Department of Physics, Institute of Advanced Studies,
Meerut University, Meerut 250 001

*Permanent address: Department of Physics, M M H College, Ghaziabad 201 001

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Abstract. Elastic scattering of electrons by hydrogen molecules has been investigated in the intermediate energy range 100–2000 eV. The direct scattering amplitude consists of first Börn and second Börn minus distortion term. The contribution of exchange has been included through Ochkur approximation. The elastic differential cross-sections agree with experimental data.

Keywords. Elastic scattering; electrons; hydrogen molecules.

1. Introduction

The scattering of electrons by molecular hydrogen is the simplest electron-molecule scattering process and a number of theoretical studies have been carried out. However, only recently the absolute differential cross-sections (DCS) for electron-hydrogen molecule ($e\text{-H}_2$) elastic scattering over a wide range of intermediate impact energies (100–2000 eV) have been measured by van Wingerden *et al* (1977). The earlier measurements of Williams (1969), Lloyd *et al* (1974) and Fink *et al* (1975) were all relative. van Wingerden *et al* compared their data with various theoretical results obtained in Börn (Ford and Browne 1973), Born-exchange (Khare and Moiseiwitsch 1965), Börn-exchange-polarisation (Truhler and Rice 1970, 1971, 1974; Khare and Shoba 1974) and eikonal (Bhattacharyya and Ghosh 1975) approximations and found that the best agreement is obtained with the results of Khare and Shobha. The Börn-exchange-polarisation approximation of Khare and Shobha which is known as Khare-Shoba approximation (KSA) includes the exchange through Ochkur approximation (Ochkur 1964) and the polarisation of the target through an energy-independent dynamic polarisation potential. Recently, studies on the independent atom model have been carried out (Jain and Khare 1977; Huang and Chen 1977; Hayashi and Kuchitsu 1977; Srivastava *et al* 1978, Jain *et al* 1979). Gupta and Khare (1978) have employed KSA with an energy-dependent polarisation potential and obtained better results than those obtained with energy-independent polarisation potential. It may, however, be noted that both the second order polarisation potentials of KSA are empirical and real. Further the absorption effects are completely neglected. Dhal *et al* (1979) have employed optical eikonal approximation to investigate $e\text{-H}_2$ elastic scattering at 50, 100 and 200 eV. Their second order optical potential contains polarisation as well as absorption effects and in the averaging process, all possible orientation of the molecular axis are taken into consideration. The inclusion of absorption effects

and the averaging over all the angles should improve the agreement between theory and experiment. However, the eikonal results of Dhal *et al* (1979) do not exhibit this trend.

In the present investigation, following Bonham (1971), the second Börn scattering amplitude minus the distortion term is employed to include polarisation and absorption effects.

2. Theory

Let us consider the elastic scattering of electrons by hydrogen molecules with its two nuclei being separated by the equilibrium distance R ($=1.4$ Au). Let $\mathbf{R}(\mathbf{R}, \theta_0, \phi_0)$ describe the orientation of the internuclear molecular axis with reference to some polar axis fixed in space. If $\sigma(\theta, \phi; \theta_0, \phi_0)$ represents the DCS for the particular orientation of the internuclear axis, where (θ, ϕ) describes the direction of scattering, then the differential cross-section averaged over all molecular orientations is given by

$$I(\theta, \phi) = \frac{1}{4\pi} \int \sigma(\theta, \phi; \theta_0, \phi_0) \sin \theta_0 d\theta_0 d\phi_0. \quad (1)$$

Following Bonham (1971) and neglecting the second order exchange effects, the DCS including polarisation and absorption effects within the framework of Börn approximation is given by

$$\sigma(\theta, \phi; \theta_0, \phi_0) = |f_{B1} - g + f_{pa}|^2. \quad (2)$$

where f_{B1} and g are the first order Börn and exchange scattering amplitudes respectively. The second order scattering amplitude f_{pa} is given by the second Börn scattering amplitude from which the distortion term is omitted (Bonham 1971).

The first Börn scattering amplitude for e - H_2 elastic scattering is given by (in atomic units)

$$f_{B1} = -\frac{1}{4\pi} \int \exp(-i\mathbf{k}_f \cdot \mathbf{r}) \psi_0^*(\mathbf{r}_1, \mathbf{r}_2) V(\mathbf{r}; \mathbf{r}_1, \mathbf{r}_2) \psi_0(\mathbf{r}_1, \mathbf{r}_2) \\ \times \exp(i\mathbf{k}_0 \cdot \mathbf{r}) d\mathbf{r} d\mathbf{r}_1 d\mathbf{r}_2 \quad (3)$$

where \mathbf{k}_0 and \mathbf{k}_f are the initial and final momenta of the scattered electron and

$$V(\mathbf{r}; \mathbf{r}_1, \mathbf{r}_2) = -2/|\mathbf{r} - \mathbf{R}/2| - 2/|\mathbf{r} + \mathbf{R}/2| + \sum_{i=1}^2 2/|\mathbf{r} - \mathbf{r}_i|. \quad (4)$$

In the above equations (3) and (4) $\psi_0(\mathbf{r}_1, \mathbf{r}_2)$ is the electronic ground state wave function of H_2 and the distances are measured from the molecular midpoint. Substituting (4) in (3) and using Bethe integral, we obtain

$$f_{B1} = (4/K^2) [\cos(\mathbf{K} \cdot \mathbf{R}/2) - J], \quad (5)$$

where $\mathbf{K} = \mathbf{k}_0 - \mathbf{k}_f$, the momentum transfer during the collision and

$$J = \int \exp(i\mathbf{K} \cdot \mathbf{r}_1) |\psi_0(\mathbf{r}_1, \mathbf{r}_2)|^2 d\mathbf{r}_1 d\mathbf{r}_2. \quad (6)$$

The first order exchange scattering amplitude in Ochkur approximation is given by (Khare and Shobha 1974)

$$g = -(2/k_0^2)J. \quad (7)$$

The second order scattering amplitude f_{pa} is given by

$$f_{pa} = (32\pi^4)^{-1} S'_n \int d\mathbf{q} \frac{\langle O, \mathbf{k}_f | V | n, \mathbf{q} \rangle \langle n, \mathbf{q} | V | O, \mathbf{k}_0 \rangle}{q^2 - k_n^2 - i\epsilon}, \quad (8)$$

$$\begin{aligned} \text{with } \langle 0, \mathbf{k}_1 | V | n, \mathbf{K}_2 \rangle &= \int \exp(-i\mathbf{k}_1 \cdot \mathbf{r}) \psi_0^*(\mathbf{r}_1, \mathbf{r}_2) V(\mathbf{r}; \mathbf{r}_1, \mathbf{r}_2) \\ &\times \psi_n(\mathbf{r}_1, \mathbf{r}_2) \exp(i\mathbf{k}_2 \cdot \mathbf{r}) d\mathbf{r} d\mathbf{r}_1 d\mathbf{r}_2 \end{aligned} \quad (9)$$

$$\text{and } k_n^2 = k_0^2 - \delta_n; \quad (10)$$

δ_n being the n th electronic excitation threshold energy. The prime on summation in (8) denotes that the distortion term ($n = 0$) is excluded and wherever ϵ appears $\epsilon \rightarrow 0^+$ is implied.

We substitute (4) in (9) and use Bethe integral to obtain

$$\langle 0, \mathbf{k}_1 | V | n, \mathbf{k}_2 \rangle = \frac{8\pi}{S^2} \langle 0 | -2 \cos(\mathbf{S} \cdot \mathbf{R}/2) \delta_{on} + \sum_{i=1}^2 \exp(i\mathbf{S} \cdot \mathbf{r}_i) | n \rangle, \quad (11)$$

with $\mathbf{S} = \mathbf{k}_2 - \mathbf{k}_1$. δ_{on} is the Kronecker delta symbol. Since $n \neq 0$ in our case, the first term on the right side of (11) vanishes. We use (11) to reduce (8) to

$$f_{pa} = (2/\pi^2) S'_n \int d\mathbf{q} \frac{\langle 0 | A(\mathbf{K}_1) | n \rangle \langle n | A(\mathbf{K}_2) | 0 \rangle}{(q^2 - k_n^2 - i\epsilon) K_1^2 K_2^2}, \quad (12)$$

where we have defined

$$\mathbf{K}_1 = \mathbf{k}_0 - \mathbf{q}; \quad \mathbf{K}_2 = \mathbf{q} - \mathbf{k}_f,$$

$$\text{and } A(\mathbf{t}) = \sum_{j=1}^2 \exp(i\mathbf{t} \cdot \mathbf{r}_j). \quad (13)$$

To sum the infinite series (12), we replace k_n^2 by $p^2 (= k_0^2 - \delta)$ and then use the closure relation. δ is the mean excitation energy and for H_2 has the value 1.08 R. The value is obtained by taking (Jhanwar and Khare 1974)

$$a = -\frac{4}{\pi} \left(\frac{\partial}{\partial K} R_e f_{pa} \right)_{K=0}.$$

Thus we obtain

$$f_{pa} = \frac{2}{\pi^2} \int dq \frac{\langle 0 | A(\mathbf{K}_1) A(\mathbf{K}_2) | 0 \rangle - \langle 0 | A(\mathbf{K}_1) | 0 \rangle \langle 0 | A(\mathbf{K}_2) | 0 \rangle}{(q^2 - p^2 - i\epsilon) K_1^2 K_2^2}. \quad (14)$$

It is evident from (5), (6), (7) and (14) that a suitable ground state wave function $\psi_0(\mathbf{r}_1, \mathbf{r}_2)$ of H_2 is required to evaluate f_{B1} , g and f_{pa} . In the present investigation, to evaluate f_{B1} and g , we employ a highly accurate 57-term single centre-wave function of Hayes (1967). It may be noted that the first Börn cross-sections are in good agreement with the experimental data at large angles for intermediate and high energies (Khare and Shobha 1974; Gupta and Khare 1978). This may be due to the fact that for large momentum transfer the impact parameter is small. Hence, the effective electron-molecule interaction is close to coulombian in nature for which the first Börn approximation yields exact results. However, the first Börn underestimates the cross-section at low angles. The inclusion of exchange and second order Börn terms improves the agreement between the theory and experiment at low angles but leaves the large angle cross-sections practically unchanged. If we use the 57-term Hayes wave function to obtain f_{pa} , the calculation becomes complicated. Fortunately, at small angles the contribution from the non-spherical terms of the wave function is negligible and it only grows with the angle of scattering (Bhattacharyya and Ghosh 1975; Gupta 1978). Hence to keep the calculation tractable, we obtain f_{pa} by employing simple spherical single centre wave function of Carter *et al* (1958). It is expected that such a procedure will not introduce any appreciable error. The details of evaluation of f_{B1} and g with Hayes wave function are given by Gupta and Khare (1978) and are not repeated here. The spherical single centre-wave function of Carter *et al* is given by

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \phi(\mathbf{r}_1) \phi(\mathbf{r}_2), \quad (15)$$

$$\text{with } \phi(\mathbf{r}) = (1/\sqrt{4\pi})P(r)/r. \quad (16)$$

Carter *et al* have tabulated the numerical values of $P(r)$ for a number of discrete values of r . These values may be fitted (within 2%) to the form

$$\phi(r) = (N/\sqrt{\pi}) [\exp(-a_1 r) + C \exp(-a_2 r)], \quad (17)$$

$$\text{with } N = 1.15098, C = -0.45073, a_1 = 1.07315 \text{ and } a_2 = 3.92868.$$

Now, to evaluate f_{pa} we substitute (15) and (17) in (14) and obtain

$$\begin{aligned} f_{pa} = & 8 \sum_{j=1}^3 \left[\frac{8N^2 a_j \beta_j}{(K^2 + \beta_j^2)^2} - 1 \right] A(0, 0) + \sum_{j=1}^3 \frac{128}{\beta_j^3} a_j [A_p(\beta_j, 0) - \beta_j^2 D_j A_p(\beta_j, 0)] \\ & - \sum_{i,j=1}^3 \frac{512 N^4 a_i a_j}{\beta_i^3 \beta_j^3} [A_p(\beta_i, \beta_j) - \beta_i^2 D_i A_p(\beta_i, \beta_j) - \beta_j^2 D_j A_p(\beta_i, \beta_j) \\ & + \beta_i^2 \beta_j^2 D_i D_j A_p(\beta_i, \beta_j)], \end{aligned} \quad (18)$$

where $a_1=1$, $a_2=C^2$, $a_3=2C$, $\beta_1=2a_1$, $\beta_2=2a_2$, $\beta_3=a_1+a_2$, $D_n=\partial/\partial\beta_n^2$ and

$$A_p(\alpha, \beta) = \frac{1}{2\pi^2} \int dq \frac{1}{(q^2 - p^2 - i\epsilon)(K_0^2 + \alpha^2)(K_f^2 + \beta^2)}. \quad (19)$$

The integral $A_p(\alpha, \beta)$ can be evaluated using Dalitz (1951) technique and Feynman identity is used to reduce the integral over q to an one-dimensional integral (Holt and Moiseiwitsch 1968; Bonham 1971; Byron and Joachain 1973). This one-dimensional integral can then be separated into real and imaginary parts. Byron and Joachain suggested the numerical evaluation of these integrals. However, we found difficulty in the numerical evaluation of the real part of $A_p(\alpha, \beta)$ when either α or β is zero. Holt and Moiseiwitsch have also pointed out a similar difficulty. Bonham (1971) evaluated analytically both real and imaginary parts of $A_p(\alpha, \beta)$ and discussed their various special cases. However, his expressions are so lengthy that the analytical evaluation of f_{pa} , as given by (18), becomes very cumbersome.

In the present investigation we follow Lewis (1956) who considered the integral:

$$I(\lambda; \mathbf{q}_1, \alpha; \mathbf{q}_2, \beta) = \int d\mathbf{q} [(q^2 + \lambda^2)(|\mathbf{q} - \mathbf{q}_1|^2 + \alpha^2)(|\mathbf{q} - \mathbf{q}_2|^2 + \beta^2)]^{-1}, \quad (20)$$

and evaluated it analytically to obtain

$$I(\lambda; \mathbf{q}_1, \alpha; \mathbf{q}_2, \beta) = \frac{\pi^2}{(b^2 - ac)^{1/2}} \ln \left\{ \frac{b + (b^2 - ac)^{1/2}}{b - (b^2 - ac)^{1/2}} \right\}, \quad (21)$$

where $ac = [|\mathbf{q}_1 - \mathbf{q}_2|^2 + (\alpha + \beta)^2] [q_1^2 + (\alpha + \lambda)^2] [q_2^2 + (\beta + \lambda)^2]$,

$$b = \lambda [|\mathbf{q}_1 - \mathbf{q}_2|^2 + (\alpha + \beta)^2] + \beta[\lambda^2 + q_1^2 + \alpha^2] + \alpha[\lambda^2 + q_2^2 + \beta^2] \quad (22)$$

The function $I(\lambda; \mathbf{q}_1, \alpha; \mathbf{q}_2, \beta)$ as given by (21) is clearly analytic even for the complex values of λ , α and β . Regarding the specification of the branch of logarithm, Lewis pointed out that the arguments of the numerator and denominator must be taken from $-\pi$ to $+\pi$.

Comparison of (19) with (20) shows that

$$A_p(\alpha, \beta) = \frac{1}{2\pi^2} I(-ip; \mathbf{k}_0, \alpha; \mathbf{k}_f, \beta), \quad (23)$$

Thus a general analytical expression for $A_p(\alpha, \beta)$ can be obtained. In the particular case of the elastic scattering ($|\mathbf{k}_0| = |\mathbf{k}_f|$), it is given by

$$A_p(\alpha, \beta) = \frac{1}{2iC} \ln \left\{ \frac{A + i(C - B)}{A - i(C + B)} \right\}, \quad (24)$$

$$A = \beta(\delta + \alpha^2) + \alpha(\delta + \beta^2),$$

$$B = p[K^2 + (\alpha + \beta)^2],$$

$$C^2 = K^2 [p^2 K^2 + (p^2 + k_0^2)(\alpha^2 + \beta^2) + (\delta^2 + \alpha^2 \beta^2)]. \quad (25)$$

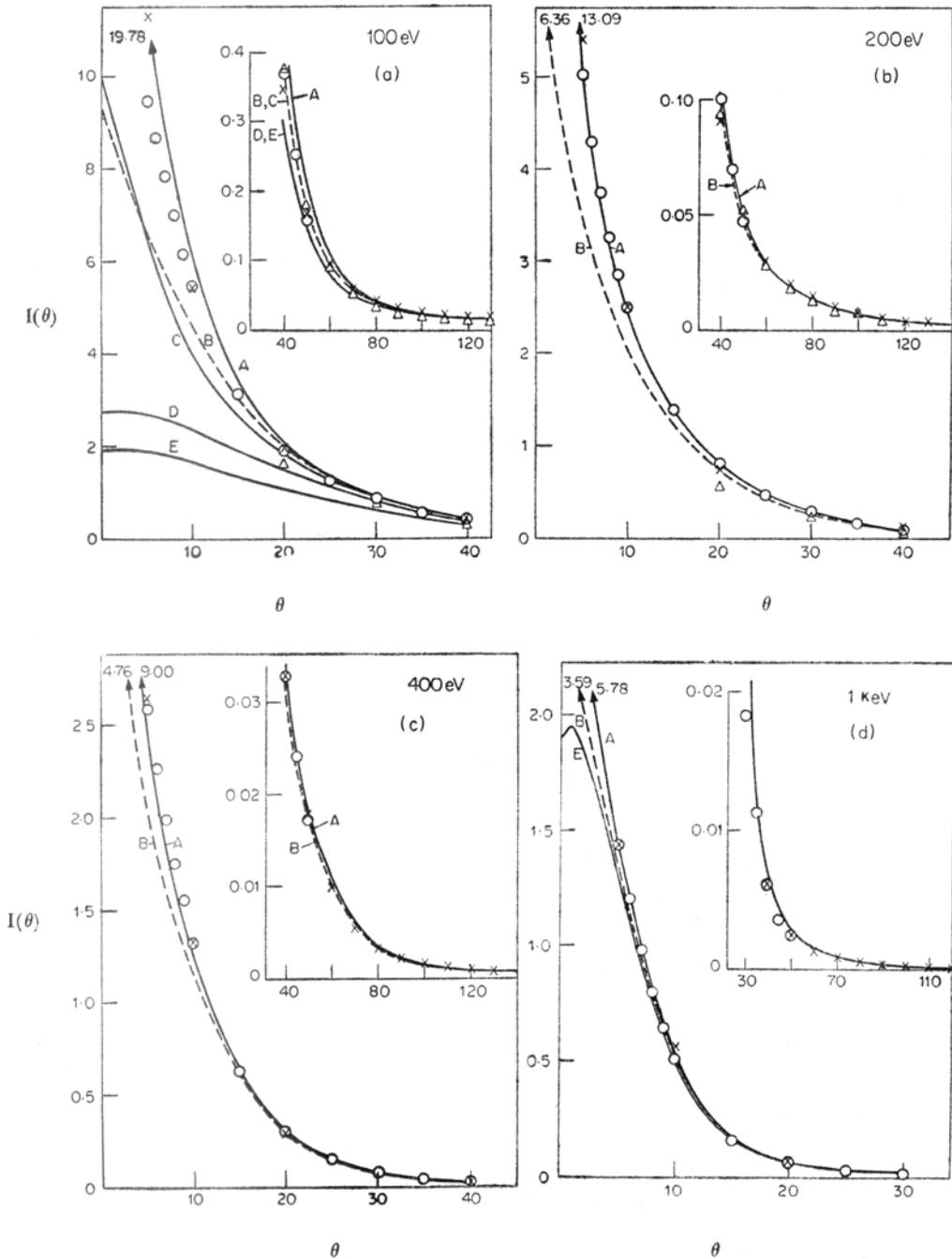


Figure 1. Differential cross-section for electrons elastically scattered by hydrogen molecules for incident energies 100 eV to 1 keV. \circ Experimental results of van Wingerden *et al* (1977). \times , \triangle ; Experimental results of Fink *et al* (1975) and Lloyd *et al* (1974) respectively as renormalised by van Wingerden *et al* (1977). A. Present results. B. Results of Gupta and Khare (1978). C. Present results upto third order (Börn-exchange polarisation). D. Results upto second order (Börn-exchange). E. First Börn results.

As noted earlier δ is the mean excitation energy. The special cases of $A_p(\alpha, \beta)$, relevant to the present calculations can be obtained from (24). As a check, all the special cases listed by Bonham have been reproduced from (24).

3. Calculations, results and discussions

Equation (18) along with (24) is employed to obtain analytic expressions for the real and imaginary parts of f_{pa} . The averaged DCS are then calculated from equations (2) and (1) for impact energies varying from 100 eV to 2 keV and the results at a few energies are given in figures 1(a) to 1(d) (curves A). The results obtained by Gupta and Khare (1978) (curve B) and the absolute experimental data of van Wingerden *et al* (1977) and of Fink *et al* (1975) and Lloyd *et al* (1974) (both renormalised by van Wingerden *et al* 1977) are also shown for comparison. At 100 eV few additional results are shown by curve E (Börn), curve D (Börn-exchange) and curve C (Börn-exchange and real part of f_{pa} and DCS correct upto third order only) to show the contribution of the different terms.

It is evident that all the approximations yield practically the same results at large angles. This confirms our earlier remark that at large angles the contributions of exchange and second order Börn terms are negligible. However, curves E and D as shown in figure 1(a) grossly underestimate the cross-sections at low angles. The inclusion of real part of f_{pa} (polarisation effects, curve C) greatly improves the agreement between the theory and experiments. But, still curve C underestimates the experimental results. Finally the curve A which includes real as well as imaginary parts of f_{pa} yields good agreement with the experimental data over the whole angular range. This clearly shows the importance of polarisation and absorption effects at low scattering angles. A similar agreement is obtained at other energies also. As expected, the angular region in which A differs from E decreases with the increase of energy, for example at 1 keV, the difference between A and E is limited to $\theta < 10^\circ$. This clearly indicates that the exchange, polarisation and absorption effects decrease with energy. It may also be pointed out that curves B and C are fairly close to each other. This indicates that the empirical polarisation potential employed by Gupta and Khare (1978) to obtain third order DCS is reasonable. The present investigation also shows that Börn calculations using higher order terms can be carried out using appropriate single centre wave functions.

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