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Elastic scattering of electrons by molecular hydrogen at intermediate and high energies

Ashok Jain, A. N. Tripathi, and M. K. Srivastava
Department of Physics, University of Roorkee, Roorkee-247672, India

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Differential cross sections for the elastic scattering of electrons from molecular hydrogen are calculated within the independent-atom model. The required differential cross sections of atomic hydrogen have been obtained by using the eikonal-Born-series method. The effect of the molecular binding is also considered. The present results compare well with recent absolute experimental measurements.

I. INTRODUCTION

Recent precise absolute experimental elastic e-H_2 differential cross-section measurements in the intermediate and high-energy region studied by Srivastava *et al.*[1] and Wingerden *et al.*[2] have focused the attention of many workers on the critical examination of the applicability of different theoretical approaches. Earlier studies investigating the elastic scattering of electrons by H_2 molecules were based on the Born approximation.[3] Many attempts have been made to improve upon the Born approximation. Khare and Moiseiwitsch[4] have included the exchange effects and later Khare and Shobha,[5] Trajmar *et al.*,[6] and Truhlar and Rice[7] accounted for the long-range interactions, i.e., polarization effect within the framework of the Born approximation. The results of their calculations are in good agreement with the experimental findings. Ford and Browne[8] and Liu and Smith[9] have also studied this process in the Born approximation using an accurate wave function for the hydrogen molecule and found that the results of different calculations basically differ only in the small-angle scattering region. Recently, Truhlar *et al.*[10] have carried out a calculation of inelastic scattering (rotational excitation) of electrons by molecular hydrogen in the energy range 10–40 eV using an effective potential (including static contribution, polarization, and exchange effects) and treating the process in the infinite-order-sudden (IOS) approximation. Truhlar and Brandt[11] have also studied the elastic and rotational excitation differential cross sections for electron-hydrogen molecule in the same energy region using the two-state close-coupling approximation with the same effective potential. Their results are in good agreement with the experiment except for elastic scattering in the small-angle region, where perhaps the data are not yet very reliable. They have reviewed (see the paper of Truhlar and Brandt[11] and references therein) in detail the different calculations carried out in this energy region. The eikonal and related approximations[12-15] have also been recently applied to investigate the elastic scattering of electrons by the hydrogen molecule.

Scattering at medium and high energies is adequately described by a coherent superposition of the contributions from individual atomic scattering centers. This approach, often referred to as the independent-atom model (IAM), is applicable for $R \ll k_i a^2$, where k_i is the magnitude of the incident wave vector, a is the range of the potential of an atom of the molecule, and R is the most probable internuclear distance. In applying this model the main aim of the workers has been to obtain a better description of the e-H_2 scattering by starting from reliable differential cross sections for the single (in this case hydrogen) atom. However, due to neglect of the binding effects, the results of IAM calculations differ from the experimental data. The importance of these effects has in fact been observed in the past by Bonham and Iijima.[16] They have used Wang[17] and Weinbaum[18] molecular wave functions in their study of e-H_2 elastic scattering and found that even at a very high incident energy of the projectile, the effect of the distortion of atomic charge distribution reduces the chemical bond of the system. This effect has recently been analyzed by Jain and Khare[19] within the framework of IAM. They have calculated atomic hydrogen differential cross section using the static-field approximation with effective charge[16] $Z = 1.193$ for the atomic orbital e^{-Zr} and including polarization and exchange contributions. This choice of Z, which is the effective nuclear charge for the single hydrogenic orbital on each center, accounts for the effect of molecular binding (valence-bond effects).

The eikonal-Born-series (EBS) method recently developed by Byron and Joachain[20] has been very successful in obtaining accurate electron-hydrogen differential cross sections in the intermediate energy region. This method has been discussed in great detail in a recent review by Byron and Joachain.[21] In view of very good EBS results in the atomic case, we think it is worthwhile to use it along with the molecular-binding correction to investigate the e-H_2 elastic scattering within the IAM model. In Sec. II we outline the IAM model and in Sec. III, we present the results of our calculation and compare them with the recent experimental data.

II. THEORY

In IAM the differential cross section for the e-H_2 scattering is given by[15]

$$\left(\frac{d\sigma}{d\Omega}\right)_{e\text{-}H_2}=2[(|f|^2+|g|^2)+(|f|^2-|g|^2)j_0(qR)], \quad (1)$$

where j_0 is the spherical Bessel function of zeroth order, $\vec{q}=\vec{k}_i-\vec{k}_f$ is the momentum transfer, and $\vec{k}_i$ and $\vec{k}_f$ are, respectively, the momenta of the incident and the scattered electrons. The scattering amplitudes f and g correspond to the direct and exchange scattering by the hydrogen atoms. If the exchange effects are small, Eq. (1) reduces to the form[22]

$$\left(\frac{d\sigma}{d\Omega}\right)_{e\text{-}H_2}=2|f|^2[1+j_0(qR)] . \quad (2)$$

The direct amplitude is evaluated in the EBS approximation

$$f=f_{B1}+f_{B2}+f_{G3}, \quad (3)$$

where f_{B1} is the first Born term, f_{B2} is the second Born term, and f_{G3} the third-order Glauber term. The exchange amplitude is taken into account in the Ochkur[23] approximation. The details of evaluating these have been discussed in a series of papers by Byron and Joachain.[21] The only difference here is that we have used the effective nuclear charge $Z=1.193$ instead of one to account for the molecular-binding effects.

III. RESULTS AND DISCUSSION

We have calculated the elastic differential cross sections (DCS) for e-H_2 scattering using Eqs. (1) and (3) and including exchange in the Ochkur approximation at 75, 100, 200, 400, and 700 eV and compared the results with the recent available absolute experimental measurements. At 75 eV the comparison has been made with the absolute measurements of Srivastava *et al.*[1] The results obtained by using $Z=1$ and $Z=1.193$ have been displayed in Fig. 1. It is clear that the results with $Z=1.193$ compare better with the measurements throughout the angular range. At 100, 200, 400, and 700 eV, we compare our results with the recent absolute measurements of Wingerden *et al.*[2] up to 50° and with the measurements of Fink *et al.*[24] normalized to the measurements of Wingerden *et al.* beyond 50°. It is clear from Figs. 1 and 2 that the present results with $Z=1.193$ agree on the average to within about 5% of the experimental data throughout the angular range considered. The measurements of Fink *et al.*[24] yield somewhat higher value of the cross section in comparison with the measurements of Wingerden *et al.*[2] We have not shown the data points of Lloyd *et al.*[25] since there is hardly any difference between the results of Lloyd *et al.* and Fink *et al.*, particularly in the region of intermediate and large scattering angles, i.e., beyond 60°.

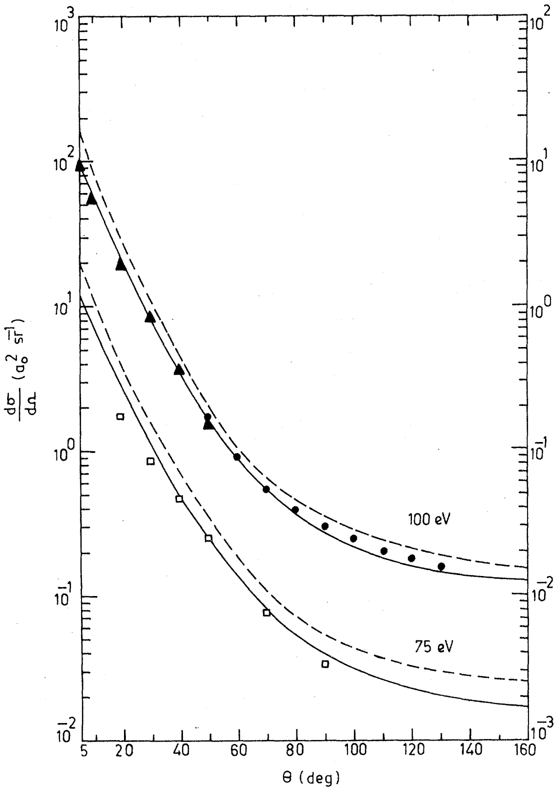

FIG. 1. Differential cross sections for elastic scattering of electrons by molecular hydrogen in its ground state at 75 eV (left-hand scale) and 100 eV (right-hand scale). Present calculations: ——— with $Z=1.193$, ---- with $Z=1$. Experimental data: □, Srivastava *et al.* (Ref. 1); ▲, Wingerden *et al.* (Ref. 2); ●, Fink *et al.* (Ref. 24).

In the energy region $E>200$ eV (Fig. 2) there is practically no difference, as expected, between the results obtained with and without (not shown) exchange effects. However, the difference between the two calculations, one using $Z=1$ and the other using $Z=1.193$, continues to persist even up to 700 eV. This difference in DCS due to the different choices of the atomic orbitals goes on decreasing with the increase in the incident energy. It is observed that a departure of the order of about

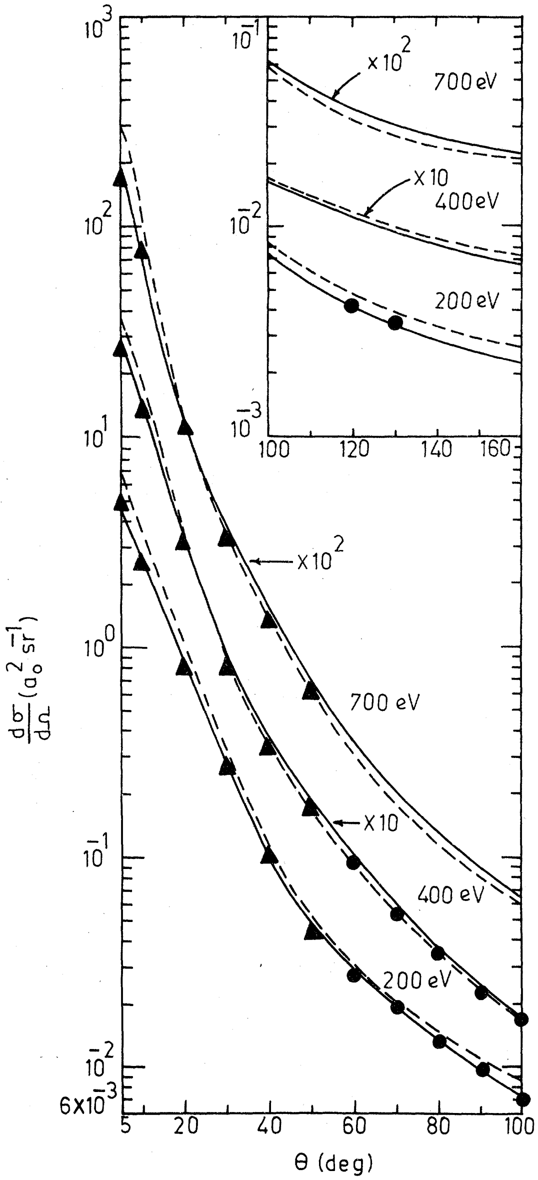

FIG. 2. Same as Fig. 1, but for 200, 400, and 700 eV. Results for 400 eV and 700 eV have been multiplied by factors of 10 and 100, respectively, as shown.

20% in the exponent of the atomic orbital from the free-atom value causes on the average about 30% reduction in the DCS at 100 eV for the atomic hydrogen in the entire angular region. In all the cases the results obtained with $Z = 1.193$ are in better agreement with the experimental data.

Another assessment of our IAM results, with the EBS for atomic scattering and the incorporation of the binding effects is provided by Fig. 3. It displays, at 100 and 200 eV, a comparison of the ratio R_{expt} of the experimental elastic scattering cross section from atomic hydrogen to the experimental one from molecular hydrogen[2,25] with the ratios

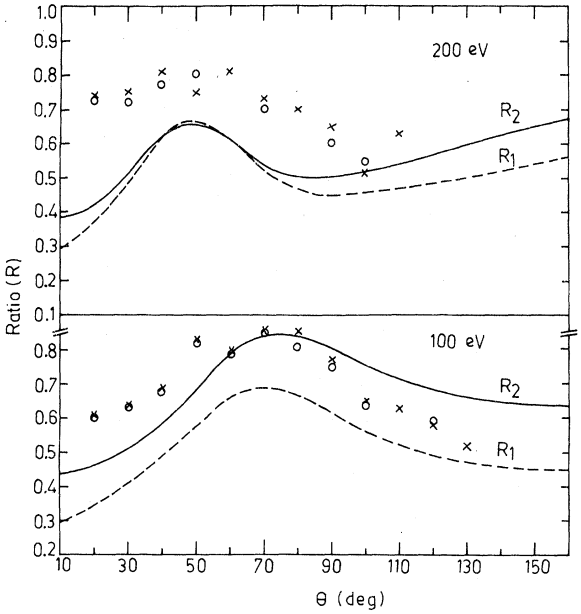

FIG. 3. Ratios (R) of electrons elastically scattered from atomic hydrogen to those elastically scattered from molecular hydrogen at different angles for 100- and 200-eV incident energies. Present calculations: —— with $Z=1.193$, ----- with $Z=1$. Experimental ratios: ×, Lloyd *et al.* (Ref. 25); O, Wingerden *et al.* (Ref. 2).

$$R_1 = \sigma_H(Z=1)/\sigma_{H_2}(Z=1), \tag{4}$$

$$R_2 = \sigma_H(Z=1)/\sigma_{H_2}(Z=1.193) \tag{5}$$

obtained from our results. It is found that the ratio R_{expt} and the theoretical ones R_1 and R_2 exhibit the same general trend. The experimental maxima and minima are more closely reproduced by R_2. The value $Z = 1.193$ shifts the curve substantially and shows that the chemical binding effects are important in this energy range. A similar feature is also observed in a recent study by Jain and Khare.[19] The maximum in the curve goes on shifting towards smaller and smaller scattering angles as the incident energy increases.

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