Elastic positron—hydrogen-molecule scattering using the eikonal approximation

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An eikonal approximation has been used to investigate the elastic positron–hydrogen-molecule scattering problem. The effective potential used here includes the static as well as the polarization potentials. The spherical and the nonspherical parts of both potentials are taken into consideration. The results have been obtained from 0.1 to 50 eV. The results for the elastic cross section are found to be very close to the experimental findings below the positronium-formation threshold. The effect of the polarization potential is found to be appreciable even up to 50 eV.

I. INTRODUCTION

Recently, the positron has become an effective probe for studying atomic and molecular collisions.[1] For theoreticians the problem of collisions induced by positrons is quite interesting since in this case the Pauli exclusion principle does not come into play. Hence the details of the effect of positrons on the atomic or molecular wave function as it penetrates the electron cloud of the target become significant. Secondly, in positron scattering the effects of the undistorted and the distorted targets are opposite in nature, unlike in electron scattering, so that the differential scattering cross section depends sensitively on the degree of cancellation of the two effects. Until recently, the production of low-energy positron beams of reasonable intensity and resolution has been a problem. This problem having been overcome,[2] there are now experimental data for atoms[2] and even molecules.[3] However, the experimental data are still very scarce.

The hydrogen molecule is the simplest molecular system and naturally this system is the first choice for any theoretical investigation. Unfortunately, only a few theoretical attempts[3,4] have been made to study positron–hydrogen-molecule scattering. Lodge *et al.*[4] have investigated the problem in the adiabatic-nuclei approximation. They used the single-center static as well as the spherical and the nonspherical polarization potentials for the hydrogen molecule, and reported results below the first electronic excitation threshold. Baille *et al.*[3] extended their work to include the rotational excitation of the hydrogen molecule as well. Hara[4] has performed similar calculations using the two-center formalism. However, their results are not in very good agreement with the only available experimental data due to Coleman.[3]

In this paper we have applied the eikonal approximation to investigate the elastic scattering of positrons by hydrogen molecules. It has been prompted by our success in describing electron–hydrogen-molecule scattering, in the intermediate energy region, using the same approximation.[5] Moreover, Saha *et al.*[6] have shown that the total cross section for the positron-helium system, calculated through the eikonal approximation, gives a reasonable fit to experimental observations below the threshold for positronium formation. The soundness and applicability of the approximation have been discussed in paper I. In the present work we have considered the short-range static potential in the two-center formalism. The quadrupole tail of the static potential has been replaced by a semiempirical quadrupole potential. The effects of polarization, both spherical and nonspherical, have been accommodated through model potentials. Two such potentials, one used in paper I and the other due to Henry and Lane,[7] have been used. However, we have not considered the positronium channel in our calculations.

II. THEORY

The elastic-scattering amplitude in the eikonal approximation as a function of the scattering angle θ is given by[8]

$$F(\theta, \theta_m, \varphi_m) = \frac{ik_i}{2\pi} \int e^{i\vec{q}\cdot\vec{b}_3}(e^{-i\chi(b_3, \varphi_3, \theta_m, \varphi_m)} - 1)d^2b_3,$$

(1)

where $\vec{q} = \vec{k}_i - \vec{k}_f$, $\vec{k}_i$ and $\vec{k}_f$ being the initial and the final momenta, and $\vec{b}_3$ is the impact-parameter vector. We have taken the polar axis to be in the direction $\vec{k}_i$. θ_m and φ_m are the angles between the polar axis and the molecular axis. $\chi(b_3, \varphi_3, \theta_m, \varphi_m)$ is the phase-shift function,

$$\chi(b_3,\varphi_3,\theta_m,\varphi_m) = \frac{1}{v_i}\int_{-\infty}^{\infty} V_{opt}(\vec{r}_3,\theta_m,\varphi_m)dz_3, \qquad (2)$$

where $\vec{v}_i$ is the velocity of the incident electron, and $\vec{r}_3$ denotes the position vector of the incoming electron relative to the center of mass,

$$\vec{r}_3 = \vec{b}_3 + \hat{k}_i z_3. \qquad (3)$$

In terms of the static potential $V_s(\vec{r}_3,\theta_m,\varphi_m)$ and the polarization potential $V_p(\vec{r}_3,\theta_m,\varphi_m)$, the optical potential $V_{opt}(\vec{r}_3,\theta_m,\varphi_m)$ is given by

$$V_{opt}(\vec{r}_3,\theta_m,\varphi_m) = V_s(\vec{r}_3,\theta_m,\varphi_m) + V_p(\vec{r}_3,\theta_m,\varphi_m), \qquad (4)$$

with

$$V_s(\vec{r}_3,\theta_m,\varphi_m) = -V_s^0(r_3) - [V_s^2(r_3) + V_q^2(r_3)]P_2(\cos\theta_{3m}),$$

$$V_p(\vec{r}_3,\theta_m,\varphi_m) = V_p^0(r_3) + V_p^2(r_3)P_2(\cos\theta_{3m}),$$

where $V_q^2(r_3)$ represents the quadrupole tail of the static potential, $V_p^0(r_3)$ and $V_p^2(r_3)$ are, respectively, the spherical and nonspherical parts of the polarization potential, and θ_{3m} is the angle between $\vec{r}_3$ and the molecular axis, given by

$$\cos\theta_{3m} = \cos\theta_3\cos\theta_m + \sin\theta_3\sin\theta_m\cos(\varphi_3 - \varphi_m). \qquad (5)$$

Explicit expressions for $V_s^0(r_3)$ and $V_s^2(r_3)$ are given in paper I. To perform the averaging over the

molecular orientations, we have selected three perpendicular orientations[9]: $(0,0)$, $(\frac{1}{2}\pi,0)$, and $(\frac{1}{2}\pi,\frac{1}{2}\pi)$. For the orientation $(0,0)$ (i.e., $\theta_m=0$ and $\varphi_m=0$), it is evident from expressions (5) and (4) that the phase-shift function χ [Eq. (2)] does not depend upon φ_3. Hence, for this particular orientation, the φ_3 integration in Eq. (1) can be easily carried out. For the remaining two orientations, $(\frac{1}{2}\pi,0)$ and $(\frac{1}{2}\pi,\frac{1}{2}\pi)$, we insert Eq. (5) (upon substitution of the appropriate set of values for θ_m and φ_m) and Eq. (4) in Eq. (2), and a simple calculation gives

$$\chi(b_3,\varphi_3,\tfrac{1}{2}\pi,0) = A(\vec{b}_3) + B(\vec{b}_3)\cos2\varphi_3, \qquad (6a)$$

$$\chi(b_3,\varphi_3,\tfrac{1}{2}\pi,\tfrac{1}{2}\pi) = A(\vec{b}_3) - B(\vec{b}_3)\cos2\varphi_3, \qquad (6b)$$

with

$$A(\vec{b}_3) = \frac{2}{v_i}\int_0^{\infty}\{-V_s^0(r_3) + V_p^0(r_3) + \tfrac{1}{4}(3\sin^2\theta_3 - 2)$$
$$\times[V_p^2(r_3) - V_s^2(r_3) - V_q^2(r_3)]\}\,dz_3,$$

$$B(\vec{b}_3) = \frac{3}{2v_i}\int_0^{\infty}\sin^2\theta_3[V_p^2(r_3) - V_s^2(r_3) - V_q^2(r_3)]dz_3.$$

Using Eqs. (1) and (6), expanding $\exp[i(qb_3\cos\varphi_3 \mp B\cos2\varphi_3)]$ in terms of Bessel functions, and carrying out the integration over φ_3, we obtain

$$F(\theta,\theta_m,\varphi_m) = -ik_i\int\left[\left(J_0(qb_3)J_0(B) + 2\sum_{m=1}^{\infty}(\pm)^m J_{2m}(qb_3)J_m(B)\right)e^{-iA} - J_0(qb_3)\right]b_3\,db_3, \qquad (7)$$

where the J_n's are the Bessel functions of order n, and the plus and minus signs in the summation are for the orientations $(\frac{1}{2}\pi,0)$ and $(\frac{1}{2}\pi,\frac{1}{2}\pi)$, respectively.

Finally, averaged differential cross sections $\langle I(\theta)\rangle$ and the averaged total cross sections $\langle\sigma\rangle$ are calculated from the expressions

$$\langle I(\theta)\rangle = \tfrac{1}{3}[\,|F(\theta,0,0)|^2 + |F(\theta,\tfrac{1}{2}\pi,0)|^2 + |F(\theta,\tfrac{1}{2}\pi,\tfrac{1}{2}\pi)|^2\,],$$

$$\langle\sigma(\theta)\rangle = \tfrac{1}{3}[\sigma(0,0) + \sigma(\tfrac{1}{2}\pi,0) + \sigma(\tfrac{1}{2}\pi,\tfrac{1}{2}\pi)]. \qquad (8)$$

It should be noted that the averaged cross sections defined by the relations (8) are essentially the sum of the elastic and the rotational excitation cross sections.

III. RESULTS AND DISCUSSION

The expressions A and B in Eqs. (6) and the integrand in Eq. (7) have been solved numerically using the Gaussian quadrature method. The convergence of the series involving Bessel functions in the scattering amplitude has been tested. It was found that only three terms are sufficient for accurate results.

In the present investigation the following forms are used for $V_q^2(r_3)$, $V_p^0(r_3)$ and $V_p^2(r_3)$:

Model A.

$$V_q^2(r_3) = -Qr_3^3(r_3^2 + R_0^2)^{-3}, \quad V_p^0(r_3) = -\tfrac{1}{2}\alpha_0(r_3^2 + R_0^2)^{-2},$$

$$V_p^2(r_3) = -\tfrac{1}{2}\alpha_2 r_3^2(r_3^2 + R_0^2)^{-3},$$

where the cutoff parameter R_0 is taken to be equal[10] to $1.6a_0$,

Model B.

$$V_q^2(r_3) = -Qr_3^{-3}(1 - e^{-(r_3/r_0)^6}),$$

$$V_p^0(r_3) = -\tfrac{1}{2}\alpha_0(r_3^2 + R_1^2)^{-2}(1 - e^{-(r_3/R_a)^3}),$$

$$V_p^2(r_3) = \begin{cases} -\tfrac{1}{2}\alpha_2(r_3^2 - R_2^2)^{-2}(1 - e^{-(r_3/R_b)^4}), & r_3 \geq 0.5a_0 \\ 0, & r_3 < 0.5a_0, \end{cases}$$

where $R_1 = 1.22a_0$, $R_2 = 0.1a_0$, $R_a = 1.7a_0$, $R_b = 2.0a_0$, and $r_0 = 1.8a_0$. In both models A and B above, the quadrupole moment[11] Q, the spherical part of the static dipole polarizability[12] α_0, and the nonspherical part of the static dipole polarizabilty[12] α_2, are
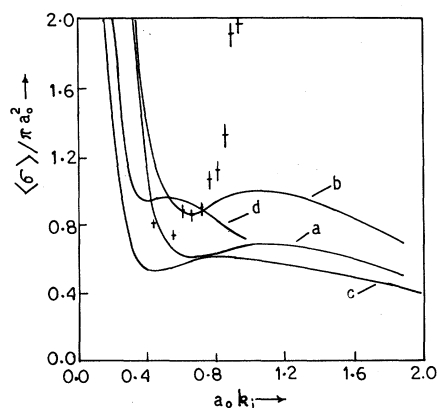
FIG. 1. Averaged total cross section for positrons scattered by hydrogen molecules. (a) Results with potential A; (b) results with potential B; (c) results of Baille et $al.$ (Ref. 3); and (d) results of Hara (Ref. 4). The experimental points are the total cross sections (sum of the elastic and inelastic cross sections) due to Coleman (Ref. 3).

FIG. 2. Momentum-transfer cross sections. Labeling of the curves is the same as in Fig. 1.

taken to be $0.490e^2a_0^2$, $5.1786e^2a_0^3$, and $1.2019e^2a_0^3$, respectively. Model A has been considered in paper I with a less-accurate value[13] of $0.464e^2a_0^2$ for Q. The analytic form of model B was given by Henry and Lane.[7] For the short-range static potential, we have chosen the ground-state wave function of the hydrogen molecule as used by Hara.[10] In this respect, we would like to mention that at positron energies greater than 10.0 eV there is very little to choose among the short-range potentials[3] derived from different molecular wave functions found in the literature.

In Fig. 1, curves a and b represent the averaged total cross sections computed with the potentials A and B, respectively. Curve c gives the results of Baille et $al,$[3] while curve d shows those of Hara.[4] Baille et $al.$ used Wang's[14] wave function; Hara, on the other hand, used the five-term self-consistent molecular orbital due to Kolos and Roothaan[13] for the ground-state wave function of the hydrogen molecule. However, both the above authors con-
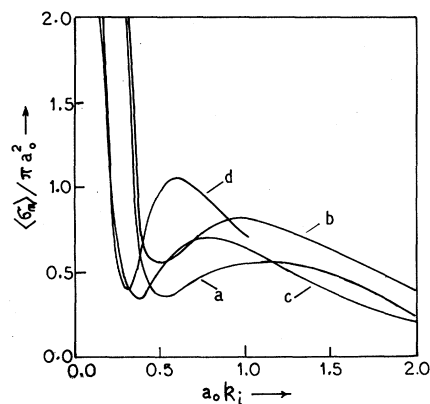
sidered the polarization potentials as given in model B. The experimental observations for the total cross sections of Coleman[3] have also been plotted for comparison. The shape of our curves a and b are more or less the same as that obtained by Baille et $al.$ and Hara. However, it is interesting to note from our two curves that the long-range potentials have considerable effects even for positron energies as high as 50.0 eV. This is in contradiction to the observations made by Baille et $al.$ Furthermore, the positions of the minima for the total cross sections have been shifted toward higher energies compared to those found by earlier theoretical workers. Below the threshold for positron formation ($k_i = 0.8$ a_0^{-1}), our results with the Henry and Lane polarization potential seem to give better fits to the experimental observations than other theoretical results. Above the threshold, our curves, like those of Baille et $al.$ and Hara, differ appreciably from the experimental curve. This is due to the fact that the observed cross sections are the sum of the elastic cross sections and the inelastic cross sections which are energetically permissible.

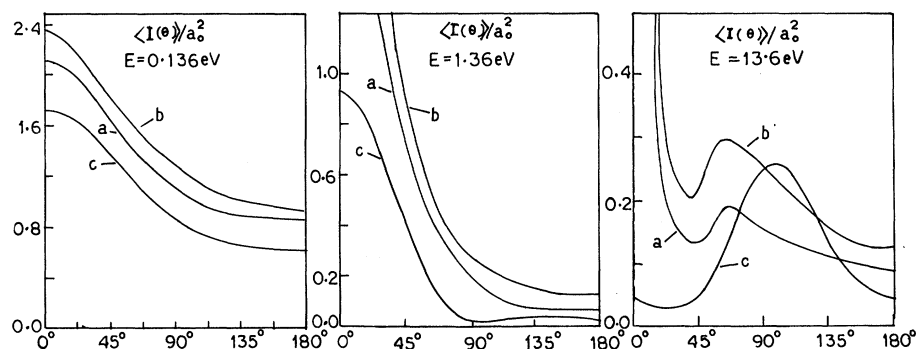Figure 2 gives the momentum-transfer cross sections. The labeling of the curves is identical

FIG. 3. Differential scattering cross sections at 0.136, 1.36, and 13.6 eV. The labeling of the curves is the same as in Fig. 1.

with that in Fig. 1. The qualitative features of our curves, as well as their relative behavior with respect to those due to Baille *et al.* and Hara, are the same as have been observed in the case of the averaged total cross section.

Figure 3 represents the averaged differential cross section plotted against scattering angle at incident positron energies of 0.136, 1.36, and 13.6 eV. A comparison is made with the theoretical results obtained earlier by Baille *et al.* (curves labeled *c*) at the similar energies. In the absence of any experimental data it is very difficult to conclude which of the two theoretical calculations, if any, gives proper angular dependence of the differential cross sections.

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