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Scattering of low- to intermediate-energy positrons from molecular hydrogen

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Using a complex model potential, we have calculated the total, integrated elastic, momentum transfer, absorption, and differential cross sections for positrons scattered from molecular hydrogen. The widely available software package GAUSSIAN is used to generate the radial electronic charge density of the molecule which is used to produce the interaction potentials. The quasifree absorption potential, previously developed and used for positron-atom scattering, is extended to positron scattering from molecular targets. It is shown that this model potential approach produces accurate results even into the low-energy regime.

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I. INTRODUCTION

The scattering of positrons from atomic and molecular targets continues to be an area of active investigation in both experimental and theoretical collision studies. As the ability to produce controlled positron beams continues to be refined and such beams become available in more laboratories, a larger variety of positron-gas systems are being studied experimentally with improving results. The state of theoretical calculations in this area can be divided into four impact-energy (E) regimes. These are very-low-energy ($E \lesssim 0.1$ eV), low-energy ($0.1 \text{ eV} < E < E_{Ps}$) where E_{Ps} is the threshold for positronium formation, intermediate-energy ($E_{Ps} < E < 1000$ eV), and high-energy ($E > 1000$ eV) regimes. Low- and very-low-energy calculations are typically performed at the *ab initio* level rather than with model potentials partly because in this energy regime one does not have to take into account several inelastic channels which are complicated to handle exactly [1]. Furthermore, calculations using model potentials have performed only moderately well or even poorly at lower energies because the projectile spends more time near the target, causing the results to be more sensitive to the details of the interaction. However, the reverse is true at intermediate energies. Because of the predominance of many inelastic processes, particularly positronium formation, electronic excitation, and ionization, calculations at the *ab initio* level become extremely difficult. Also, in this energy regime, high-energy approximations, such as Born-Bethe theory, cannot yet be trusted.

We will show in this paper that use of complex model potentials can produce accurate intermediate-energy results even for positron-molecule scattering, as they have for the scattering of both electrons and positrons in atomic gases [2]. However, despite the success of this approach for atomic targets at intermediate energies, use of model potentials runs into difficulties that limit their applicability to molecular targets. First, generation of molecular charge densities is substantially more difficult than generation of atomic charge densities; therefore, many of the previous calculations for molecules employed the independent-atom model [3,4] in

which the scattering process from a molecule is treated by combining the scattering processes from the individual atoms that make up the molecule. This approach necessarily breaks down at lower energies, depending on the geometry of the molecule, because when the de Broglie wavelength of the incident positrons is of the order of the size of the bond lengths between the atoms in the molecule they cannot possibly “see” the molecule as a set of individual atoms. Furthermore, model potentials that assume that the electrons of the target atom can be treated as a free-electron gas are not accurate for atomic hydrogen containing only one electron. Therefore, in this case, the independent-atom approximation for molecules containing the hydrogen atom is not expected to be very good. Second, no good model absorption potential specifically designed for positron scattering has existed until only recently [5]. Having no viable option, previous positron-molecule collision calculations, using the model potential approach, were carried out either using model absorption potentials that were designed for electron scattering or modifying those electron absorption potentials in purely empirical ways [6].

Because of the issues just described and despite the fact that electron scattering from molecular hydrogen is a well-studied problem, to the best of our knowledge, there are only three published calculations of total cross sections for positron scattering from H_2 at intermediate impact energies [4,6,7]. In this paper, we study positron- H_2 scattering in a way that addresses both of the difficulties discussed in the previous paragraph. First, as will be discussed in more detail below, the present calculations use *molecular* charge densities to calculate the model potentials. By doing so, we bypass all of the issues concerning use of the independent-atom model. As a result, not only are we able to obtain good cross-section results for scattering from H_2 at intermediate impact energies, but surprisingly, our results are also quite good well into the low-energy regime. Second, we demonstrate the successful extension of the quasifree model absorption potential developed for positron-atom scattering to the scattering of positrons from molecular targets. Using a more appropriate positron absorption potential gives better overall results with much less need for empiricism.

This paper is organized into four parts. Following the present introductory remarks, we explain in Sec. II the theoretical framework for our calculations. First, in Sec. II A, we describe the interaction potentials used and discuss the relevant issues concerning the extension of the quasifree model to molecular targets. Section II B is devoted to a discussion of how we generated the molecular charge densities (and static potential) of the target using the commercially available software GAUSSIAN [8]. The details of how these calculations were performed are then given in Sec. II C. In Sec. III, we present our results for total, integrated elastic, momentum transfer, absorption, and differential cross sections from low to intermediate impact energies. Finally, we make some concluding remarks in Sec. IV. Unless otherwise specified, we use atomic units ($\hbar = e = m_e = 1$) throughout this paper.

II. THEORY

A. Interaction potentials

In the present calculations we model the positron-target system by a complex interaction potential $V(r)$, which consists of three parts. These parts are the static potential $V_{st}(r)$, the polarization potential $V_{pol}(r)$, and the absorption potential $V_{abs}(r)$, such that

$$V(r) = V_{st}(r) + V_{pol}(r) + iV_{abs}(r). \quad (1)$$

Each interaction potential is determined by the radially averaged electron charge density of the target molecule, $\rho(r)$, which is obtained using the method discussed in Sec. II B below. The static potential is given by

$$V_{st}(r) = \left\langle \frac{Z}{|\mathbf{r} - \mathbf{b}|} \right\rangle - 4\pi \int_0^\infty \frac{\rho(r')}{r_>} r'^2 dr', \quad (2)$$

where Z is the number of protons of the target ($Z=2$ in the present case), $\mathbf{b}$ is a vector that points from the center of the molecule to a nucleus, and $r_>$ is the larger of r and r' .

Following De Fazio *et al.* [9], the polarization interaction is given, in terms of the electron density, as

$$V_{pol}(r) = -D_4(r) \frac{\alpha_d}{2r^4} - D_6(r) \frac{\alpha_q}{2r^6} - D_8(r) \frac{\alpha_o}{2r^8}, \quad (3)$$

where α_d , α_q , and α_o are the dipole, quadrupole, and octopole polarizabilities of the target molecule, respectively. In Table I, the values of the polarizabilities and their sources, as well as other parameters used in these calculations, are provided. In Eq. (3) the functions $D_{2n}(r)$ are damping functions whose purpose is to guarantee that $V_{pol} \rightarrow 0$ as $r \rightarrow 0$; these functions are given by

$$D_{2n}(r) = \frac{\int_0^r \rho(r') r'^{2n} dr'}{\int_0^\infty \rho(r') r'^{2n} dr'}. \quad (4)$$

Note that $D_{2n}(r) \rightarrow 1$ as $r \rightarrow \infty$.

TABLE I. The values of various parameters used in this work and their sources.

Quantity	Value	Source
Bond length	$1.401a_0$	Ref. [10]
α_d	$5.18a_0^3$	Ref. [11]
α_q	$7.88a_0^5$	Ref. [11]
α_o	$3.85a_0^7$	Ref. [12]
E_{Ps}	8.63 eV	This work
E_{diss}	4.52 eV	Ref. [13]
Δ	6.57 eV	This work

The absorption potential used in this work is an extension of the quasifree model for positron-atom scattering that was given in our previous work [5]. The form of this interaction potential is

$$V_{abs} = -\frac{1}{2} \rho \bar{\sigma}_b v, \quad (5)$$

where v is the local speed of the incident positron and $\bar{\sigma}_b$ is the average cross section for binary collisions between the positron and electrons of the target molecule. For positron scattering the binary collision cross section $\bar{\sigma}_b$ of Eq. (5) is given by [5,14]

$$\bar{\sigma}_b = \frac{\pi}{(\epsilon E_F)^2} \begin{cases} f(0), & \epsilon^2 - \delta \leq 0, \\ f(\sqrt{\epsilon^2 - \delta}), & 0 < \epsilon^2 - \delta \leq 1, \\ f(1), & 1 < \epsilon^2 - \delta, \end{cases} \quad (6)$$

where

$$f(x) = \frac{2}{\delta} x^3 + 6x + 3\epsilon \ln \left(\frac{\epsilon - x}{\epsilon + x} \right) \quad (7)$$

and

$$\delta = \frac{\Delta}{E_F}, \quad \epsilon = \sqrt{\frac{E}{E_F}}. \quad (8)$$

The quantities $E_F = \hbar^2 k_F^2 / 2m$ and $k_F = (3\pi^2 \rho)^{1/3}$ are the Fermi energy and the Fermi wave number (or momentum) corresponding to the target radial electron density ρ .

One of the important aspects of the present study is to formulate an extension of this model interaction potential to the case of molecular targets. Besides the electron density, the only other target-dependent quantity used in the absorption potential is the energy gap Δ . Within the quasifree binary collision model, Δ plays a dual role as both (a) the energy gap between the initial state and the final energy state of the originally bound electron and (b) the lowest-energy threshold for inelastic processes. For *electron*-atom scattering, these two roles are consistent with each other if Δ is set equal to the excitation threshold (E_{exc}) of the target atom. However, for *positron*-atom scattering the formation of positronium introduces another inelastic threshold which can be lower than the threshold for excitation. As an example, for positron scattering from alkali-metal atoms the threshold for positronium formation (E_{Ps}) is zero [14]. In the quasifree

model the absorption cross section diverges as $\Delta \rightarrow 0$. Thus, for many positron-atom systems one has to find a reasonable choice for Δ that will be sufficiently close to the true inelastic threshold so as to minimize the absence of low-energy absorption in the calculations, but not so small that cross sections begin to diverge. Our previous investigations of positron-atom scattering [5,14] have suggested that the appropriate choice for Δ is to set it equal to the lowest *nonzero* inelastic threshold.

In the case of positron scattering from molecular targets the inelastic threshold is effectively always open because of rovibrational excitation thresholds of the target molecules. Besides the rovibrational modes, the possibility of the dissociation of the molecule adds an additional inelastic process with threshold E_{diss} . In the derivation of the quasifree model, the only inelastic processes that are considered are those that can result from a binary collision between the incident positron and a target electron: namely, electronic excitation and ionization by positron impact and positronium formation. Obviously, rovibrational excitation and dissociative processes are not part of the binary collision. This would most directly suggest that the energy gap be set equal to E_{Ps} . However, the above considerations must be balanced against the other role of Δ as the threshold at which *any* inelastic scattering occurs. Therefore, in the present study we have taken Δ to equal the average of E_{Ps} and the threshold of dissociation,

$$\Delta = \frac{1}{2}(E_{Ps} + E_{diss}). \quad (9)$$

B. Electronic charge density

In the present calculations, the electronic charge density in the hydrogen molecule is calculated with GAUSSIAN [8] using the full configuration interaction method with both single and double substitutions [15]. This code is now fast and readily available. Using the CUBE=DENSITY command in GAUSSIAN, we first generated the electronic charge density $\rho(\mathbf{r})$ on a sufficiently large three-dimensional cubic grid to cover the needed range of the calculation with a step size of $0.04a_0$ in each direction. By interpolation [16], we then obtained values of $\rho(\mathbf{r})$ over the surface of a sphere of radius r centered upon the geometric center of the molecule; Fig. 1 illustrates this procedure. For visual clarity, Fig. 1 only shows points on a plane; in fact, the symmetry of H_2 only requires generation of $\rho(\mathbf{r})$ over one quadrant of such a plane. The value of the radial charge density at r is then calculated by numerical integration:

$$\rho(r) = \frac{1}{4\pi} \int_0^{2\pi} d\phi \int_0^\pi \rho(\mathbf{r}) \sin \theta d\theta. \quad (10)$$

In this manner, values of $\rho(r)$ are calculated for every value of r needed in the integration of the radial Schrödinger equation to be discussed in the next subsection.

C. Calculations

For the spherically symmetric potential of Eq. (1) the scattering process is symmetric about the direction of the

FIG. 1. (Color online) Points on a plane of the configuration used to generate the radial electron charge density of H_2 . The two small circles present the protons in the hydrogen molecule. The large circle represents points on the surface of a sphere of radius r . The dots represent points at which $\rho(\mathbf{r})$ is determined by GAUSSIAN and these values are used to calculate $\rho(r)$ at 40 000 points on the sphere by interpolation. The radial charge density is then determined using Eq. (10).

incident positron. The solution $u_\ell(r)$, therefore, is generated by the radial Schrödinger equation (in atomic units)

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + 2[E - V(r)] \right] u_\ell(r) = 0, \quad (11)$$

where $E = \hbar^2 k^2 / 2m$ is the impact energy of the collision and ℓ is the angular momentum quantum number which also represents the order of the partial wave [17].

Equation (11) is integrated out to a distance of 10 bohr radii from the center of the molecule via the Numerov technique [18]. The first 51 ($\ell_{\max} = 50$) phase shifts are calculated exactly by comparing u_ℓ , the radial wave function of the target plus positron system, at two adjacent points r and $r_+ = r + h$:

$$\tan(\delta_\ell) = \frac{r_+ u_\ell(r) j_\ell(kr_+) - r u_\ell(r_+) j_\ell(kr)}{r u_\ell(r_+) n_\ell(kr) - r_+ u_\ell(r) n_\ell(kr_+)}, \quad (12)$$

where h is the step size ($h = 0.00075a_0$) of the calculation, and j_ℓ and n_ℓ are the spherical Bessel and Neumann functions evaluated using the algorithm of Gillman and Fiebig [19].

The scattering amplitude is obtained from the phase shifts by

$$f(\theta) = \frac{1}{2ik} \sum_{\ell=0}^{\ell_{\max}} (2\ell+1) [\exp(2i\delta_\ell) - 1] P_\ell(\cos \theta) + f_4(\theta) + f_6(\theta) + f_8(\theta). \quad (13)$$

The functions f_4 , f_6 , and f_8 are the higher- ℓ contributions from the Born phase shifts for the dipole ($\sim 1/r^4$), quadrupole ($\sim 1/r^6$), and octopole ($1/r^8$) parts of the asymptotic polarization potential, respectively. The closed-form expressions for these functions are [20]

$$f_4(\theta) = -\pi k \alpha_d \left(\frac{\sin(\theta/2)}{2} + \sum_{\ell=0}^{\ell_{\max}} \frac{P_{\ell}(\cos \theta)}{(2\ell+3)(2\ell-1)} \right), \quad (14)$$

$$f_6(\theta) = -3\pi k^3 \alpha_q \left(-\frac{\sin^3(\theta/2)}{18} + \sum_{\ell=0}^{\ell_{\max}} \frac{P_{\ell}(\cos \theta)}{(2\ell+5)(2\ell+3)(2\ell-1)(2\ell-3)} \right), \quad (15)$$

and

$$f_8(\theta) = -10\pi k^5 \alpha_o \left(\frac{\sin^5(\theta/2)}{450} + \sum_{\ell=0}^{\ell_{\max}} \frac{P_{\ell}(\cos \theta)}{(2\ell+7)(2\ell+5)(2\ell+3)(2\ell-1)(2\ell-3)(2\ell-5)} \right). \quad (16)$$

Once the scattering amplitude is known, the various cross sections can be determined. The total cross sections, which include both elastic and inelastic scattering, are obtained from the forward scattering amplitude by

$$\sigma_{tot} = \frac{4\pi}{k} \text{Im}[f(0)]. \quad (17)$$

The cross sections for elastic scattering are found by integrating the scattering amplitude

$$\sigma_{elas} = 2\pi \int_0^{\pi} |f(\theta)|^2 \sin \theta d\theta. \quad (18)$$

The absorption cross sections (the cross section for inelastic scattering) are determined by the difference

$$\sigma_{abs} = \sigma_{tot} - \sigma_{elas}. \quad (19)$$

The differential cross sections for the angular distribution of the scattered positrons are given by

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2. \quad (20)$$

Finally, the momentum transfer cross sections are found using

$$\sigma_{mom} = 2\pi \int_0^{\pi} (1 - \cos \theta) |f(\theta)|^2 \sin \theta d\theta. \quad (21)$$

III. RESULTS

Figure 2 shows the present results of the total cross sections for the scattering of positrons by H_2 compared with several experimental measurements and other theoretical calculations. The experimental measurements of the total cross sections have been made by several groups. In particular, the positron impact energies ranging from 1 to 500 eV are covered by Hoffmann *et al.* [21], from 1.5 to 301 eV by Zhou *et al.* [22], from 14 to 600 eV by Charlton *et al.* [23], from 2.15 to 20.84 eV by Charlton *et al.* [24], and from 8 to 400 eV by Deuring *et al.* [25]. To the best of our knowledge, no other theoretical calculations of total cross sections have been able to predict the structure in this curve over as

large a range of positron energies as in the present calculations. These structures extending across the low- to intermediate-energy ranges are reasonably reproduced. The present results correctly predict the local minimum in the low-energy regime of 4–9 eV and the local maximum in the intermediate-energy regime near 25 eV. In the range of around 9 eV–11 eV the present results stray outside of the error bars, overestimating the experimental values. However, in this connection, it should be noted that cross-section measurements are expected to be affected by the inability to discriminate projectiles elastically scattered through small forward angles. This lack of discrimination in a transmission experiment results in the measurement of total cross sections that are lower than the actual values. The two experimental aspects leading to this error are the size of the exit aperture of the scattering cell and the use of a retarding potential grid, located behind the scattering cell, that the transmitted projectiles need to overcome [21]. To get the best indication of the quality of the present calculations, the error bars shown in Fig. 2 are the “maximum errors” as reported in Refs. [21,22] and not just the statistical uncertainties. Error bars for the other experimental data are not shown as the errors reported were not of comparable detail.

FIG. 2. (Color online) The present total cross sections for the scattering of low- to intermediate-energy positrons by H_2 compared with several experimental measurements and other theoretical calculations. The error bars are the “maximum error” as reported by the relevant authors.

FIG. 3. (Color online) The present absorption cross sections for the scattering of positrons by H_2 compared with experimental results. The experimental results and the associated uncertainties are a summation of partial cross section measurements from different experiments. The squares are for positronium formation plus first ionization by Fromme *et al.* [29]; the circles are for positronium formation by Zhou *et al.* [22] plus first ionization by Ashley *et al.* [30] plus excitation to the $B^1\Sigma$ state by Sullivan *et al.* [31].

On the theoretical side, very few calculations of the total cross sections for the scattering of positrons by molecular hydrogen have been done. In the low-energy regime (below the positronium formation threshold of 8.63 eV), calculations of positron scattering by H_2 were done by Danby and Tennyson [26] using the *R*-matrix method, by Armour *et al.* [27] using the generalized Kohn method, and by Gibson [28]

using the distributed positron model. Contributions to the total cross section from partial cross sections of different symmetries, each symmetry corresponding to an irreducible representation of the molecular point group, were included. In their calculations, Armour *et al.* included four symmetries, Danby and Tennyson included six symmetries, and Gibson included ten symmetries of the H_2 molecule. The calculated total cross sections of Armour *et al.* and of Danby and Tennyson underestimated the experimental cross sections. This underestimation can be attributed to the limitations of the trial function used in the Kohn method and to the inadequacy of polarization in the *R*-matrix method. The elastic cross sections calculated by Gibson agreed reasonably well with the corresponding experimental data below the threshold for positronium formation. In the intermediate-energy range (from positronium formation threshold to about 1000 eV), positron-hydrogen molecule scattering cross sections have been calculated using a local spherical complex potential [6], using the additivity rule of the independent-atom model [4] and using the coupled-channel calculations [7]. None of these calculations are correctly able to predict the rise in the total cross section values as the positron energy is decreased below the positronium formation threshold. The reason for this shortcoming in the work of Baluja and Jain [6] may be the use of a variation of *electron* absorption potential for *positron* scattering. The absorption potential used in the present work, Eqs. (5)–(8), is developed specifically for positron scattering. Raizada and Baluja [4], in addition, use the approximation that molecular hydrogen can be treated as a set of two independent atoms which clearly breaks down at

TABLE II. Differential, integrated elastic, and momentum transfer cross sections (in atomic units) at selected intermediate impact energies. The notation $a [b]$ means $a \times 10^b$.

Angle (deg)	50 eV	100 eV	200 eV	300 eV	400 eV	500 eV
0	5.88 [0]	5.23 [0]	3.51 [0]	2.92 [0]	2.38 [0]	2.26 [0]
10	4.40 [0]	3.44 [0]	2.00 [0]	1.69 [0]	1.32 [0]	1.06 [0]
20	2.62 [0]	1.69 [0]	7.63 [−1]	6.01 [−1]	3.92 [−1]	2.88 [−1]
30	1.38 [0]	6.67 [−1]	1.99 [−1]	1.57 [−1]	9.85 [−2]	6.51 [−2]
40	6.09 [−1]	2.04 [−1]	3.79 [−2]	5.22 [−2]	3.72 [−2]	2.96 [−2]
50	2.20 [−1]	5.04 [−2]	5.68 [−3]	2.98 [−2]	2.57 [−2]	2.28 [−2]
60	6.43 [−2]	1.05 [−2]	8.76 [−4]	2.41 [−2]	2.27 [−2]	2.13 [−2]
70	1.44 [−2]	2.42 [−3]	4.03 [−4]	2.19 [−2]	2.16 [−2]	2.10 [−2]
80	2.68 [−3]	1.14 [−3]	3.41 [−4]	2.08 [−2]	2.13 [−2]	2.13 [−2]
90	1.22 [−3]	8.81 [−4]	2.67 [−4]	2.03 [−2]	2.14 [−2]	2.18 [−2]
100	1.40 [−3]	6.88 [−4]	2.02 [−4]	2.01 [−2]	2.17 [−2]	2.23 [−2]
110	1.34 [−3]	5.00 [−4]	1.52 [−4]	2.01 [−2]	2.20 [−2]	2.26 [−2]
120	1.10 [−3]	3.65 [−4]	1.12 [−4]	2.02 [−2]	2.23 [−2]	2.29 [−2]
130	8.23 [−4]	2.69 [−4]	8.55 [−5]	2.03 [−2]	2.26 [−2]	2.30 [−2]
140	5.67 [−4]	2.07 [−4]	6.92 [−5]	2.04 [−2]	2.27 [−2]	2.30 [−2]
150	3.92 [−4]	1.75 [−4]	5.71 [−5]	2.06 [−2]	2.29 [−2]	2.31 [−2]
160	2.93 [−4]	1.60 [−4]	4.85 [−5]	2.07 [−2]	2.29 [−2]	2.30 [−2]
170	2.44 [−4]	1.48 [−4]	4.42 [−5]	2.07 [−2]	2.30 [−2]	2.30 [−2]
180	2.17 [−4]	1.35 [−4]	4.06 [−5]	2.07 [−2]	2.30 [−2]	2.31 [−2]
σ_{elas}	3.37 [0]	1.94 [0]	8.80 [−1]	9.59 [−1]	7.64 [−1]	6.41 [−1]
σ_{mom}	3.92 [−1]	1.57 [−1]	4.79 [−2]	2.95 [−1]	3.01 [−1]	2.96 [−1]

FIG. 4. (Color online) The present low-energy differential cross sections (solid line) for the scattering of positrons by H_2 compared with the *ab initio* calculations of Lino *et al.* [1] (dashed line). The positron energy ranges from 1.36 eV to 6.9 eV.

low impact energies at which the positron de Broglie wavelength becomes comparable to the molecular bond length. In the work of Biswas *et al.* [7], the positronium formation cross sections agree well with the measured data but the low-energy total scattering cross sections deviate significantly from the measured cross sections due to absence of long-range polarization effects.

In Fig. 3, we show our absorption (or total inelastic) cross-section results compared to estimates based on various measurements. The experimental points are a combination of different experiments for measurements of inelastic processes made at common, or nearly common, impact energies. The inelastic processes in H_2 for which experimental cross sections are available include ionization by positron impact [29,30], excitation by positron impact [31], and positronium formation [22,29]. The present results show good agreement with the experimental cross sections in the region of overlap. The fact that our results overestimate the experimental points at every energy is to be expected because the experimental data do not include all partial cross sections. In particular, the ionization cross sections are only for the first ionization of H_2 , the excitation cross sections only account for excitations to the $B^1\Sigma$ state, and there are no experimental values added for other excitation processes (although they are expected to be small at these energies). As one would expect, the absorption cross sections are quite sensitive to the absorption potential; the fact that we have such good agreement for the total inelastic cross section confirms the applicability of the quasifree model for molecular targets.

Our demonstration, in Figs. 2 and 3, that the present total and absorption cross sections are good also confirms the quality of our integrated elastic cross sections at intermediate energies. In Table II, we provide the values of our differential, integrated elastic, and momentum transfer cross sections at intermediate impact energies. As mentioned in Sec. I, we note that the present model potential results are reliable well into the low-energy regime. This is confirmed partly by the quality of the low-energy total cross sections in Fig. 2. However, a much more stringent test is made by differential cross sections. To date, there are no measurements of differential cross sections for positron scattering from H_2 . Thus, in Fig. 4, we compare our present low-energy differential cross sections against the *ab initio* calculations of Lino *et al.* using the Schwinger multichannel method [1]. Despite the fact that, at small scattering angles, our calculations show a slight dip, the present results show reasonable agreement with their calculations at every energy for which a comparison has been made.

IV. CONCLUSIONS

In the present calculations, we have presented calculations of various cross sections for positrons scattered from H_2 . Using a single model-potential approach, we have presented accurate total cross sections through both the low- and intermediate-energy regimes, correctly matching the detailed structure in this curve. To the best of our knowledge, this is the first theoretical calculation to cover this extended positron energy range. We have also demonstrated that, with a very minor modification, the positron quasifree absorption potential can perform equally well, or better, for scattering in molecular gases as it has in atomic gases. Furthermore, we have introduced a simple scheme for obtaining accurate molecular charge densities using GAUSSIAN that can be applied to almost any molecule bypassing the need for the independent-atom model.

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