Ionization of atomic hydrogen by slow protons

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A theoretical model is suggested for the calculation of ionization cross sections in heavy particle collisions in the impact parameter formalism, considering the influence of coupling with the important bound states in direct as well as in rearrangement channels in a two-centered atomic state expansion. We solve the relevant time-dependent Schrödinger equation by a variational method in the two-state approximation. In the present paper, we calculate total ionization cross sections of a hydrogen atom by 5–300-keV proton impact. The results thus obtained are compared with the measured data and existing theoretical findings. [S1050-2947(98)04112-2]

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I. INTRODUCTION

One of the many diverse reactions which may take place as a consequence of collisions between a bare ion and an atom is that of single ionization, where an electron initially in a bound state is ejected to the continuum with a well-defined asymptotic value of the momentum. The simplest ionization process is the ejection of an electron from a hydrogen atom during a collision with a proton. Unlike electron impact collisions, there is no exchange interaction of target and projectile to complicate the picture, and the projectile transfers a small fraction of its momentum and energy during the collision. Furthermore, the proton carries no electron to add complications to the interaction. In spite of its simplicity, the reaction of the $H^+ + H$ system is still a three-body system in its final state, and hence does not allow any analytical solution. One has to use approximations to solve the dynamical problem.

From a theoretical point of view, the main difficulty is the representation of the final electronic state, where the emitted electron travels in the presence of two Coulomb potentials (projectile and residual target). Due to the long-range nature of the Coulomb potential, the free-particle state cannot be represented only by a plane wave. An exact solution for the problem is difficult to obtain. However, its exact asymptotic form can be found (cf. Refs. [1,2]).

To consider ionization, we should note that, in addition to ionization, there are always possibilities of elastic scattering, excitation, and charge transfer which may influence the ionization cross section, especially in the low-energy region. A knowledge of ionization cross sections is of importance in many applications such as in fusion reactors, radiation damage in biological matters, energy loss of heavy ions in solid targets, etc.

The first detailed calculation on a total ionization cross section (TICS) for $^1H^+$-H system was carried out by Bates and Griffing [3] using the first Born approximation. Their calculation was in good agreement with the measurements of Gilbody and Ireland [4] at high energies. The classical-trajectory Monte Carlo approach (CTMC) used in Ref. [5] to describe the ionization cross sections in a H^+-H collision were found to be in good agreement with the experimental values of Shah and Gilbody [6] only at intermediate energies from about 50 to 200 keV.

The continuum distorted-wave (CDW) approximation, originally introduced by Cheshire [7] to describe charge-transfer cross sections in a H^+-H collision, was extended to the ionization process by Belkić [2]. The calculated values were found to exceed the measured values [6] by about 16% at 200 keV and 104% at 40 keV. The values calculated by Hardie and Olson [8] using the CTMC method, which were extended down to about 25 keV only, were much larger and in poor agreement with the experiment. Winter and Lin [9] proposed a triple center atomic state expansion method for describing ionization at low energies. The method accounts for the mechanism in which the electron is not removed until it is asymptotically at the point of unstable equilibrium between the nuclei (third center). Values calculated below 15 keV using this approach were larger than the experimental values of Ref. [10], and fell less steeply with decreasing energy. The values obtained by Fritsh and Lin [11] in their double-center 46 atomic-state-plus-pseudostate calculations, which were extended down to 9 keV, were found to be smaller. The double-center calculations of Shakeshaft [12], based on the use of 70 scaled hydrogenic pseudostates, were in reasonable agreement with the experiment at energies in the region of the cross-section peak, but below 20 keV the cross sections were found to decrease a little too rapidly. Recently a multistate close-coupling approach using a triple-center basis set together with a selective perturbative method was used in Ref. [13] to calculate the cross sections for excitation and capture processes into $n=1$, 2, and 3 states. These authors also calculated the cross sections for ionization at intermediate energies for a collision of a proton with atomic hydrogen. The cross-section values for ionization obtained by the above approach were found to be higher compared to the data of Ref. [10].

The experimental data on the ionization cross sections obtained by Fite *et al.* [14] in the range 0.04–40 keV were derived by reference to the sum of previously measured cross sections for charge transfer and ionization for H^+ in H_2. The values were of higher magnitude as compared with the data of Ref. [10]. Recently Kerby *et al.* [15] measured the total ionization cross sections for a H^+-H system in an energy range of 20–114 keV, and obtained slightly higher values than the experimental values of Ref. [10].

In the light of the above discussion, we have, in the present paper, calculated TICS's of atomic hydrogen by im-

pact with a proton at low and intermediate energies, taking the charge-transfer channel into consideration. The present calculated results are compared with the experimental values of Refs. [10,15], and other existing theoretical results. In Sec. II, we describe the theoretical model used in the calculation,[1] and in Sec. III we present our results with a discussion.

II. THEORY

We consider the ionization of a hydrogen atom in a ground state by collision with protons. We adopt the impact parameter treatment, where the internuclear motion is classically treated as $\vec{R}=\vec{b}+\vec{v}t$ with impact parameter b, the relative velocity of the projectile with target being $\vec{v}$ and the midpoint of the line joining the two nuclei is chosen as origin. Time t is measured from the instant when the two nuclei are closest to each other. Let $\vec{r},\vec{r}_P,\vec{r}_T$ denote the position vectors of the electron relative to the origin, projectile, and target nuclei, respectively. The Hamiltonian H_e for the electron moving in the field of the projectile and the residual target nucleus is given by

$$H_e=-\frac{1}{2}\nabla^2-\frac{1}{r_P}-\frac{1}{r_T} \tag{1}$$

(atomic units are used throughout).

The nucleus-nucleus interaction term is omitted here as this interaction can be removed by a canonical transformation, as pointed out by Wick (cf. Jackson and Shiff [16]), and as such it should not affect any transition probability for a particular impact parameter. The development in time t of the electron wave function Ψ is given by the time-dependent Schrödinger equation

$$\left(H-i\frac{\partial}{\partial t}\right)\psi=0 \tag{2}$$

together with initial condition that, at $t=-\infty$, the electron is attached to the target nucleus in the ground state.

We write

$$\psi=\int c_{k'}\psi_{k_c'}^{-}d\vec{k}_c'+\sum_i a_i\psi_{Pi}+\sum_j b_j\psi_{Tj}, \tag{3}$$

where the first term is an integral over the continuum states and the other terms denote the discrete states in direct as well as in charge-transfer channels. The coefficients $c_{k'}$, a_i, and b_j are functions of time. On putting ψ in the time-dependent Schrödinger equation (2), we obtain

$$i\int \dot{c}_{k'}\psi_{k_c'}^{-}d\vec{k}_c'=\left(H-i\frac{\partial}{\partial t}\right)\left[\sum_i a_i\psi_{Pi}+\sum_j b_j\psi_{Tj}\right]+\int c_{k'}\left(H-i\frac{\partial}{\partial t}\right)\psi_{k_c'}^{-}d\vec{k}_c'. \tag{3a}$$

$\psi_{k_c'}^{-}$ is an approximate solution of the equation

$$\left(H-i\frac{\partial}{\partial t}\right)\psi_{k_c'}^{-}\approx 0,$$

the solution being exact asymptotically. In view of this we neglect $\int c_{k'}[H-i(\partial/\partial t)]\psi_{k_c'}^{-}d\vec{k}_c'$, considering $c_{k'}$ to be small. Further,

$$\int \psi_{k_c}^{*}\psi_{k_c'}^{-}d\vec{r}=\delta(\vec{k}_c-\vec{k}_c'). \tag{3b}$$

Now multiplying both sides of Eq. (3a) by $\psi_{k_c}^{-*}$, and integrating over space, we have

$$\frac{\partial}{\partial t}(c_k)=-i\int \psi_{k_c}^{*}\left[\left(H-i\frac{\partial}{\partial t}\right)\left(\sum_{ij}(a_i\psi_{Pi}+b_j\psi_{Tj})\right)\right]d\vec{r}. \tag{3c}$$

The ionization amplitude $c_k(t=+\infty)$ is obtained by time integration utilizing the initial condition $c_k=0$ at $t=-\infty$.

Let us denote the discrete parts of the wave function as ψ_d. Thus Eq. (3c) takes the form

$$\frac{\partial}{\partial t}(c_k)=-i\int \psi_{k_c}^{*}\left(H-i\frac{\partial}{\partial t}\right)\psi_d d\vec{r}. \tag{3d}$$

$|c_{k(t=+\infty)}|^2$ corresponds to the ionization probability.

In our work the continuum state wave function occurring in the final channel is represented by the product of two Coulomb wave functions [17], which takes into account the distortion due to Coulomb fields of both the projectile and the target nuclei:

$$\psi_{k_c}^{-}=N_1N_2e^{i\vec{k}\cdot\vec{r}}\,{}_1F_1(i\alpha_P,1;-i(k_Pr_P+\vec{k}_P\cdot\vec{r}_P))\,{}_1F_1(i\alpha_T,1;-i(k_Tr_T+\vec{k}_T\cdot\vec{r}_T))e^{-ik^2t/2}, \tag{4}$$

[1] A preliminary version of the model was published earlier [23,24].

where $\alpha_P=-1/k_P$, $\alpha_T=-1/k_T$ and $\vec{k}_P=\vec{k}-(\vec{v}/2)$, $\vec{k}_T=\vec{k}+(\vec{v}/2)$, and

$$N_1=e^{-\pi\alpha_P/2}\Gamma(1+i\alpha_P),$$

$$N_2=e^{-\pi\alpha_T/2}\Gamma(1+i\alpha_T).$$

The above continuum-state wave function asymptotically satisfies the Schrödinger equation

$$\left(-\frac{1}{2}\nabla_r^2-\frac{Z_P}{r_P}-\frac{Z_T}{r_T}-i\frac{\partial}{\partial t}\right)\psi_{\vec{k}_c}^{-}=0. \tag{5}$$

ψ_d in Eq. (3d) is to be obtained by solving the time-dependent Schrödinger equation

$$H_e\psi_d=i\frac{\partial\psi_d}{\partial t} \tag{6}$$

by a variational technique developed by Sil [18].

In order to determine ψ_d in Eq. (6), we neglect the effect of continuum states. As stated above, the time is measured from the instant when the two nuclei are nearest to each other. For the solution of the time-dependent Schrödinger equation, we consider a trial wave function ψ_T in which a number of lower most discrete states around the two moving nuclei which seem important have been incorporated. We obtain the differential equations for determination of ψ (ψ_d) by making the integral

$$I=\int\frac{1}{2}\left[\psi^*\left(i\frac{\partial}{\partial t}-H_e\right)\psi+\psi\left(-i\frac{\partial}{\partial t}-H_e\right)\psi^*\right]d\vec{r}\,dt \tag{7}$$

stationary with respect to small arbitrary variation of ψ and its complex conjugate ψ^*.

The trial wave function ψ_T here is a linear combination of the two ground-state wave functions around two protons,

$$\psi_T=a(t)\psi_1+b(t)\psi_2, \tag{8}$$

where the coefficients $a(t)$ and $b(t)$ are functions of time, and

$$\psi_1=\psi_{1\mathrm{orb}}\psi_{1\mathrm{tr}}$$
$$=(\pi)^{-1/2}\exp(-r_1+i\varepsilon_0 t)\exp\left(-\frac{i}{2}\vec{v}\cdot\vec{r}-\frac{i}{8}v^2t\right), \tag{9}$$

$$\psi_2=\psi_{2\mathrm{orb}}\psi_{2\mathrm{tr}}$$
$$=(\pi)^{-1/2}\exp(-r_2+i\epsilon_0 t)\exp\left(\frac{i}{2}\vec{v}\cdot\vec{r}-\frac{i}{8}v^2t\right). \tag{10}$$

Here ε_0 is the binding energy of the electron. ψ_1 is the normalized ground state wave function around the target proton and consists of two parts, i.e., (1) $\psi_{1\mathrm{orb}}$ due to the orbital motion of the electron around the proton, and (2) $\psi_{1\mathrm{tr}}$ due to the translatory motion of the electron, i.e., the motion which the electron shares because of its being attached to the moving proton and contains momentum transfer term $\exp(i\vec{v}\cdot\vec{r})$ and kinetic energy term $\exp[i/8(v^2t)]$. Similarly ψ_2, the normalized ground state-wave function around the incident proton, consists of two parts $\psi_{2\mathrm{orb}}$ and $\psi_{2\mathrm{tr}}$.

In the variational integral (7) we substitute the trial function ψ_T for ψ. We first perform the space integration over r. We have the freedom of arbitrary variations of $a(t)$, $a^*(t)$, $b(t)$, and $b^*(t)$. We may write

$$I=\int L\,dt, \tag{11}$$

where

$$L=(a^*a+b^*b)f_1+(a^*b+ab^*)f_2$$
$$+\frac{i}{2}(a^*\dot{a}+b^*\dot{b}-\dot{a}^*a-\dot{b}^*b)$$
$$+\frac{i}{2}(a^*\dot{b}+\dot{a}b^*-\dot{a}^*b-a\dot{b}^*)f_3, \tag{12}$$

where

$$f_1=\int\psi_1^*\frac{1}{r_2}\psi_1dV=\int\psi_2^*\frac{1}{r_1}\psi_2dV,$$
$$f_2=\frac{1}{2}\int\psi_1^*\left(\frac{1}{r_1}+\frac{1}{r_2}\right)\Psi_2dV, \tag{13}$$
$$f_3=\int\Psi_1^*\Psi_2dV.$$

Here f_2 and f_3 are real, which can be justified as follows:

$$f_2=\frac{1}{2}\int\psi_1^*\left(\frac{1}{r_1}+\frac{1}{r_2}\right)\psi_2dV.$$

By using Eqs. (9) and (10), we write

$$f_2=\frac{1}{2\pi}\int\exp[-(r_1+r_2)]\left(\frac{1}{r_1}+\frac{1}{r_2}\right)\exp(i\vec{v}\cdot\vec{r})dV.$$

By introducing a transformation $\vec{r}\rightarrow-\vec{r}$, we have $|r_1|\rightarrow|r_2|$ and $|r_2|\rightarrow|r_1|$.

In view of the invariance of any space integral under the transformation $\vec{r}\rightarrow-\vec{r}$ we have $f_2=f_2^*$, i.e., f_2 is real. Similarly, f_3 can be shown to be real. Making the integral $I=\int L\,dt$ stationary with respect to small arbitrary variations of a^* and b^*, we obtain the coupled differential equations as follows:

$$f_1a+\left(f_2+\frac{i}{2}\dot{f}_3\right)b+i\dot{a}+if_3\dot{b}=0, \tag{14}$$

$$\left(f_2+\frac{i}{2}\dot{f}_3\right)a+f_1b+if_3\dot{a}+i\dot{b}=0. \tag{15}$$

If we make the integral stationary with respect to small arbitrary variations of a and b, we may obtain complex conjugate equations corresponding to Eqs. (14) and (15).

From Eqs. (14) and (15), we obtain

$$\left(f_1+f_2+\frac{i}{2}\dot{f}_3\right)(a+b)+i(1+f_3)(\dot{a}+\dot{b})=0 \quad (16)$$

and

$$\left(f_1-f_2-\frac{i}{2}\dot{f}_3\right)(a-b)+i(1-f_3)(\dot{a}-\dot{b})=0. \quad (17)$$

It may be pointed out that McCarroll [19] obtained equations similar to Eqs. (16) and (17), but the present equations contain an additional term $\dot{f}_3=(d/dt)\int\psi_1^*\psi_2 dV$ which ensures that, for all time, even with inexact wave functions Ψ_1 and Ψ_2 (if normalized), $\int\psi_T^*\psi_T dV$ is independent of time. The condition at $t=-\infty$, when the electron is attached to the target nucleus in the initial state, ensures that this value is initially unity and will always be maintained. The details were discussed in Ref. [20].

From Eq. (16), we have

$$\frac{d}{dt}(a+b)=-\frac{1}{i(1+f_3)}\left[f_1+f_2+\frac{i}{2}\frac{df_3}{dt}\right](a+b). \quad (18)$$

Making use of the initial condition, i.e., at $t=-\infty$, $a=1$, and $b=0$, we have

$$(a+b)=\exp\left(i\int_{-\infty}^{t}\frac{(f_1+f_2)}{(1+f_3)}\,dt\right)\frac{1}{\sqrt{(1+f_3)}}. \quad (19)$$

Again, proceeding in the same manner, we obtain

$$(a-b)=\exp\left(i\int_{-\infty}^{t}\frac{(f_1-f_2)}{(1-f_3)}\,dt\right)\frac{1}{\sqrt{(1-f_3)}}. \quad (20)$$

From Eqs. (19) and (20), we can write

$$a=\frac{1}{2}\left[\frac{1}{\sqrt{1+f_3}}\exp\left(i\int_{-\infty}^{t}\frac{(f_1+f_2)dt}{(1+f_3)}\right)+\frac{1}{\sqrt{1-f_3}}\exp\left(i\int_{-\infty}^{t}\frac{(f_1-f_2)dt}{(1-f_3)}\right)\right], \quad (21)$$

$$b=\frac{1}{2}\left[\frac{1}{\sqrt{1+f_3}}\exp\left(i\int_{-\infty}^{t}\frac{(f_1+f_2)dt}{(1+f_3)}\right)-\frac{1}{\sqrt{1-f_3}}\exp\left(i\int_{-\infty}^{t}\frac{(f_1-f_2)dt}{(1-f_3)}\right)\right], \quad (22)$$

so then a and b may be written in the form

$$a,b=\frac{1}{2}\left[K_1\exp\left(i\int_{-\infty}^{t}F_1dt\right)\pm K_2\exp\left(i\int_{-\infty}^{t}F_2dt\right)\right]=\frac{1}{2}(G_1(t)\pm G_2(t))$$

(say), where

$$K_1=\frac{1}{\sqrt{1+f_3}},\quad K_2=\frac{1}{\sqrt{1-f_3}}$$

and

$$F_1=\frac{f_1+f_2}{1+f_3},\quad F_2=\frac{f_1-f_2}{1-f_3}.$$

Now the trial wave function Ψ_T in Eq. (8) can be written as

$$\Psi_T=\frac{1}{2}[(G_1(t)+G_2(t))\Psi_1+(G_1(t)-G_2(t))\Psi_2], \quad (23)$$

where Ψ_1 and Ψ_2 represent the ground-state wave functions of a hydrogen atom, as stated in Eqs. (9) and (10). In the present calculation for low and intermediate energies, we neglect the momentum-transfer terms. It should be noted that for higher energies these terms cannot be ignored.

The transition amplitude in Eq. (3d) can be written as

$$\begin{aligned}c_k(b)(t=+\infty)&=\int_{-\infty}^{+\infty}dt\int\Psi_{\vec{k}_c}^{*}\left(H-i\frac{\partial}{\partial t}\right)\frac{1}{2}[(G_1(t)+G_2(t))\Psi_1+(G_1(t)-G_2(t))\Psi_2]d\vec{r}\\&=-\frac{1}{2}\int_{-\infty}^{\infty}dt\int\Psi_{\vec{k}_c}^{*}\left[\frac{1}{r_P}\Psi_1(G_1(t)+G_2(t))+\frac{1}{r_T}\Psi_2(G_1(t)-G_2(t))\right]d\vec{r}-i\int_{-\infty}^{\infty}dt\int\Psi_{\vec{k}_c}^{*}[\Psi_1\dot{a}+\Psi_2\dot{b}]d\vec{r},\end{aligned} \quad (24)$$

where $\dot{a}$ and $\dot{b}$ are the time derivatives of a and b, respectively. From Eqs. (16) and (17), we obtain

$$\dot{a}=\frac{i}{2}\left[(G_1(t)G_3(t))+G_2(t)G_4(t)\right], \tag{25}$$

$$\dot{b}=\frac{i}{2}\left[(G_1(t)G_3(t))-G_2(t)G_4(t)\right], \tag{26}$$

where

$$G_3(t)=K_1^2\left(f_{12p}+\frac{i}{2}\dot{f}_3\right)$$

and

$$G_4(t)=K_2^2\left(f_{12m}-\frac{i}{2}\dot{f}_3\right),$$

with $f_{12p}=f_1+f_2$ and $f_{12m}=f_1-f_2$.

Equation (24) may be written as

$$c_k(b)(t=+\infty)=-\frac{1}{2}\int_{-\infty}^{\infty}dt(G_1(t)+G_2(t))\int\frac{\Psi_{k_c}^{*}\Psi_1}{r_P}d\vec{r}+(G_1(t)-G_2(t))\int\frac{\Psi_{k_c}^{*}\Psi_2}{r_T}d\vec{r}$$
$$-(G_1(t)G_3(t)+G_2(t)G_4(t))\int\Psi_{k_c}^{*}\Psi_1 d\vec{r}-(G_1(t)G_3(t)-G_2(t)G_4(t))\int\Psi_{k_c}^{*}\Psi_2 d\vec{r}. \tag{27}$$

Evaluating the space part of Eq. (27) (see the Appendix), the transition amplitude for ionization may be written as

$$c_k(b)(t=+\infty)=-\frac{1}{2}\int_{-\infty}^{\infty}dt\ \exp(i(k^2t/2+\varepsilon-v^2/8))t$$
$$\times\int\exp(i\vec{\rho}\cdot\vec{b}+ivQ_zt)dQ_zd\vec{\rho}$$
$$\times[-T_1S_1-T_2S_2-T_3S_3-T_4S_4], \tag{28}$$

where

$$T_1=(G_1(t)+G_2(t)),\quad T_2=(G_1(t)-G_2(t)),$$
$$T_3=(G_1(t)G_3(t)+G_2(t)G_4(t)),$$
$$T_4=(G_1(t)G_3(t)-G_2(t)G_4(t)),$$

and

$$S_1=\underset{\mu\to0}{Lt}\left(\frac{\partial I}{\partial\lambda}\right),\quad S_2=\underset{\lambda\to0}{Lt}\left(\frac{\partial I}{\partial\mu}\right),$$

$$S_3=\underset{\mu\to0}{Lt}\left(\frac{\partial^2 I}{\partial\lambda\partial\mu}\right),\quad S_4=\underset{\lambda\to0}{Lt}\left(\frac{\partial^2 I}{\partial\lambda\partial\mu}\right).$$

S_1, S_2, S_3, and S_4 are functions of ρ and Q_z only. Hence the total cross section is

$$\sigma_{\text{total}}=2\pi\int\frac{d^2\sigma}{dE_e d\Omega_e}\sin\theta_e d\theta_e dE_e,$$

where

$$\frac{d^2\sigma}{dE_e d\Omega_e}\cong\int db|c_k(b)(t=+\infty)|^2$$

is the differential cross section. (The symbols have their usual meaning.)

III. RESULTS AND DISCUSSION

The present results for the total ionization cross sections in the range 5–300 keV are displayed in Fig. 1. We compare

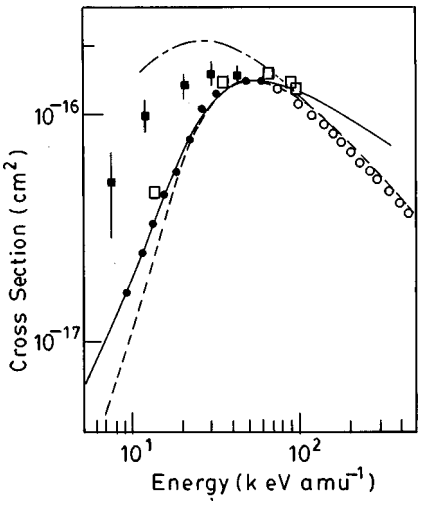

FIG. 1. Total ionization cross section of atomic hydrogen by proton impact. Present result: (——). CDW-EIS: (— — —). Born result: (— · — · —). Experimental results: Ref. [10] (●), Ref. [6] (○), Ref. [15] (□), and Ref. [14] (■).

the present results with the available experimental data and other theoretical findings which are also presented in the same figure. As shown from the figure, the present calculated values of TICS's show good agreement with the measured data of Refs. [10] and [6] up to the energy 100 keV. However, the experimental data obtained by Fite *et al.* [14] grossly overestimate the present cross section values in energy region below 40 keV. It may be pointed out that the data of Fite *et al.* were derived by reference to the sum of measured cross sections for charge transfer and ionization for H^+ in H_2. The more recent measurements of Kerby *et al.* [15] are found to be a little higher than the present results, as well as data of Refs. [10] and [6].

Values calculated by Born approximation [3] grossly overestimate the present results at energies below 100 keV. The calculated values of Crothers and McCann [21] and McCartney and Crothers [22] obtained by applying the CDW-EIS approximation in which distortion is accounted for in the entrance as well as in the exit channel show good agreement with the experiments of Refs. [6,10], and the present theoretical findings above 40 keV. Below 9.4 keV, no experimental value is available for a proton-hydrogen system. However, our curve tends to deviate from the experimental values of Shah and Gilbody [6] above 100 keV. The present model takes into account the charge-transfer channel, the effect of which is very important, particularly at low energies. The success of this model at low and intermediate energies is quite understandable. At high energies, however, the momentum-transfer term plays a very significant role, and so the present model is not expected to be very reliable at higher energies.

IV. CONCLUSION

We calculated the total ionization cross sections for the collision of hydrogen atoms in the ground state by protons over the energy region of 5–300 keV by using the two-center atomic state approximation, in which we took into consideration the influence of the coupling of the lower, most discrete, states around the two moving nuclei in order to study the low-energy collision. Our calculated values are found to be in very good agreement in low- and intermediate-energy regions, especially in the energy range from 10 to 100 keV, as predicted by the experimental data of Ref. [10]. However, the measurements of Kerby *et al.* are found to be slightly greater compared to the present results. Beyond 100 keV the present model has difficulty in accurately interpreting the experimental results of Ref. [10], which may be due to the noninclusion of the momentum-transfer term in the calculation. The present results also agree well with that of CDW-EIS values in the intermediate-energy region, whereas the values obtained using the Born approximation are found to be much higher than the present results. It is interesting to note that at low and intermediate energies the performance of our simple two-state calculation, wherein the conservation of probability has been ensured, is very encouraging, and this appears to point out that the enforcement of unitarity is rather more important than the inclusion of a large number of terms in the expansion of the wave function.

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APPENDIX

To evaluate the space part of Eq. (27), we consider the integral

$$I=\int e^{-i\vec{K}\cdot\vec{r}}e^{-\lambda_1 r_T}e^{-\mu_1 r_p}\left(\frac{1}{r_p r_T}\right)e^{i(t_1\vec{k}_p\cdot\vec{r}_p+t_2\vec{k}_T\cdot\vec{r}_T)}\cdot d\vec{r},$$

where $\lambda_1=\lambda-it_2k_T$ and $\mu_1=\mu-it_1k_P$. Using the Fourier transformation technique, we have

$$I=\frac{2}{\pi}\int\frac{e^{i\vec{Q}\cdot\vec{R}}}{(A-Bt_1)(C-Dt_2)}\,d\vec{Q},$$

where

$$A=(\vec{Q}-\vec{K}/2)^2,\quad B=\vec{K}_p\cdot(\vec{K}-2\vec{Q}),$$

$$C=(\vec{Q}+\vec{K}/2)^2+\lambda^2,$$

and

$$D=\vec{K}_T\cdot(2\vec{Q}+\vec{K})+2i\lambda K_T.$$

To simplify the integration over Q, let us consider the z axis along the direction of v; then the three-dimensional vectors can be represented in the following manner:

$$\vec{Q}=\vec{Q}_Z+\vec{\rho},\quad K=\vec{K}_Z+\vec{q},$$

where ρ and q are two-dimensional vectors, and

$$Q_Z=-\frac{E}{v}.$$

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