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$v/2$ electrons in $H^+ + H$ ionizing collisions

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Classical-trajectory Monte Carlo calculations are used to determine the velocity and angular dependence of the electron ionized in the $H^+ + H \rightarrow H^+ + H^+ + e^-$ collision. The energy range studied is 40—200 keV. At energies $E \leq 60$ keV, ionized electrons with velocities that are near one-half ($v/2$) the relative velocity v of the collision dominate the electron spectra. At higher energies the maximum position of the ionized electrons shifts and is found centered about the target nucleus.

In a previous paper[1] on ion-atom differential cross sections at intermediate energies, calculations were presented for the angular dependence of the ionized electron in the collision

$$H^+ + H \rightarrow H^+ + H^+ + e^- . \tag{1}$$

No differentiation was made as to the velocity distribution of the ionized electron. A search was made for the "electron capture to the continuum" (ECC) electrons, but the statistics of the calculations were insufficient to observe any; the ECC electrons are scattered at small angles, $\theta \sim 0°$, with a velocity close to that of the incident ion. However, it was stated in Ref. 1 that "We did note, however, a considerable number of small-angle scattering events for ejected-electron velocities approximately equal to one-half the projectile velocity. These electrons are ones that are left stranded equidistant between the projectile- and target-nucleus ions and are balanced in place by the attractive Coulomb forces of both ions." One may term these $v/2$ electrons "Wannier[2] electrons."

Because of interest in the details of collisions involving fundamental systems such as $H^+ + H$, this report quantifies our earlier comments and points to the possibility of observing Wannier electrons in intermediate-energy collisions on this system. At present there are no experimental observations of Wannier electrons nor theoretical calculations of the velocity and angular dependence of the ionized electrons.

The calculational method is the same as used in Ref. 1. An exact three-body, three-dimensional classical theory was used to obtain the angular scattering of the electrons. As is well known, one must make approximations when solving a three-body problem. The application of quantum-mechanical methods requires a truncation in the size and choice of the basis set, resulting in an incomplete description of the coupling between discrete and continuum levels. On the other hand, classical methods have, in essence, an infinite basis set to span the continuum and bound levels of an atom but enforce quantization only in the initial conditions of the atom. The classical method has been demonstrated to yield accurate values for electron capture and ionization cross sections. Such agreement is a reflection that the angular scattering by two point charges (Rutherford scattering) is the same in both the classical and quantal frameworks. Furthermore, the microcanonical distribution used for the classical description of the ground-state hydrogen-atom target exactly reproduces the quantal momentum distribution for the hydrogen 1s state. The use of a three-body, three-dimensional approach also accounts for curvilinear trajectories and incorporates the Coulomb forces between all the particles.

TABLE I. Calculated total cross sections for ionization and charge transfer [or charge exchange (cex)] in $H^+ + H$ collisions.

E (keV)	σ_{ion} (10^{-16} cm^2)	σ_{cex} (10^{-16} cm^2)
40	1.22	1.72
60	1.53	0.64
100	1.20	0.12
200	0.73	

In the classical method, the positions and momenta of the three particles are known at all times. Thus, it is possible to determine the angular position and velocity of the

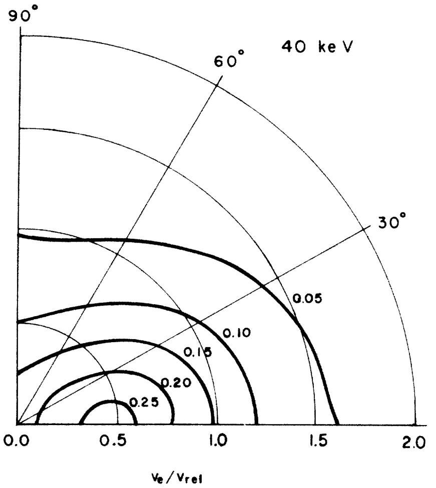

FIG. 1. Calculated spectrum in the laboratory frame for the electron ionized in $H^+ + H$ collisions. The velocity of the electron v_e is given in terms of the relative velocity of the collision v_{rel}. The scattering angles are noted. For this case, the projectile energy was 40 keV and $v_{\text{rel}} = 2.77 \times 10^8$ cm/s.

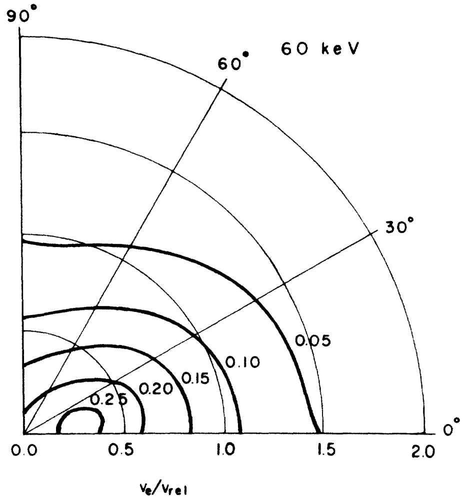

FIG. 2. Same notation as Fig. 1, except $E = 60$ keV and $v_{\rm rel} = 3.39 \times 10^8$ cm/s.

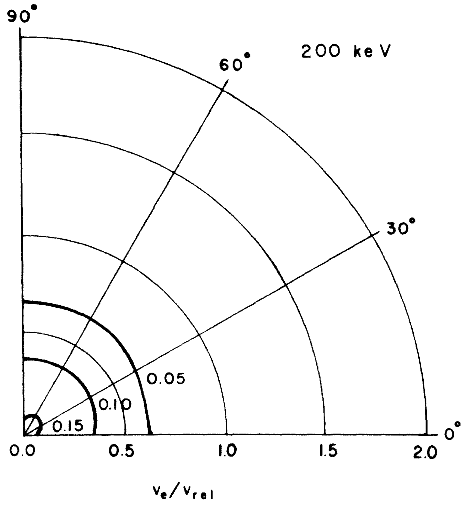

FIG. 4. Same notation as Fig. 1, except $E = 200$ keV and $v_{\rm rel} = 6.19 \times 10^8$ cm/s.

ionized electron for reaction (1). In the classical method, several thousand trajectories are run at each energy (in these systems, 10 000–20 000 trajectories) until good statistics have been accumulated for the collision process under study. As a reference, the calculated total charge transfer and ionization cross sections are listed in Table I. The ionization cross sections, which are of interest to this work, are within ±12% of the recent Shah and Gilbody experimental measurements.[3] Also, as demonstrated in Ref. 1, the calculated energy-loss spectra for ionization in $H^+ + H$ collisions are in good agreement with experimental observations.[4]

Spectra of the angular and velocity positions of the ionized electron after 40-, 60-, 100-, and 200-keV $H^+ + H$ collisions are displayed in Figs. 1—4. At 40 keV, we find the ionized electrons are centered around $v_e = v/2$, Fig. 1. As the collision energy increases to 60 keV, the peak shifts closer to the position of the target nucleus. At higher energies, 100 and 200 keV, the electron distribution becomes centered about the target nucleus. In the figures, the magnitude at the peak maximum was normalized to unity. Thus, besides the trend for the maximum to shift to center about the target nucleus with increasing energy, there is also the trend for the structure to become more sharply peaked at the higher energies.

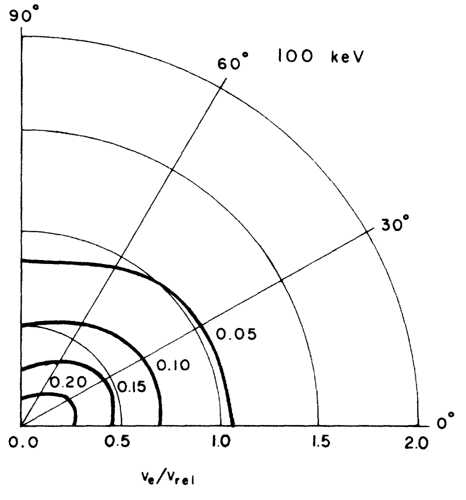

FIG. 3. Same notation as Fig. 1, except $E = 100$ keV and $v_{\rm rel} = 4.38 \times 10^8$ cm/s.

The energy dependence of the position of the peak in the electron distributions may be correlated with the importance of charge transfer in the electron loss process. If there is considerable transfer of the electrons to the projectile, there can also be a large fraction of ionized electrons left on or near the Wannier ridge. As the velocity increases and charge transfer becomes less probable, the ionized electrons become isotropically distributed about the target nucleus with the collision mechanism being simple impact ionization. The total cross sections given in Table I show the charge transfer values decrease below the ionization values above approximately 50 keV, which correlates with the shift in the ionized electron peak position.

The classical calculations presented in this paper should be an aid in the basis set determination for quantum-mechanical calculations of the ionization cross sections. It is apparent that a basis set must be flexible enough to represent the existence of Wannier electrons for $E \lesssim 60$ keV. In fact, recent low-energy quantal calculations[5] at $E \leq 15$ keV show the need to include basis functions centered at the midpoint between the nuclei in order to obtain accurate values for the ionization cross sections. At high energies, $E \gtrsim 100$ keV, the ionized electrons are centered about the target nucleus, indicating that a single-center basis set about the target should be adequate to determine the ionization cross sections.

ACKNOWLEDGMENTS

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