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Mutual neutralization in $H^+ - H^-$ collisions by electron capture

Ivan Mančev[1], Nenad Milojević[1] and Dževad Belkić[2]

[1] *Department of Physics, Faculty of Sciences and Mathematics, University of Niš - P.O. Box 224, 18000 Niš, Serbia*
[2] *Karolinska Institute - P.O. Box 260, S-171 76 Stockholm, Sweden, EU*

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Abstract – State-selective and total cross-sections for single-electron capture from H^- by H^+ covering the incident energy range from 10 to 3000 keV are computed by means of the four-body boundary corrected first Born (CB1-4B) approximation. A crucial connection between the Coulomb-distorted asymptotic state in the entrance channel and the pertinent perturbation, which causes the transition in the $H^+ - H^-$ collisions, is consistently used in our computations of the "prior" version of cross-sections. The obtained results from the CB1-4B method clearly outperform the earlier findings by the close-coupling methods for the same problem. Comparisons with the available measurements are carried out and excellent agreement with the CB1 method is recorded down to impact energies as low as 10 keV.

Introduction. – Negative ions play a major role in a number of areas of physics and chemistry. It is well known that over 80% of the naturally occurring elements are able to form stable atomic negative ions [1]. In addition, negative ions of many molecules are known to exist [2]. Massey [3] and Smirnov [4] have published monographs on the general subject of negative ions. The stability of a negative ion depends critically on the extent to which the extra electron shares the attractive field of its parent nucleus with the other electrons. There is a strong fundamental interest in negative ions. This is due to the fact that electron correlation effects play a very important role in determining the overall structure and dynamics of these ions, as reviewed in [1,5,6].

The positive and negative hydrogen ions are the main components of thermonuclear and astrophysical plasma. The basic neutralization reaction between H^+ and H^- is very important for thermonuclear research as well as for investigation of atmospheric and astrophysical processes. In the solar atmosphere, negative ions represent one of the primary sources of continuous opacity in the visible spectrum.

Mutual neutralization in the $H^+ - H^-$ collisions is the prototype reaction for electron transfer between two oppositely charged ions. It is the simplest ion-ion reaction possible. However, the simplicity of this reaction is, in fact, deceptive. Namely, the attendant two protons and two active electrons make this system a *pure four-body problem*. In practice, applications of a four-body collision theory involve laborious analytical and numerical computations even within any type of first-order approximations.

The structure of a negative ion is different from that of an atom or a positive ion in several important aspects. This difference can be traced back to the nature of the interaction which binds the outermost electron. In atoms and positive ions the valence electron moves asymptotically in the long-range Coulomb field of the associated positively charged core. The outermost electron in a negative ion experiences a much weaker, induced interaction potential of short range arising from the polarization effect of the atomic core. The induced dipole potential is shallow and typically supports only a single bound state. The weakness of this potential is reflected in the fact that binding energies, or equivalently the electron affinities of the parent atoms, are typically an order of magnitude smaller than the ionization energies of atoms [6].

At low collision energies, the split-shell $(1s1s')$ configuration description of the H^- ion has often been used. According to this picture, one of the two electrons in H^- lies in an almost hydrogenic $1s$ orbital, whereas the second loosely bound $1s'$ electron occupies a diffuse orbital whose radius is about $4a_0$. Under such circumstances,

the treatment of the $H^+ + H^-$ system can be simplified by using a model potential which describes the effluence of the "inner" onto the "outer" electron. This model reduces the original system to a problem with a simpler *one-electron* Hamiltonian. The captured electron is the outer, weakly bound electron, which moves in a combined field of the Coulomb potential due to one of the centres (H^+), and a short-range interaction associated with the other centre (H). The electron from H lying in a compact orbital is expected to yield only a weak contribution to the neutralization cross-section [7]. With this assumption, the two-centre one-electron Hamiltonian h for the process $H_a^+ + H_b^- \to H_a + H_b$ is given by $h = -\Delta/2 - 1/r_a + V_b(r_b)$, where the potential $V_b(r_b)$ for the $e^- + H_b$ interaction has the form of a nonlocal separable operator. According to this model, the tightly bound, noncaptured electron is considered as belonging to a frozen core.

One-electron Hamiltonians have already been used for descriptions of the $H^+ + H^-$ collisions by, *e.g.*, Ermolaev [8] in the atomic basis set formalism, and Sidis *et al.* [7,9] in the molecular basis expansion model. A detailed study of the one-electron molecular description of the $H^+ + H^-$ system can be found in refs. [10,11].

Theoretical cross-sections for neutralization in collisions between H^+ and H^- ions in the energy range from 0.62 to 80.0 keV were reported by Ermolaev [8]. Close-coupled computations were carried out [8], within the semiclassical impact-parameter approximations, in which the wave function was expanded in terms of a two-centre basis of traveling atomic orbitals with up to 51 states. Using a 23-state basis on each heavy particle within another coupled-channel computation, Shingal and Bransden [12] reported cross-sections for the same process at energies in a range from 0.15 to 50 keV.

The cross-sections for charge transfer in the $H^+ + H^-$ collisions have been computed using the two-centre atomic orbital close-coupling (TC-AOCC) method [13,14]. Moreover, collision dynamics of the $H^+ + H^-$ system have been studied [15] by means of the TC-AOCC method when the invoked interactions of charged particles were screened. Liu and Wang [15] used the short-range Debye-Hückel (Yukawa-type) model potential to describe the interaction between the loose electron and the neutral core. They found that the interaction screening introduces significant changes in the direct and exchange couplings, affecting the magnitude and energy behaviour of state-selective cross-sections [15]. These effects cause a change of the charge exchange spectrum, which may be applied for diagnostics of temperature and density of laboratory and astrophysical plasmas. Using one-electron Hamiltonians and expressing the wave function of the outer, weakly bound electron in terms of the Coulomb Green's function, Chibisov [16,17] has extensively investigated electron capture in slow collisions between negative and positive ions.

In all the above-cited studies on mutual neutralization, the captured electron is the loosely bound, outer electron. Simultaneously, these treatments assume that the atomic core remains mainly undisturbed throughout this process. However, at higher collision energies, such a description ceases to be valid implying that capture of the core electron has to be taken into account [8]. There are two high-energy three-body approximations which have been employed for investigating mutual neutralization. One such model is the three-body Coulomb-Born (CB-3B) approximation which has been applied [18] in the "prior" and "post" forms to compute total cross-sections for the ground–to–ground-state electron capture $H^+ + H^-(1s^2) \to H(1s) + H(1s)$ in the energy region from 25 to 100 keV. The other theory, is the three-body continuum distorted wave (CDW-3B) approximation, which has been used to determine the electron-capture cross-sections $Q(nl, n'l')$ when fast protons impinge on the H^- target system [19]. Here, the quantum numbers nl and $n'l'$ denote the electronic states of the captured and passive electrons, respectively. Further, study [19] reported the data for the states with n as well as n' equal to 1 and 2, alongside $l = 0$, 1 and $l' = 0$. These results for cross-sections from [19] were found to be highly sensitive to a change of the target wave functions. The target system was described by a variational wave function of the Hartree-Fock type using a split-shell formalism and a configuration-interaction wave function [19].

Notwithstanding the importance of the above-quoted studies, they are nevertheless all restricted to the category of three-body approximations, in which only the active electron is described in an explicit manner. As such, thus far, no theoretical computation based upon more advanced four-body models for neutralization in the $H^+ + H^-$ collisions has been carried out. On the other hand, for bound-free transitions involving H^+ and H^-, the four-body Modified Coulomb-Born (MCB) approximation [20–23] for single-electron detachment $H^+ + H^- \to H^+ + H + e$ is in an excellent agreement with all the available experimental data at incident velocities v covering a large range (0.235–12 a.u.). This is a good motivation for performing a systematic study of the allied process of single-electron capture in the $H^+ + H^-$ collisions using the CB1-4B method, which also belongs to a wide category of four-body distorted wave theories. Such a task is accomplished in the present work, which provides a comprehensive set of partial, state-selective as well as total cross-sections that have not previously been available in the literature. A further goal is to compare the existing experimental data with our theoretical total cross-sections obtained by summing over all the state-to-state transitions of the captured electron.

Atomic units will be used throughout unless otherwise stated.

Theory. – We examine single-electron capture by protons from the negative H^- ions:

$$H_a^+ + H_b^-(1s^2) \longrightarrow H_a(nlm) + H_b(1s). \qquad (1)$$

Here, indices "a" and "b" are used to make a formal distinction between the two otherwise identical protons, whereas nlm are the usual hydrogen atom quantum numbers. Let $\vec{s}_1$ and $\vec{s}_2$ ($\vec{x}_1$ and $\vec{x}_2$) be the position vectors of the first and the second electron (e_1 and e_2) relative to the projectile and target proton, respectively. We adopt the nonrelativistic spin-independent formalism in which the two electrons in (1) can be considered as distinguishable from each other. In such a case, we shall consider that e_1 is captured in the arbitrary state $H_a(nlm)$, while e_2 remains in the target rest $H_b(1s)$. We shall also need $\vec{R}$ as the vector of the internuclear axis via $\vec{R} = \vec{x}_1 - \vec{s}_1 = \vec{x}_2 - \vec{s}_2$. In the entrance channel, it is convenient to introduce $\vec{r}_i$ as the position vector of the projectile relative to the centre of mass of the target H^-. Symmetrically, in the exit channel, let $\vec{r}_f$ is the position vector of the centre of mass of $H_b(1s)$ relative to $H_a(nlm)$. The target H^- is taken to be in its ground singlet state $(1s)^2\ ^1S$ of even parity. It is commonly thought that invariably all singly charged non-molecular negative ions in the absence of external magnetic fields possess only one stable ground-state configuration. The ground state of H^- is given by the electronic configuration $(1s)^2\ ^1S$. Indeed a proof was given by Hill [24] in 1976 that H^- can have only one bound, stable state. However, much earlier in 1950, Hylleraas [25] proved the existence of the second stable state of H^- corresponding to the doubly excited state $(2s2p)\ ^3P$.

The "prior" form of the transition amplitude for process (1), in the four-body first Born approximation with correct boundary conditions (CB1-4B) can be written as

$$T_{if} = \left\langle \Phi_f^c | V_i | \Phi_i^c \right\rangle, \tag{2}$$

where Φ_i^c and Φ_f^c are the initial and final states in the entrance and exit channels, respectively. The initial state with the correct asymptotic behaviour at $r_i \to \infty$ is given by

$$\Phi_i^c = \varphi_i(\vec{x}_1, \vec{x}_2) e^{i\vec{k}_i \cdot \vec{r}_i} \mathcal{N}^+(\nu)\, {}_1F_1(i\nu, 1, ik_i r_i - i\vec{k}_i \cdot \vec{r}_i), \tag{3}$$

where $\mathcal{N}^+(\nu) = e^{\pi\nu/2}\Gamma(1 - i\nu)$ and $\nu = 1/v$ is the Sommerfeld parameter. The symbol ${}_1F_1(a, b, z)$ stands for the Gauss confluent hypergeometric function, whereas v is the incident velocity. Function $\varphi_i(\vec{x}_1, \vec{x}_2)$ represents the two-electron bound-state wave function of the H^- target, whereas $\vec{k}_i$ is the initial wave vector defined via $\vec{k}_i = \mu\vec{v}$. The reduced mass μ of the two initial aggregates is $\mu = M(M+2)/(2M+2)$, with M being the proton mass. The Coulomb wave function Φ_i^c from eq. (3) has the asymptotic form

$$\Phi_i^c(r_i \to \infty) \equiv \Phi_i^+ = \varphi_i(\vec{x}_1, \vec{x}_2) \exp(i\vec{k}_i \cdot \vec{r}_i) \times \exp[-i\nu \ln(vR - \vec{v} \cdot \vec{R})]. \tag{4}$$

It is seen from (4) that the asymptotic scattering state Φ_i^+ represents the product of the corresponding unperturbed state $\varphi_i(\vec{x}_1, \vec{x}_2) \exp(i\vec{k}_i \cdot \vec{r}_i)$ and the logarithmic phase factor $\exp[-i\nu \ln(vR - \vec{v} \cdot \vec{R})]$ due to the attractive long-range Coulomb interaction between the incident proton and the H^- ion. In eq. (4), we employed the usual mass approximation $M \gg 1$ leading to $\vec{r}_i \simeq \vec{R}$.

The asymptotic form of the final state Φ_f^c as $r_f \to \infty$ reads as

$$\Phi_f^c(r_f \to \infty) \equiv \Phi_f^- = \varphi_{nlm}(\vec{s}_1)\varphi_T(\vec{x}_2) \exp(-i\vec{k}_f \cdot \vec{r}_f). \tag{5}$$

The functions $\varphi_{nlm}(\vec{s}_1)$ and $\varphi_T(\vec{x}_2)$ in eq. (5) represent the bound-state wave functions of the atomic hydrogen in the exit channel. Furthermore, $\vec{k}_f$ is the final wave vector.

The perturbation potential V_i in the entrance channel with its asymptotic value $V_i(r_i \to \infty)$ is defined by

$$V_i = \frac{1}{R} + \frac{1}{r_i} - \frac{1}{s_1} - \frac{1}{s_2} \simeq \frac{2}{R} - \frac{1}{s_1} - \frac{1}{s_2}. \tag{6}$$

The potential V_i exhibits a short-range behaviour when $R \to \infty$. In the CB1-4B approximation, the proper connection between the long-range Coulomb distortion effect and the accompanying perturbation potential is established according to the principles of scattering theory [26]. It must be emphasized that imposing the proper Coulomb boundary conditions in the entrance and exit channels is of crucial importance for ion-atom(ion) collisions [22,27], since otherwise unphysical results could easily be incurred. This was most drastically evidenced in single-electron detachment $H^+ + H^- \to H^+ + H + e$ [23] for which the eikonal Coulomb-Born (ECB) approximation [28] overestimates the experimental data by 2-3 orders of magnitude, as opposed to the successful performance of the MCB method [20]. The ECB and MCB approximation share the same initial and final wave functions. However, the perturbation potential of the ECB model is inconsistent with the wave function of the entrance channel thus leading to the incorrect boundary condition in this approximation.

We shall use the eikonal hypothesis, since small scattering angles dominate in heavy-particle collisions. This implies that $\vec{k}_i \cdot \vec{r}_i + \vec{k}_f \cdot \vec{r}_f = -\vec{\alpha} \cdot \vec{R} - \vec{v} \cdot \vec{x}_1$. Here, $\vec{\alpha}$ is the momentum transfer $\vec{\alpha}$ defined by: $\vec{\alpha} = \vec{\eta} - (v/2 - \Delta E/v)\hat{\vec{v}}$, with, $\Delta E = E_i - E_f$, $E_f = -1/(2n^2) - 1/2$, where E_i is the binding energy of the H^- target. The transverse component of the change in the relative linear momentum of heavy particles is denoted by: $\vec{\eta} = (\eta\cos\phi_\eta, \eta\sin\phi_\eta, 0)$, $\vec{\eta} \cdot \vec{v} = 0$. Hence, the "prior" form of the transition amplitude for process (1), in the CB1-4B method can be expressed as the following nine-dimensional integral:

$$T_{if}(\vec{\eta}) = \int\int\int \mathrm{d}\vec{R}\mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2 \varphi_{nlm}^*(\vec{s}_1)\varphi_T^*(\vec{x}_2) \times \varphi_i(\vec{x}_1, \vec{x}_2) \left[\frac{2}{R} - \frac{1}{s_1} - \frac{1}{s_2}\right] \times \exp(-i\vec{\alpha} \cdot \vec{R} - i\vec{v} \cdot \vec{x}_1)(vR + \vec{v} \cdot \vec{R})^{i\nu}. \tag{7}$$

Here, the set $\{\vec{R}, \vec{x}_1, \vec{x}_2\}$ of the Jacobi independent variables is utilized, since the full kinetic energy operator is

diagonal in this set of variables. The total cross-section in the CB1-4B method is given by

$$Q_{if}(\pi a_0^2) = \frac{1}{2\pi^2 v^2} \int_0^\infty \mathrm{d}\eta\eta |T_{if}|^2 \,. \tag{8}$$

Following the derivation presented in ref. [29], the matrix elements T_{if} from eq. (7) can be reduced to a two-dimensional integral over real variables from 0 to 1. Thus, for computations of total cross-sections, only three-dimensional quadratures are required to be performed numerically. Theoretical total cross-sections from eq. (8) refer to capture of one electron. In a nonrelativistic theory, the target electrons are distinguishable. Therefore, cross-sections from eq. (8) are multiplied by 2, since each of the two electrons from the same K-shell of the H^- ion can be captured with equal probability.

Results and discussions. – In the present work, we shall use the four-parameter wave function of Löwdin [30] for the ground state of the $H^-(^1S)$ ion: $\varphi_i(\vec{x}_1, \vec{x}_2) = N(a_1 \mathrm{e}^{-b_1 x_1} + a_2 \mathrm{e}^{-b_2 x_1})(a_1 \mathrm{e}^{-b_1 x_2} + a_2 \mathrm{e}^{-b_2 x_2})$, where $a_1 = 0.30025$, $a_2 = 1.0001$, $b_1 = 0.4228$, $b_2 = 0.9794$, and N is the normalization constant. All the results of the present numerical computations are obtained by means of the Gauss-Legendre quadrature for the remaining triple integral. An appropriate change of variable is introduced in the integration over η to take full advantage of the fact that the main contribution stems from a narrow forward cone [31]. At every considered impact energy, a total of 160 integration points was used for each of the three quadratures in order to achieve convergence to the preassigned two decimal places.

Cross-sections for mutual neutralization in the $H^+ + H^-$ collisions (1) for a number of final states characterized by quantum numbers (n, l), as well as by those for the sum over all the final states of the captured electron are listed in table 1 in the energy range from 10 to 3000 keV. In particular, the results Q_{tot} from table 1 are obtained by summing over the contributions from all the individual shells and sub-shells of the captured electron up to $n = 4$ using the following expression:

$$Q_{\mathrm{tot}} \simeq Q_1 + Q_2 + Q_3 + 2.561 Q_4 \,, \tag{9}$$

where $Q_n = \sum_{l=0}^{n-1} Q_{nl}$, $Q_{nl} = \sum_{m=-l}^{+l} Q_{nlm}$. Numerical factor 2.561 in (9) comes from the Oppenheimer n^{-3} scaling law which takes approximately into account all the levels $n \geqslant 5$. By reference to the distribution of the cross-sections for various angular momenta l computed at a fixed principal quantum number n, table 1 reveals that $Q_{2s} > Q_{2p}$ at impact energies $E \geqslant 100$ keV, $Q_{3s} > Q_{3p}$ and $Q_{4s} > Q_{4p}$ at $E \geqslant 150$ keV, $Q_{3p} > Q_{3d}$ at $E \geqslant 20$ keV, as well as $Q_{4d} > Q_{4f}$ at all the considered energies. The results from table 1 are also depicted graphically in fig. 1. Shown are the distributions of the partial cross-sections Q_n for capture into the individual final states with the given principal quantum number n. It is seen in this figure that electron capture into the ground state ($n = 1$) gives the largest contribution at impact energies above 20 keV. At present, there are no experimental data for state-selective

Table 1: Total cross-sections (in units of cm^2) in the CB1-4B method for electron capture by protons from $H^-(1s^2)$ as a function of the laboratory impact energy E (keV). The rows labeled Q_{tot} represent the cross-sections summed over the bound states of the captured electron $H(nlm)$ by using eq. (9). Notation $X[-N]$ implies $X \times 10^{-N}$.

nl/E	10	20	50	75
$1s$	3.78[−16]	1.74[−16]	3.07[−17]	1.04[−17]
$2s$	1.38[−16]	3.33[−17]	5.03[−18]	1.72[−18]
$2p$	4.71[−16]	1.41[−16]	1.07[−17]	2.34[−18]
Q_2	6.09[−16]	1.74[−16]	1.58[−17]	4.06[−18]
$3s$	4.30[−17]	1.12[−17]	1.59[−18]	5.42[−19]
$3p$	1.11[−16]	3.90[−17]	3.61[−18]	8.18[−19]
$3d$	1.28[−16]	2.57[−17]	8.92[−19]	1.35[−19]
Q_3	2.83[−16]	7.59[−17]	6.09[−18]	1.49[−18]
$4s$	1.86[−17]	4.99[−18]	6.90[−19]	2.34[−19]
$4p$	4.60[−17]	1.63[−17]	1.58[−18]	3.64[−19]
$4d$	4.72[−17]	1.25[−17]	5.07[−19]	7.87[−20]
$4f$	2.58[−17]	2.93[−18]	4.17[−20]	4.28[−21]
Q_4	1.37[−16]	3.67[−17]	2.82[−18]	6.80[−19]
Q_{tot}	1.62[−15]	5.18[−16]	5.98[−17]	1.77[−17]
nl/E	100	150	200	500
$1s$	4.22[−18]	9.92[−19]	3.13[−19]	4.41[−21]
$2s$	7.01[−19]	1.61[−19]	4.97[−20]	6.30[−22]
$2p$	6.90[−19]	1.01[−19]	2.27[−20]	1.08[−22]
Q_2	1.39[−18]	2.62[−19]	7.24[−20]	7.38[−22]
$3s$	2.20[−19]	5.04[−20]	1.54[−20]	1.92[−22]
$3p$	2.45[−19]	3.63[−20]	8.17[−21]	3.86[−23]
$3d$	3.04[−20]	3.03[−21]	5.15[−22]	9.74[−25]
Q_3	4.95[−19]	8.97[−20]	2.41[−20]	2.31[−22]
$4s$	9.47[−20]	2.16[−20]	6.61[−21]	8.15[−23]
$4p$	1.09[−19]	1.63[−20]	3.67[−21]	1.73[−23]
$4d$	1.80[−20]	1.81[−21]	3.09[−22]	5.87[−25]
$4f$	7.38[−22]	5.03[−23]	6.49[−24]	4.99[−27]
Q_4	2.23[−19]	3.98[−20]	1.06[−20]	9.94[−23]
Q_{tot}	6.68[−18]	1.45[−18]	4.37[−19]	5.63[−21]
nl/E	750	1000	1500	3000
$1s$	5.37[−22]	1.15[−22]	1.23[−23]	2.46[−25]
$2s$	7.39[−23]	1.54[−23]	1.61[−24]	3.16[−26]
$2p$	8.28[−24]	1.28[−24]	8.74[−26]	8.29[−28]
Q_2	8.22[−23]	1.67[−23]	1.70[−24]	3.24[−26]
$3s$	2.23[−23]	4.63[−24]	4.83[−25]	9.39[−27]
$3p$	2.94[−24]	4.52[−25]	3.09[−26]	2.92[−28]
$3d$	4.91[−26]	5.62[−27]	2.53[−28]	1.18[−30]
Q_3	2.53[−23]	5.09[−24]	5.14[−25]	9.69[−27]
$4s$	9.47[−24]	1.96[−24]	2.04[−25]	3.98[−27]
$4p$	1.32[−24]	2.02[−25]	1.38[−26]	1.30[−28]
$4d$	2.96[−26]	3.38[−27]	1.52[−28]	7.06[−31]
$4f$	1.67[−28]	1.42[−29]	4.23[−31]	9.69[−34]
Q_4	1.08[−23]	2.17[−24]	2.18[−25]	4.11[−27]
Q_{tot}	6.72[−22]	1.42[−22]	1.51[−23]	2.99[−25]

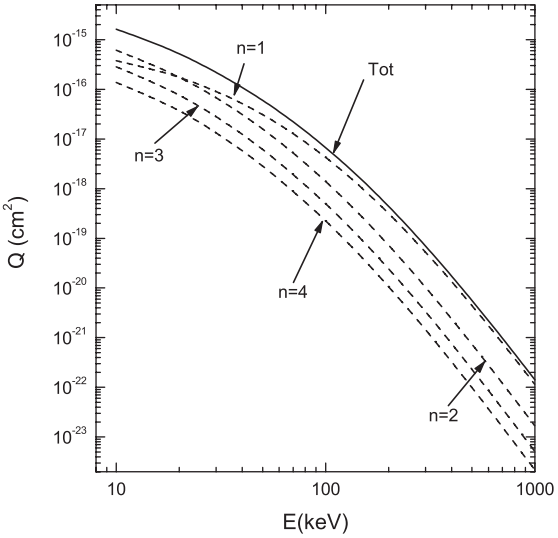

Fig. 1: Total cross-sections (in cm^2) as a function of the laboratory incident energy E (keV) for reaction $H_a^+ + H_b^-(1s^2) \to H_a(nlm) + H_b(1s)$. The full line represents the total cross-sections $Q_{tot} \simeq Q_1 + Q_2 + Q_3 + 2.561Q_4$ obtained by means of the CB1-4B method using the Oppenheimer n^{-3} scaling law for an approximate account of all the levels $n \geqslant 5$ that are not explicitly computed. The dashed lines show the partial cross-Q_n for the fixed principal quantum number n of the captured electron, as indicated by the arrows in the figure.

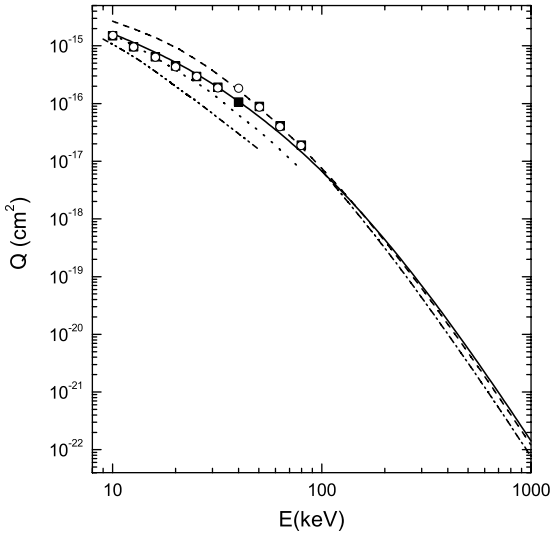

Fig. 2: Total cross-sections (in cm^2) as a function of the laboratory incident energy E (keV) for mutual neutralization in the $H^+ + H^-$ collisions by electron capture from the target. The full curve shows the results for the total cross-sections $Q_{tot} \simeq Q_1 + Q_2 + Q_3 + 2.561Q_4$ that are computed using the CB1-4B approximation. The dashed curve: the CB1-3B model (present computations), the dot-dashed curve: the CDW-3B model [19], the double-dot–dashed curve: the coupled-channel model of Shingal and Bransden [12], the dotted curve: the TC-AOCC method [14]. Experimental data: Schön *et al.* [35] (■); Melchert *et al.* [36] (○).

cross-sections to assess the accuracy of predictions of the CB1-4B method for partial cross-sections Q_n. It is highly desirable that measurements of these state-selective cross-sections Q_n are made in the nearest future.

On the other hand, experimental data exist for total cross-sections Q_{tot} [32–36] that are summed over all the final states nlm of the captured electron in the exit channel of process (1). The most recent of these data from measurements are depicted in fig. 2 and compared with the corresponding theoretical results. The target H^- ion in this collisional event can become a neutral H atom either by electron detachment with a cross-section Q_D, or by mutual neutralization with a cross-section Q_M (to avoid clutter, in the above expressions and figures subscript M is omitted from cross-sections). If the symbol Q_T is chosen to denote the absolute cross-section for the total production of the hydrogen atoms, then it follows that $Q_T = Q_D + Q_M$, since the lost electron can be ionized or captured. Schön *et al.* [35] measured Q_T and Q_M and deduced the detachment cross-sections by $Q_D = Q_T - Q_M$. Peart *et al.* [34] in 1976 measured Q_T at centre-of-mass energies between 1.49 and 35.2 keV. In order to investigate electron detachment, they subtracted cross-sections Q_M from their data for Q_T. However, in 1976, no cross-sections Q_M were measured in the relevant energy range, such that Peart *et al.* had to extrapolate the earlier low-energy experimental data (below 10 keV) [32,33] for Q_M to higher collision energies. In 1987, Schön *et al.* [35] showed that this extrapolation resulted in a significant overestimation. For this reason, such extrapolated data of Peart *et al.* [34] have not been plotted in fig. 2.

The results for Q_{tot} from the CB1-4B approximation graphed in fig. 2 are obtained by means of eq. (9). As can be seen from this figure, the CB1-4B theory is very successful in describing the experimental data of Schön *et al.* [35] and Melchert *et al.* [36]. The results from experiments reported in [36] practically coincide with measurements from [35]. The exception occurs only at energy $E_{lab} = 40$ keV, where the measured cross-section from ref. [35] is $1.06 \pm 0.16\,[-16]$ cm^2, whereas ref. [36] gives the corresponding value of $1.85 \pm 0.185\,[-16]$ cm^2. Additional experimental cross-sections at higher impact energies would be welcome to provide further important tests for the present theory. In order to compare our results with some quantum-mechanical three-body models, we have employed the general computer code of Belkić [31] for the CB1-3B approximation by choosing the hydrogen-like wave function for the target ion with the effective charge $Z_T^{eff} = 0.6875$. The obtained results with the captured states $n \leqslant 4$, summed over all the ml-sublevels, are shown in fig. 2 by the dashed line. At higher impact energies, both the CB1-3B and CB1-4B methods give similar results. However, at lower energies, the CB1-4B method exhibits a significantly better agreement with the measurements. The results of the CDW-3B model from ref. [19] obtained at energies above 100 keV with the same

effective charge (0.6875) are depicted in fig. 2 by the dot-dashed line. The results of the CDW-3B method lie below the cross-sections of the CB1 model due to the inclusion of continuum intermediate states of the captured electron. As to the other theories, it is clear from fig. 2 that the results obtained by the coupled-channel method using a 23-state basis on each heavy particle [12] considerably underestimate the experimental data. A systematically increased deviation of these cross-sections of the close-coupling model from the measured findings is seen to occur as the impact energy is augmented. Extension of the basis size may increase the computed cross-sections. Thus, Liu and Wang [14] carried out the computations by using the TC-AOCC method with a 50- and 77-state basis set functions at $E > 52.06$ keV and $E \leqslant 52.06$ keV, respectively. Their results shown as the dotted line in fig. 2 are above those of Shingal and Bransden [12] and lie below the experimental data at higher energies.

Conclusion. – We have investigated the problem of mutual neutralization in the $H^+ + H^-$ collisions via single-electron capture from the target ion H^- at energies between 10 and 3000 keV by means of the CB1-4B approximation. The CB1-4B method is a fully quantum-mechanical four-body formalism, since it explicitly considers each individual particle and all the interactions among them in the collision under investigation. The CB1-4B theory strictly preserves the correct boundary conditions in both collisional channels according to the principles of scattering theory and the asymptotic convergence problem. Our computations provide detailed information on the partial cross-sections to each individual *nl* shell of the captured electron in the final state. These data are summed to obtain the corresponding total cross-sections for comparison with the available experimental data. Excellent agreement is found between the total cross-sections from the CB1-4B method and the associated findings from the measurements.

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