Atomic and molecular transport processes in a cool hydrogen plasma

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Abstract. Recent developments concerning the relatively cool and dense divertor region of magnetically confined tokamak fusion plasma devices might play a key role in the realization of useful energy production. Atomic and molecular processes, in turn, critically influence the performance of the divertor. In particular, charge transfer from vibrationally excited hydrogen molecules as well as elastic processes and charge transfer between various ground state hydrogen species (ions, atoms and molecules, in isotopic combinations) could be of critical importance for the momentum transport mechanisms and charge balance in this region. We show here the benchmarking results of our fully quantal calculations for a great number of the relevant processes.

INTRODUCTION

The transport of particles and, in particular, the exchange of momentum, in cool hydrogen plasma/gas can be dominantly determined by elastic scattering and resonant charge capture among hydrogen ions, atoms, and molecules. For example, recent emphasis on the engineering design of fusion reactors has focused attention on these issues regarding the so-called divertor region in which high density, low temperature hydrogen plasma is produced to bring about the neutralization and heat exhaust from the burning plasma in the core region [1–7]. Furthermore, elastic scattering as well as spin exchange between neutrals has been shown to be an important process in numerous astrophysical environments, for example, in planetary ionospheres [8], the heliospheric shock at the interface of our solar system and the local interstellar medium [9,10], comet bow shocks (see e.g. [11]), and non-radiative shocks in supernovae ejecta (see e.g. [12]). Interest generated by the recent experimental observations of Bose-Einstein condensates has also spurred the need for accurate description of very low temperature elastic and spin exchange scattering (e.g. for H+H scattering see [13,14]).

To address the need for comprehensive and accurate data for the relevant elastic, charge transfer, and transport cross sections, we have recently undertaken a very large set of fully quantal calculations. Moreover, we have included consideration of the full range of possible scattering angles, since all angles contribute in the calcula-

tion of the higher (transport relevant) moments of the integral elastic cross section, and since large angles contribute to the charge transfer and spin exchange. Four types of systems, ion-atom (A^++B), atom-atom (A+B), ion-molecule (A^++BC) and atom-molecule (A+BC) have been studied, where A,B, and C are any of the hydrogen atom isotopes (H, D, or T). In addition, A^++He systems were studied, where A is any of the isotopes of H. The hydrogen molecules are assumed to be initially in their ground vibrational states. These constitute 51 distinct collision systems. We base our discussion here on recent [15–17] fully quantal calculations of more than 2800 differential and more than 200 integral cross sections spanning the center of mass (CM) collision energy range of 0.1-100 eV. Besides utilizing the best available potential energy surfaces and carefully checking numerical convergences to achieve high accuracy in the calculations, the good quality of the data was also verified by extensive comparison with the theoretical and experimental data available in the literature. The differential cross sections were calculated for 768 CM scattering angles in interval $(0, \pi)$, starting from angles as small as 6×10^{-6} rad to facility Gauss-Legendre quadrature. The calculated differential and integral cross sections can be viewed in both graphical and tabular forms through the WWW site of the ORNL Controlled Fusion Atomic Data Center (`www-cfadc.phy.ornl.gov`). As a further aid to plasma modeling, convenient analytical fitting coefficients to describe the differential and integral cross sections were also tabulated [18]. We note here that all collision energies and scattering angles used are given in the center of mass system. Atomic units (a.u.) are used throughout the text unless stated otherwise.

There has been considerable inconsistency in the definition of the elastic (el) cross section as well as its higher moments, the momentum transfer (mt) and viscosity (vi) cross sections, with respect to the quantum indistinguishability of colliding particles (QIP) at low collision energies in symmetric systems such as H^++H or H+H [19–25,13]. This indistinguishability is manifested by an overlap of the wavefunctions at low collision energies and thus by significant interference between the elastic and charge transfer channels in the case of ion-atom scattering (Fig. 1a), or by the direct elastic and recoil channels for the atom-atom case. With increasing collision energy the overlap decreases and pronounced peaks for forward and backward scattering are displayed by the differential cross sections (Fig. 1b). These peaks correspond in this limit to elastic scattering (forward) and either charge transfer (backward) for the ion-atom case or target recoil (backward) for the atom-atom case, thus enabling classical distinguishability of the particles (CDP), i.e. labeling of the projectile and the target.

Since in practice, most experiments, as well as plasma modeling, assume unpolarized beams of projectiles and unpolarized targets, the relevant theory of elastic scattering should take into account the spin statistics of the nuclei [22,19,25]. This results in an elastic cross section which, for high collision energies, tends to the "total" cross section for scattering of projectiles, rather than to the elastic one, thus representing an experiment in which direct and recoil channels are not separated even for energies where CDP is in effect. Particularly sensitive to this definition

is the momentum transfer cross section, derived by integration of the elastic differential cross section weighted by $1 - \cos\theta$, where θ is the scattering angle. Since the weighting factor emphasizes the backward scattering angles, the momentum transfer cross section could be considerably larger if recoil scattering is present in the elastic cross section.

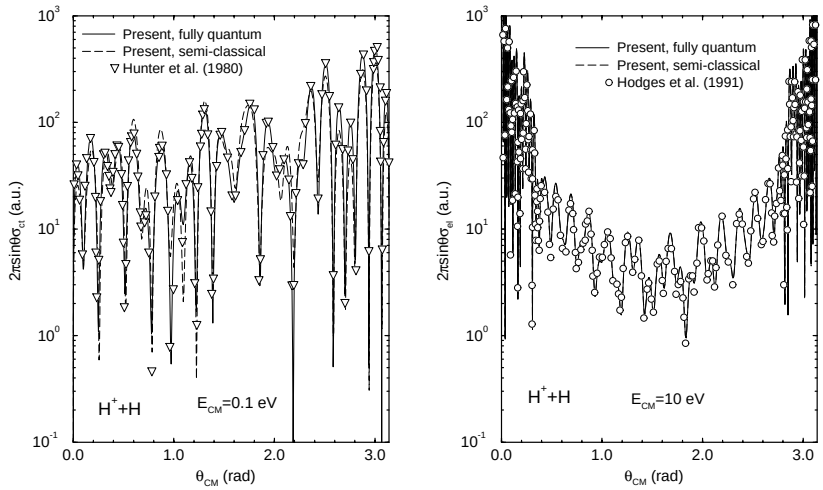

Fig. 1 Differential cross section for elastic scattering of H^+ on H.

Thus the usual quantum-mechanical definition of the elastic cross section as well as of its higher moments for the symmetric (nuclei) systems do not have the classical limit, defined by CDP, even when the latter can be reached in an experiment ($E_{CM} > 1$ eV). Alternately, inability to distinguish projectiles ions from ions coming from the target by charge transfer (ct) leads one to define the "spin-exchange" (se) cross section, assuming the scattering of a polarized beam of projectiles on an unpolarized target [19,25]. If the scattered particle is detected with changed nuclear spin, and spin-coupling is not present, this particle has certainly come from the target. The spin exchange cross section does have the correct classical limit which would smoothly become equivalent to the charge transfer cross section in the CDP limit. One may analogously define the spin exchange cross section for identical atom-atom scattering [22,13,26].

To maintain a quantum mechanically correct definition consistent with conventions well established in the literature in the energy range considered here, we treat the identical nuclei in ion-atom and atom-atom scattering as indistinguishable, even for $E_{CM} > 1$ eV, when the "elastic" cross section transitions to the total scattering cross section, containing the non-overlapping sum of direct and recoil channels.

Two significantly different sets of elastic and transport cross sections could be produced for the symmetric collision systems even at higher energies, depending on the assumption of QIP or CDP. Although each of the sets is internally consistent, they could potentially introduce a confusion in plasma modeling applications,

resulting from double counting. Under the assumption of quantum indistinguishability, modeling of particle transport in plasmas should not additionally include momentum transfer through resonant charge transfer, because this is already contained in the total elastic cross section. However, to separate the recoil processes in the integral cross sections for $H^+ + H$, one can subtract the charge transfer cross section from the total elastic cross section, arriving at the elastic cross section in the distinguishable particle sense, which is, of course, well defined only at "high" energies. Similarly, the elastic differential cross sections may be approximated as the absolute value of the difference of the total and charge transfer differential cross sections. This can then be used to recalculate the integral quantities, such as the momentum transfer and viscosity cross sections to obtain results that have the correct classical limit. We have shown elsewhere [16] that the distinguishability of the particles introduced in such a way does not lead to more than about 10% uncertainty in the integral cross sections for the systems considered here at energies above 0.1 eV. As a convenience to plasma modeling, we have calculated the integral cross sections for symmetric systems with both QIP and CDP assumptions, and these are separatelly available at `www-cfadc.phy.ornl.gov`.

Calculation of these differential and integral cross sections has been described in detail recently [15–17] and only the essential features of the numerical methods are summarized briefly here. For example, common to the calculational techniques for all systems considered is the solution of the relevant Schrödinger radial equation or system of equations (in cases that involve molecular targets). These have been solved using the method described by Johnson [32] based on the use of the logarithmic derivative. The step size used in the numerical mesh was between 0.001 and 0.0001 while the convergence of a solution for the elastic amplitude a_ℓ in the number of partial waves, ℓ, was established for each energy by requiring that $1 - \mathrm{Re}\{a_\ell\} \leq 10^{-5}$, $\mathrm{Im}^2\{a_\ell\} \leq 10^{-5}$ for at least ten successive partial waves. The number of partial waves needed for convergence of the elastic amplitudes was usually significantly larger than the amount needed for the corresponding convergence of inelastic amplitudes, reflecting the importance of the region of large internuclear distance in elastic scattering. The converged amplitudes were matched to the standard plane wave boundary conditions in order to define the K matrix and subsequently the unitarized S matrix [32].

The integral elastic cross section, σ_{el}, and its higher moments [33], the momentum transfer σ_{mt} and viscosity σ_{vi} cross sections were found by numerical and (where possible) analytic integration over scattering angles

$$\sigma_{el} = 2\pi \int_0^\pi d\theta \sin\theta \frac{d\sigma_{el}}{d\Omega} \tag{1}$$

$$\sigma_{mt} = 2\pi \int_0^\pi d\theta \sin\theta (1 - \cos\theta) \frac{d\sigma_{el}}{d\Omega} \tag{2}$$

$$\sigma_{vi} = 2\pi \int_0^\pi d\theta \sin^3\theta \frac{d\sigma_{el}}{d\Omega}. \tag{3}$$

In Section I we present a review of consistent, spin-averaged formulas for calculation of differential and integral cross sections for the ion-atom and atom-atom systems considered here. We also discuss the level of physical accuracy of the calculations. Some detail on the results obtained for scattering of ions and atoms on molecules are discussed in Section II.

The establishment of the detached plasma regimes in the divertor, which is essential for minimization of plasma-divertor plate interaction and the associated material erosion and material properties degradation effects, can be faciliated by inclusion of certain fast volume plasma recombination mechanisms. One of the reaction schemes proposed is "ion conversion" [34], which involves capture of an electron by a proton from a vibrationally excited H_2, followed by dissociative recombination of H_2^+ with a plasma electron. The present state of information for many of the processes involving excited molecular states does not allow the construction of a collisional-radiative model for the H_2/H gas. In Section III we present our preliminary fully quantal results for the process $H^+ + H_2(\nu) \rightarrow H + H_2^+$, where ν is an arbitrary vibrational state.

I ION-ATOM AND ATOM-ATOM COLLISIONS

In symmetric neutral-neutral scattering (for example H+H), both nuclear and electron spin statistics have to be taken into account for proper derivation of the QIP elastic differential cross sections. It is interersting to note that while H^+ and T^+ are fermions (spin 1/2), D^+ is a boson (with spin 1), which lead to different expressions for the cross sections. Specifically,

$$\frac{d\sigma_{el}}{d\Omega} = \frac{1}{k^2}\left[\alpha_s\Gamma_s^+ + \alpha_t\Gamma_t^+ + \beta_s\Gamma_s^- + \beta_t\Gamma_t^-\right] \tag{4}$$

where

$$\Gamma_{s,t}^{\pm} = \left|\sum_{\ell=\pm}(2\ell+1)(\exp(i\delta_\ell^{s,t})\sin\delta_\ell^{s,t}P_\ell(\cos\theta)\right|^2 . \tag{5}$$

The "+" and " −" signs denote even and odd values of ℓ, respectively, $\delta_\ell^{s,t}$ is the elastic partial phase shift for singlet (s) and triplet (t) electronic states, and k is the CM collisional momentum. The values of the coefficients α and β are shown in Table I for all of these cases (i.e. for H+H, T+T, and D+D).

System	α_s	α_t	β_s	β_t
H+H, T+T	1/4	9/4	3/4	3/4
D+D	2/3	1	1/3	2

Table I. Parameters in Eq. (4) defining the elastic differential cross section $d\sigma_{el}/d\Omega$ for neutral-atom–neutral-atom scattering.

Among the most notable work considering elastic scattering in H+H collisions in the literature, Jamieson *et al.* [13] introduced an additional factor of 1/2 in order to adjust the cross section to become identical to that derivable in the high energy, classical limit (Boltzmann statistics). We adopt this convention here as well. Upon integration over the scattering angle, this yields for the total integral elastic cross section [22,13] for H+H and T+T

$$\sigma_{el} = \frac{2\pi}{k^2}[\sum_{\ell=even}(2\ell+1)(\frac{1}{4}\sin^2\delta_\ell^s + \frac{9}{4}\sin^2\delta_\ell^t) + \sum_{\ell=odd}(2\ell+1)(\frac{3}{4}\sin^2\delta_\ell^s + \frac{3}{4}\sin^2\delta_\ell^t)]. \tag{6}$$

The momentum transfer cross section, defined in Eq. (2) yields the result

$$\sigma_{mt} = \sigma_{el} \tag{7}$$

which is a consequence of full symmetry of the QIP elastic differential cross section about $\theta = \pi/2$.

An alternative definition of the momentum transfer cross section may be considered for H + H scattering at higher energies if one assumes full distinguishability of the projectile and target nuclei (i.e. Boltzmann statistics [22]), and therefore applying only electronic spin statistics. This yields

$$\sigma_{mt,B} = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(\ell+1)(\frac{1}{4}\sin^2\Delta_\ell^s + \frac{3}{4}\sin^2\Delta_\ell^t). \tag{8}$$

For D+D scattering, assuming distinguishability of nuclei, the Boltzmann statistics momentum transfer cross section takes on the same form as in the H + H and T + T cases. Moreover, in this limit all differential and integral cross sections take similar forms, irrespective of the type of nuclei.

We note that the viscosity cross section [16] obtained from Eq. (3) is in full agreement with that obtained by Jamieson *et al.* [13] and that we have summarized the formulas for the integral elastic, momentum transfer, and viscosity cross sections elsewhere [16].Sumarizing the atom-atom cases, the integral cross sections can be written in the form [13]

$$\sigma = \frac{2\pi}{k^2}\sum_{\ell=\pm} g(\ell)(\omega_1^\pm \sin^2\eta_1 + \omega_2^\pm \sin^2\eta_2) \tag{9}$$

where the coefficients $g(\ell)$, $\omega_{1,2}^\pm$ and $\eta_{1,2}$ are given in Table II.

In the case of ion-atom scattering, the spin statistics is less involved, including only nuclei. Expanding this definition using the expressions above for the amplitudes we find that the elastic differential cross section can be written in the form

$$\frac{d\sigma_{el}}{d\Omega} = \frac{1}{4k^2}[\alpha_g\left|\Gamma_g^+\right|^2 + 3\alpha_u\left|\Gamma_u^+\right|^2 + \beta_u\left|\Gamma_u^-\right|^2 + 3\beta_g\left|\Gamma_g^-\right|^2 + 2\mathrm{Re}\{\gamma_{gu}\Gamma_{\mathrm{g}}^{+*}\Gamma_{\mathrm{u}}^- + 3\gamma_{ug}\Gamma_{\mathrm{g}}^{-*}\Gamma_{\mathrm{u}}^+\}] \tag{10}$$

where $\Gamma^{\pm}_{g,u}$ was defined in Eq. (5), and the coefficients α, β and γ are given in Table III. The subscripts g and u mean here *gerade* and *ungerade* electronic states,

Type	g	η_1	η_2
elastic	$2\ell+1$	δ^s_ℓ	δ^t_ℓ
momentum transfer	$2\ell+1$	δ^s_ℓ	δ^t_ℓ
viscosity	$\frac{(\ell+1)(\ell+2)}{2\ell+3}$	$\delta^s_{\ell+2}-\delta^s_\ell$	$\delta^t_{\ell+2}-\delta^t_\ell$

	H^++H,T^++T				D^++D			
Type	ω_1^+	ω_2^+	ω_1^-	ω_2^-	ω_1^+	ω_2^+	ω_1^-	ω_2^-
total	1/4	9/4	3/4	3/4	2/3	1	1/3	2
momentum transfer	1/4	9/4	3/4	3/4	2/3	1	1/3	2
viscosity	1/4	9/4	3/4	3/4	2/3	1	1/3	2

Table II. Parameters in Eq. (9) for spin averaged integral elastic cross sections in symmetric atom-atom systems.

respectively. Due to the presence of the interference term in this expression, the momentum transfer integral cross section is not equal to the integral elastic cross section [16].

System	α_g	α_u	β_g	β_u	γ_{gu}	γ_{ug}
H^++H, T^++T	1/4	3/4	3/4	1/4	1/4	3/4
D^++D	2/3	1/3	1/3	2/3	2/3	1/3

Table III. Parameters for the for the Eq. (10) defining the elastic differential cross section $d\sigma_{el}/d\Omega$ for ion–neutral-atom scattering.

When the nuclei are of different masses we consider them as CDP, so that the cross sections can be calculated by considering scattering without regard to the nuclear spins.

For the symmetric (*sym*) ion-atom systems, performing integration over scattering angles analytically, the formulas obtained for the integral elastic cross section and its higher moments take the same form,

$$\sigma_{tot,sym} = \frac{4\pi}{k^2}\sum_{\ell=\pm} g(\ell)(\omega_1^{\pm}\sin^2\eta_1 + \omega_2^{\pm}\sin^2\eta_2) \tag{11}$$

where the coefficients are summarized in Table IV, while charge transfer is given by

$$\sigma_{ct,sym} = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2(\delta^g_\ell - \delta^u_\ell). \tag{12}$$

Type	g	η_1	η_2
total	$2\ell+1$	δ^g_ℓ	δ^u_ℓ
momentum transfer	$\ell+1$	$\delta^g_\ell - \delta^u_{\ell+1}$	$\delta^u_\ell - \delta^u_{\ell+1}$
viscosity	$\frac{(\ell+1)(\ell+2)}{2\ell+3}$	$\delta^g_{\ell+2} - \delta^g_\ell$	$\delta^u_{\ell+2} - \delta^u_\ell$

	H^++H,T^++T				D^++D			
Type	ω_1^+	ω_2^+	ω_1^-	ω_2^-	ω_1^+	ω_2^+	ω_1^-	ω_2^-
total	1/4	3/4	3/4	1/4	2/3	1/3	1/3	2/3
momentum transfer	1/4	3/4	3/4	1/4	2/3	1/3	1/3	2/3
viscosity	1/4	3/4	3/4	1/4	2/3	1/3	1/3	2/3

Table IV. Parameters in Eq. (11) for spin averaged integral elastic cross sections in symmetric ion-atom systems.

The QIP cross sections, defined by Eq. (9) and (11) do not tend to the CDP (like, for example, the D^++H case, where projectile and target can be distinguished by different masses), even when the energy is high enough for coherent superposition of the amplitudes in Eq. (10). For example $\sigma^{(el)}_{tot,sym}$ for H^++H is approximately a factor of $\sqrt{2}$ larger than σ_{el} calculated using Boltzman spin statistics like in Eq. (8), over almost the entire range of energies considered, although both are referred to as "elastic" cross sections in the literature. Still, it is possible to construct an elastic cross section even for symmetric systems, which has the correct CDP limit and, as we show in Section II, has a reasonable interpretation even at energies as low as 0.1 eV. In the rest of the text we will call this the "elastic" cross section for symmetric ion-atom scattering, i.e.

$$\sigma_{el,sym} = \sigma^{el}_{tot,sym} - \sigma_{ct,sym}. \tag{13}$$

To define the momentum transfer and viscosity cross sections with the correct CDP limit, it is convenient to define the "elastic" differential cross section by subtracting $d\sigma_{ct,sym}/d\Omega$ from $d\sigma_{tot,sym}/d\Omega$ and applying the weighted integration in Eqs.(2) and (3).

Obviously, the elastic differential cross section so defined for a symmetric system differs from the CDP cross section by the interference term, which vanishes in the CDP limit. Although $d\sigma_{el}/d\Omega$ can be negative for some angles and energies, at least in principle, it results in integral cross sections with the correct CDP limit, as we illustrate in Section II.

In spite of the high numerical accuracy of the present calculations, the assumption of a weak coupling of the ground gerade ($1s\sigma_g$) and ungerade ($2p\sigma_u$) states with the excited molecular states of H_2^+ could result in physical inaccuracies of the elastic and charge transfer ion-atom differential cross sections for the higher portion of the energy range considered. In particular, it is well known [35,36] that strong Coriolis (rotational) coupling between the $2p\sigma_u$ and $2p\pi_u$ states at small internuclear distances may influence the cross sections if the product of the collision

energy and scattering angle (Eθ) is greater than 1 keVdeg. We have investigated the influence of this coupling for the ion-atom case, where the consequence of the effect is expected to be more pronounced. At worst (E_{CM}=100 eV), we found about a 3% correction for the viscosity cross section and less than 1.5% corrections for the momentum transfer and integral elastic cross sections.

We sumarize our results for the integral elastic, momentum transfer and viscosity cross sections in Fig. 2.

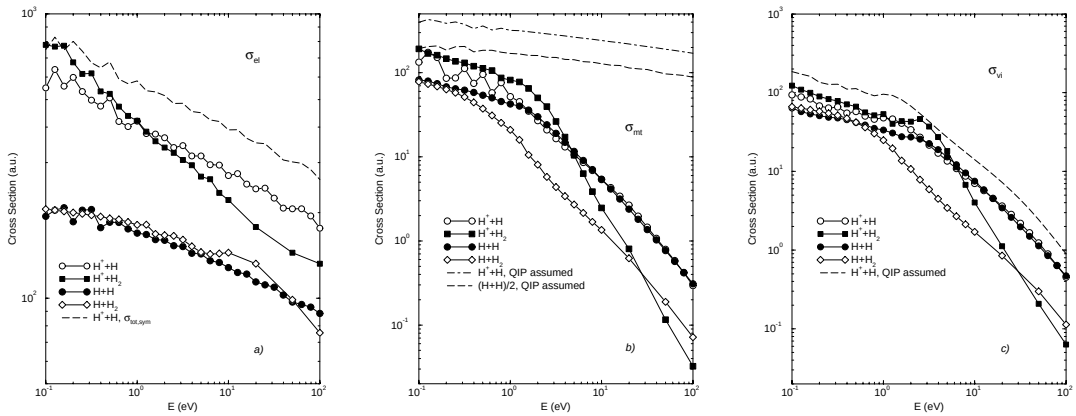

Fig. 2 Integral a) elastic, b) momentum transfer, and c) viscosity cross sections for typical cases considered.

II ION/ATOM-MOLECULE SYSTEMS

Elastic neutral-neutral (atom-atom) collisions have been the least studied among the systems considered here, while data for scattering from molecular systems are almost entirely unavailable. To our knowledge, only one comprehensive set of data is available for the latter over an extended energy range (0.067-6670 eV). This data are the momentum transfer cross sections for H+H_2 collisions found by Phelps [37] who interpolated between experimentally derived data at low energies and theoretical results (Smith *et al.* [38]) at high energies. However, a certain amount of data is available at temperatures lower than those of the present interest [39] regarding, in particular, rotational excitations needed for interpretation of the infrared emission and cooling of interstellar clouds. In contrast, the H^++H_2, being the most fundamental and simplest ion-molecule system collision system, has been often studied [40–48] from sub-eV to keV energies, with regard to elastic scattering, rotational and vibrational excitation, and charge transfer, but not in a comprehensive manner

The H^++H_2 charge transfer reaction, although endoergic, has a low threshold energy (1.83 eV), and is strongly coupled to the mechanism of vibrational excitation to states that are high enough ($\nu \geq 4$) to overcome the barrier. Thus, this reaction

is a second order process, for energies < 200 eV [37], with an integral cross section that is more than ten times lower than the cross section for excitation to the first excited state of H_2 . On the other hand, in order for the electron to make a transition to the excited surface ($H+H_2^+$), the H_2 bond must stretch while the projectile is still close enough to the H_2 molecule. Collisions that involve nuclear rearrangements will almost always lead to scattering at larger angles which will not significantly contribute to the presently considered elastic cross section results, but could influence to some extent the transport cross sections below about 1 eV due to their emphasis of large angle scattering. Thus, in the energy range considered here, it is satisfactory to treat elastic scattering and vibrational excitations with inclusion of only the ground electronic energy surface with the appropriate caution (i.e. using the transformation to the diabatic surface in the $H^+ + H_2$ case). This is the first assumption made in the present calculations. Moreover, the energy gap for any reaction that involves an electronic transition is much larger for neutral-neutral collisions, which allows greater certainty in the results obtained with only one electronic surface.

The second simplifying approximation is a variation of the so-called sudden approximation, known as the infinite order sudden approximation (IOSA) [49,50,40,41]. When the rotational motion is adiabatic with respect to the relative translational motion of the molecule and a colliding particle, the projectile effectively interacts with a molecule that has no rotational angular momentum. Such a physical situation allows the complete decoupling of the diatomic rotational and projectile orbital angular momenta in the scattering system and leads to an enormous simplification in the equations of motion. Hence, the rotationally summed cross sections only depend on the initial ground rotational state. The Hamiltonian contains only a vibrational kinetic energy operator as a "signature" of the molecular target, but also depends parametrically on the molecular orientation which is fixed during the collision. The calculations need to be repeated for a range of orientations and the resulting cross sections averaged. This approach has been followed for both fully quantal and semi-classical formulations and has been shown to be strictly valid only for systems with short range rotational coupling. Thus the sudden approximation is most applicable to the neutral-neutral system ($H+H_2$) where the anisotropy of the interaction is short-ranged.

Specifically, we have used the IOSA over the whole energy range considered and find that it suffices to expand the wavefunction in a truncated basis of 9 vibrational states. For $H^+ + H_2$ this allows convergence of the results for at least 3 excited states and 5 for $H+H_2$. However, for ion-molecule systems additional caution is needed, since the sudden approximation is expected to be valid for the $H^+ + H_2$ system above a collision energy of about 3 eV [45], while for lower energies its validity remains undetermined due to the lack of more elaborate calculations or measurements. Nevertheless, since typical rotational energies for H_2 are of the order of 0.01 eV or less, the classical argument of freezing molecular rotations for the duration of the collision for $E_{CM} > 0.1$ eV indicates that acceptable results may be obtained as long as rotationally averaged cross sections are calculated.

Some of the existing calculations for $H^+ + H_2$ collisions utilize the "time-dependent" or "impact-parameter" formalism which assumes a classical or often straight-line motion of the projectile [46]. While the straight-line trajectory method could be an acceptable approximation for small scattering angles, it poorly describes the scattering at larger angles. As demonstrated below, the scattering angles following vibrational excitation for both proton and neutral atom impact are shifted significantly toward larger values in comparison to the behavior displayed by elastic scattering. Thus we chose a fully quantal approach for both the projectile and diatomic vibrational motion.

It turns out that the principal mechanism for vibrational excitation in the $H^+ + H_2$ system is well understood [44] and is mainly an effect of "bond dilution" – the temporary depletion of electron density from the molecular bond by the passing proton. The vibrational excitation is caused by the stretching force which acts simultaneously on both of the H_2 nuclei, which becomes significant at small distances, thus causing the largest contribution to the cross section for large scattering angles. The mechanism is apparently weaker in $H+H_2$ scattering and the incident atom interacts predominantly with the nearest atom of the molecule. This is elucidated [17] through comparison with the elastic cross sections in the H+H system (Fig. 2a), as well as with the dependence on the molecular orientation.

III $\mathbf{H}^+ + \mathrm{H}_2(\nu) \rightarrow \mathrm{H} + \mathrm{H}_2$

Because of its potential significance in the chain of reactions in "molecular assisted recombination" leading to plasma detachment, we are studying charge transfer involving vibrationally excited H_2. Our preliminary results, summed over all final vibrational states of H_2^+, are presented in Fig. 3. The mechanism is expected to be

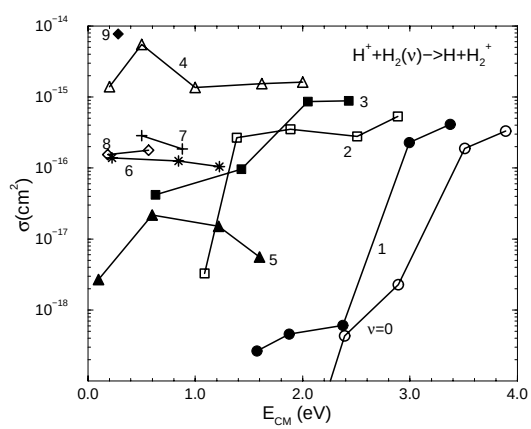

Fig. 3 Total cross sections for charge transfer in collisions of vibrationally excited $H_2(\nu)$ with H^+. The curves are indexed by initial state ν.

operative for plasma temperatures in the range 1-2 eV (close to the divertor plates) and thus, a fully quantum approach to the problem is required. When $\nu \geq 4$, the electron capture is realized without a threshold energy, resulting in large cross sections. The rate coefficients, estimated from the present results are 3-4$\times 10^{-9}$ cm^3/s for $\nu \geq 4$.

The cross sections in Fig. 3 were obtained by solving the molecular orbital close coupling equations within a set of all vibrational states of H_2 and H_2^+, using the IOSA [41] approximation. The averaging over the diatom orientations is done *a posteriori*. The exclusion of the vibrational continuum from the calculation may artifically enhance the results, since the dissociation from the excited vibrational states of H_2 is energetically accessible even for 1 eV energies. Treatment of the process, with inclusion of the dissociative channels is underway.

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