Elastic, excitation, ionization and charge transfer cross sections of current interest in fusion energy research

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Abstract

Due to the present interest in modeling and diagnosing the edge and divertor plasma regions in magnetically confined fusion devices, we have sought to provide new calculations regarding the elastic, excitation, ionization, and charge transfer cross sections in collisions among relevant ions, neutrals, and isotopes in the low-to intermediate-energy regime. We summarize here some of our recent work.

1 Introduction

In pursuit of ever more realistic, accurate models and diagnostic methods for fusion energy research, complete databases of heavy particle cross sections for excitation, ionization, charge transfer, and recombination have been sought for many years. While great progress has been made along these lines, the type of reactions and the collision energy range has been dictated primarily by the need to understand the physics of the central, core plasma in such magnetically confined plasma devices as tokamaks. Contemporary interest in developing so-called "next-step" experimental reactors, such as ITER, however, has highlighted the needed for the study of new atomic and molecular collision regimes. As described in great detail elsewhere [1], engineering and physics issues are focussed on (*i*) the edge plasma, which must be tailored to suppress the ingress of impurities into the core and to entrain them, and (*ii*) the divertor, which will be used for hydrogen recycling and heat (power) and particle (impurities, helium ash) exhaust. Since these plasma regimes are characterized by greatly lower temperatures and higher densities than the core, correspondingly different atomic, and even molecular, reactions play crucial roles.

2 Elastic scattering

Due to these necessarily lower temperatures and higher densities in the edge and divertor regions, significant amounts of neutrals will be present. Since the cross section for elastic ion-ion, ion-neutral, and neutral-neutral scattering can be large compared to the

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inelastic channels at very low collision energies, these processes play a dominant role in the momentum balance of these regions. In the production of atomic data relevant to fusion energy research, a database for elastic and other cross sections related to transport properties has not been compiled in light of the heretofore heavy emphasis on inelastic, intermediate to high energy collisions. In particular, these slow, neutral particles are important due to their role in radiating and dissipating power and in providing a high recycling region which shields plasma facing components from the high heat and particle fluxes. (For a description of various aspects of modeling neutral gas transport in edge and divertor plasmas, see for example Ref. [2]).

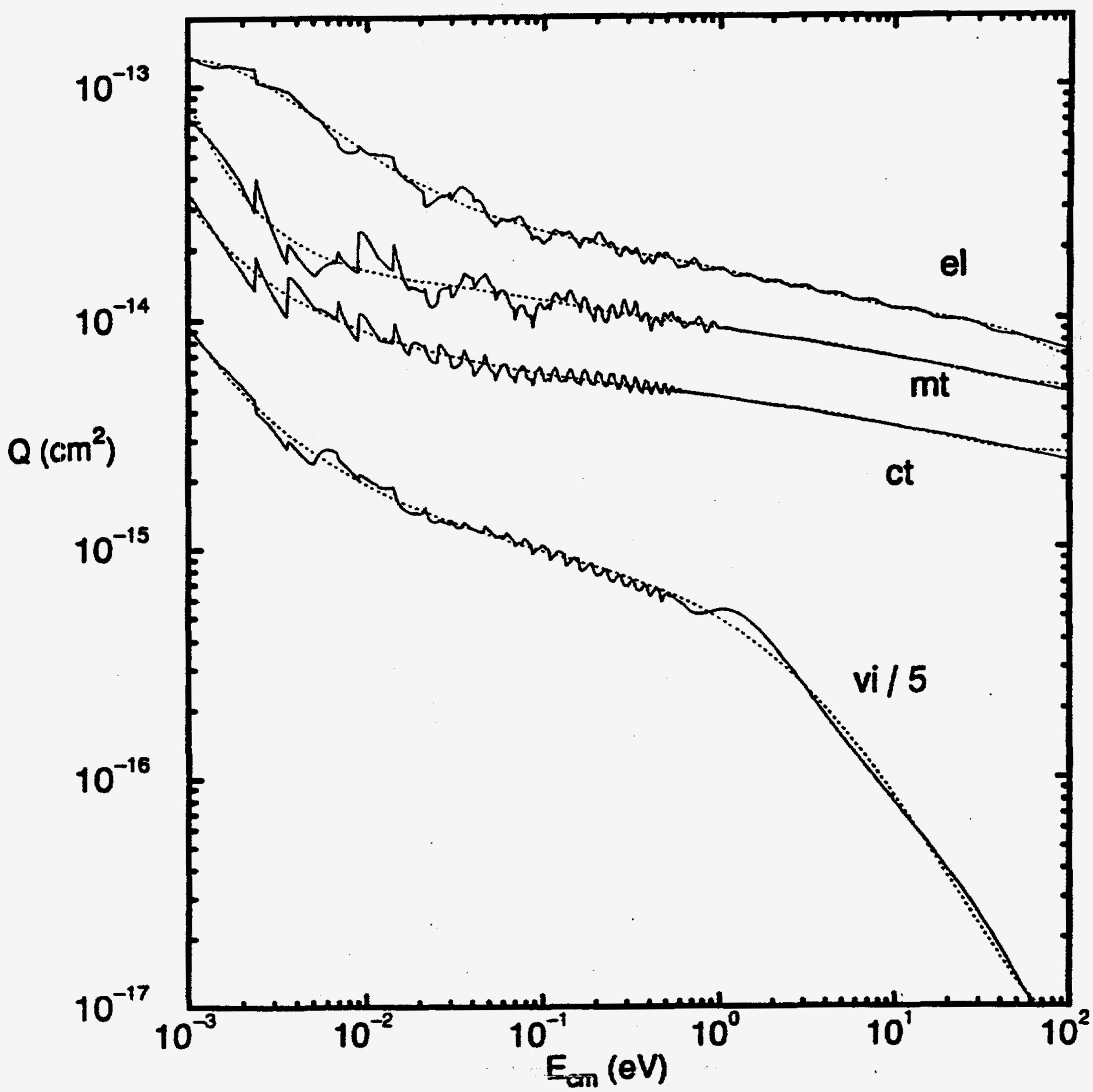
It was therefore our purpose in a recent work [3] to tabulate in a useful way data that can be found in the literature and to provide new calculations of the relevant cross sections where the data is not available, or when it has not be presented in a way which can be readily utilized. A significant contribution to such efforts has been made as well by Bachmann and Belitz [4] who utilized a classical approximation to compute cross sections for proton impact of H, H_2, and He, and for collisions of He^+ with He.

Since the edge and divertor regions will be rich in neutral atomic hydrogen, and molecular hydrogen recycled after recombination at the walls or introduced for fueling, these species have been of primary interest. In addition, since the ash of the fusion process must also be removed at the divertor, significant amounts of helium should also be present. Thus, we considered collisions among the various relevant ions and isotopes of H, H_2, and He. Since the edge plasma temperature is on the order of, say, 10 to 300 eV, and that of the divertor 1-50 eV, we consider center mass collision energies in the range $0.001 \leq E_{\rm cm} \leq 100$ eV. This range accommodates the fact that often the cross sections must be averaged over Maxwellian distributions so that knowledge of the cross section over a slightly larger range is useful. In addition, the extent of this range to the low end often allows a point of comparison to be made with data of astrophysical interest, and thus an additional benchmark.

For example, in Figure 1 we present the result of our (semiclassical) calculation of the elastic cross section compared with the classical approach of Bachmann and Belitz noted above and with the simple Massey-Mohr approximation. A very accurate quantum mechanically solution to the elastic scattering and charge transfer problem in the energy range of interest has been provided for $H^+ + H$ and [5, 6] and for $H^+ + D$ and $D^+ + H$ [7] by Hunter and Kuriyan. These works provided a benchmark for the development of our semiclassical approach, and we find very good agreement with the phase shifts they tabulated extensively [5]. In addition, we find good agreement with the elastic and charge transfer total and differential cross sections contained in these works. In addition, quite recently, Hodges and Breig [8] have performed numerical integrations of the radial Schrödinger equation for Hunter and Kuriyan's potential energy curves, and confirm their results independently. Our semiclassical results agree very well with their published elastic, momentum transfer, and charge transfer cross sections.

Furthermore, other related cross sections are actually of greater practical use. They

Figure 2. The elastic, momentum transfer, viscosity, and charge transfer cross sections for $H^+ + H$ along with smooth fits.



may be measured through various parameters of the gas or plasma transport (see e.g. Ref. [9]) or calculated from the elastic differential cross section. Of these, we will be particularly concerned with the momentum transfer (Q_{mt}) and viscosity (Q_{vi}) cross sections.

One of the most important fundamental quantities in the study of the mobility and diffusion of neutral or charged particles in a gas or plasma is the momentum transfer cross section, Q_{mt}, defined by

$$Q_{mt} = \int (1 - cos\theta) \frac{d\sigma_{el}}{d\Omega} d\Omega \tag{1}$$

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

To see how this quantity is related to momentum transfer, consider the elastic collision between two particles a and b. The linear momentum of particle a is simply μv_a. If θ is again the center of mass scattering angle, the change in the forward momentum of the particle is $\mu v_a(1 - cos\theta)$. Thus, Q_{mt} is a measure of the average forward momentum lost in such collisions. Since backscattering retards the diffusion of particles in a gas or plasma, this loss of forward momentum thus determines the rate of diffusion and therefore Q_{mt} is often referred to as the "diffusion cross section." Other important measures may be defined in terms of Q_{mt}, such as the momentum transfer mean free path, collision frequency, and fractional energy loss per collision [9].

If the elastic differential cross section is dominated by forward scattering, then owing to the factor $(1 - cos\theta)$ in the definition of the momentum transfer cross section, $Q_{el} > Q_{mt}$. Conversely, if backscattering dominates, $Q_{mt} > Q_{el}$. If the elastic cross section diverges as $\theta \rightarrow 0$, this factor may lead to a finite value of Q_{mt}.

Inversely related to the heat conductivity and viscosity of a gas or plasma is the "viscosity cross section." It too is defined as the integral over solid angle of the elastic differential cross section, weighted by a factor of $sin^2\theta$ instead of $(1 - cos\theta)$. Thus,

$$Q_{vi} = \int sin^2\theta \frac{d\sigma_{el}}{d\Omega} d\Omega \tag{3}$$

$$= 2\pi \int_0^\pi sin^3\theta \frac{d\sigma_{el}}{d\Omega} d\theta \ . \tag{4}$$

Since the $sin^2\theta$ factor is maximum at $\theta = \pi/2$ and goes to zero for $\theta \rightarrow 0$ or π, this factor emphasizes scattering near $\pi/2$ while deemphasizing either forward or backward scattering. Collisions resulting in scattering to center of mass angles near $\pi/2$ are more effective in inhibiting conductivity since such collisions tend to equalize the energy, and therefore, the greater the rate of collisional equalization of energy, the smaller the viscosity and heat conduction. Clearly, if the elastic differential cross section is dominated by forward scattering, the viscosity cross section is much smaller than the elastic total cross section.

Figure 2 shows our computed elastic, momentum transfer, viscosity, and charge transfer cross sections, along with smooth fits which are needed by modeling codes. These fits

Figure 3. The potential energy curves, elastic differential cross section, and the elastic and related transport total cross sections for Be^{2+} + H.

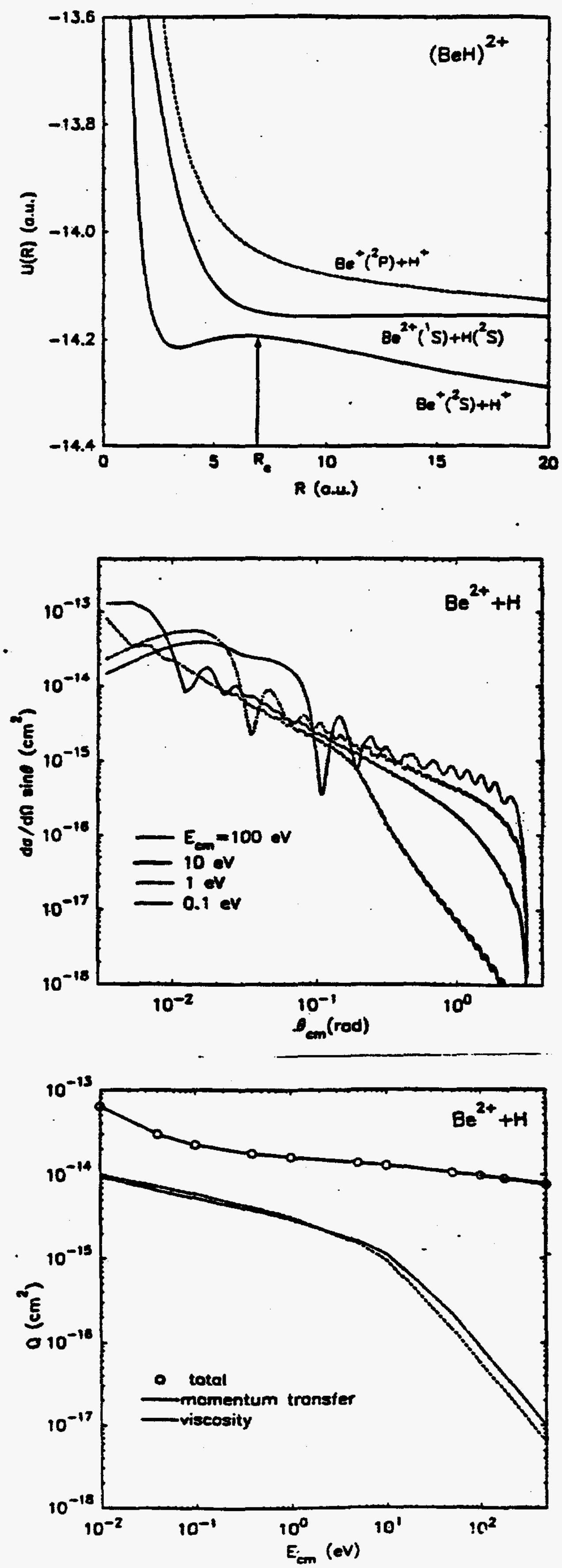
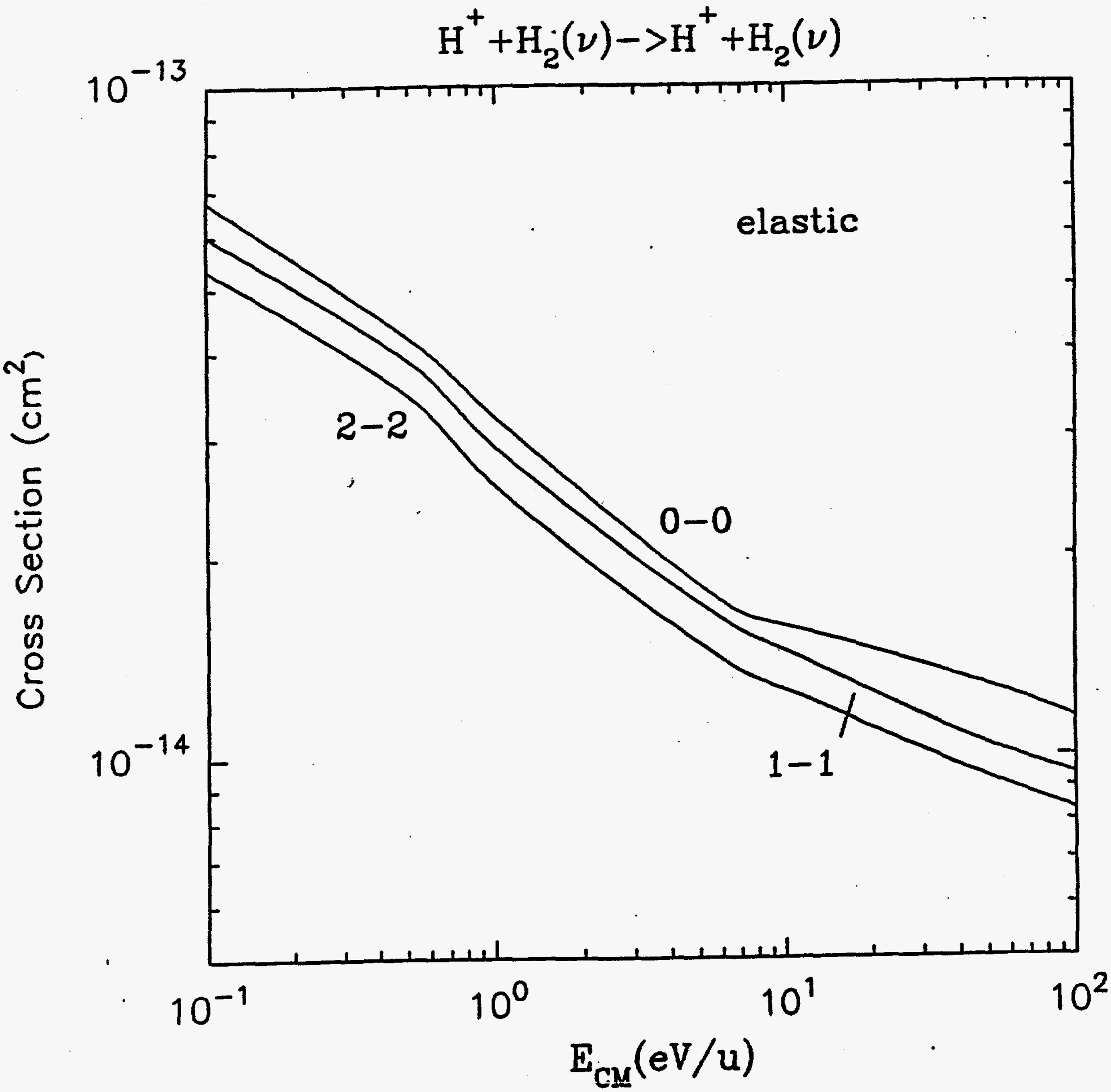


Figure 4. Preliminary result for elastic scattering from the ground and low-lying vibrationally excited states of H_2 by proton impact.



are tabulated, along with similar results for H + H, H + He, and other systems in Refs. [3, 4].

Other collision systems of current interest involve beryllium and its ions. Beryllium is a potentially useful plasma facing component since it is of low-Z, and therefore engenders low deleterious radiation losses, and has good physical/chemical properties. Therefore, beryllium neutrals and ions will be present in the divertor which may be lined with this material. Calculation of the elastic and transport cross sections requires accurate potential energy curves for the ground and low-lying states of $(BeH)^{q+}$. Such calculations are presently the object of state-of-the-art approaches. Therefore, we have applied an unrestricted Hartree-Fock calculation using Gaussian bases and a subsequent single configuration interaction approach to fill in the gaps in existing accurate data for these potentials. Finally, to facilitate our one- and two-state calculations of the elastic phase shifts, we have fit these potentials using a 6-parameter formula. This procedure and our results for scattering of Be^{2+}, Be^{+}, and Be from H are given in a recent article [10] and in Figure 3 we display the potential energy curves, typical differential cross sections, and the total elastic, momentum transfer, and viscosity cross sections for Be^{2+} + H.

Also of particular interest recently is the elastic and related transport cross sections for protons colliding with H_2. Slow collisions of these species will be quite prevalent in the divertor as hydrogen plasma is neutralized, partly through recombination on the walls. In order to calculate elastic cross sections for scattering of protons on H_2 molecules in various initial vibrational states, an Infinite Order Sudden Approximation (IOSA) was used. In effect, rotational motion of the H_2 molecule is considered frozen during the collision, allowing averaging of the cross sections obtained for fixed H_2 orientations. Adiabatic surfaces $U(R, \rho, \gamma)$ were calculated *ab initio* using the quantum chemistry program package GAMESS in its RHF-Full CI options, with 54 S, P Gaussian basis states. The calculation is done for 5200 geometrical configurations of H_3^+, varying R in the range from 60 to 0 a.u., and ρ from 0.6 to 5.4 a.u., for $\gamma = 0^o, 30^o, 60^o$, and 90^o. The semiclassical phase shifts η_l were calculated for each fixed (ρ, γ) combination $(0 \leq l \leq 3000)$, thus forming the $\rho-$dependent scattering amplitude. For each H_2 orientation, the amplitude was averaged over the normalized wave function of the relevant vibrational state ν. Finally, the resulting differential and total elastic cross sections were averaged over the full solid angle of the H_2 orientations. Results of these calculations will be published soon and in Figure 4 we present our preliminary result for the elastic cross section.

3 Ionization in collisions of H with H

Owing to the relatively low plasma temperatures of the edge and divertor regions and to conditions present in certain astrophysical environments, recent interest has turned to ionization in slow collisions of H with H. To treat this collision system, we have generalized the method of hidden crossings [11] to treat mutlielectron, multicenter systems utilizing molecular Hartree-Fock and single configuration interaction methods extended into the

Figure 5. Single ionization in H + H collisions. Displayed are results of the multicenter, multielectron hidden crossings approach (solid line), measurements by Gealy *et al.* (diamonds) and by McClure (squares), theoretical results of Shingal *et al.* (dash-dot line), and Shingal *et al.*'s correction for simultaneous ionization of one electron and excitation of the other (dashed line).

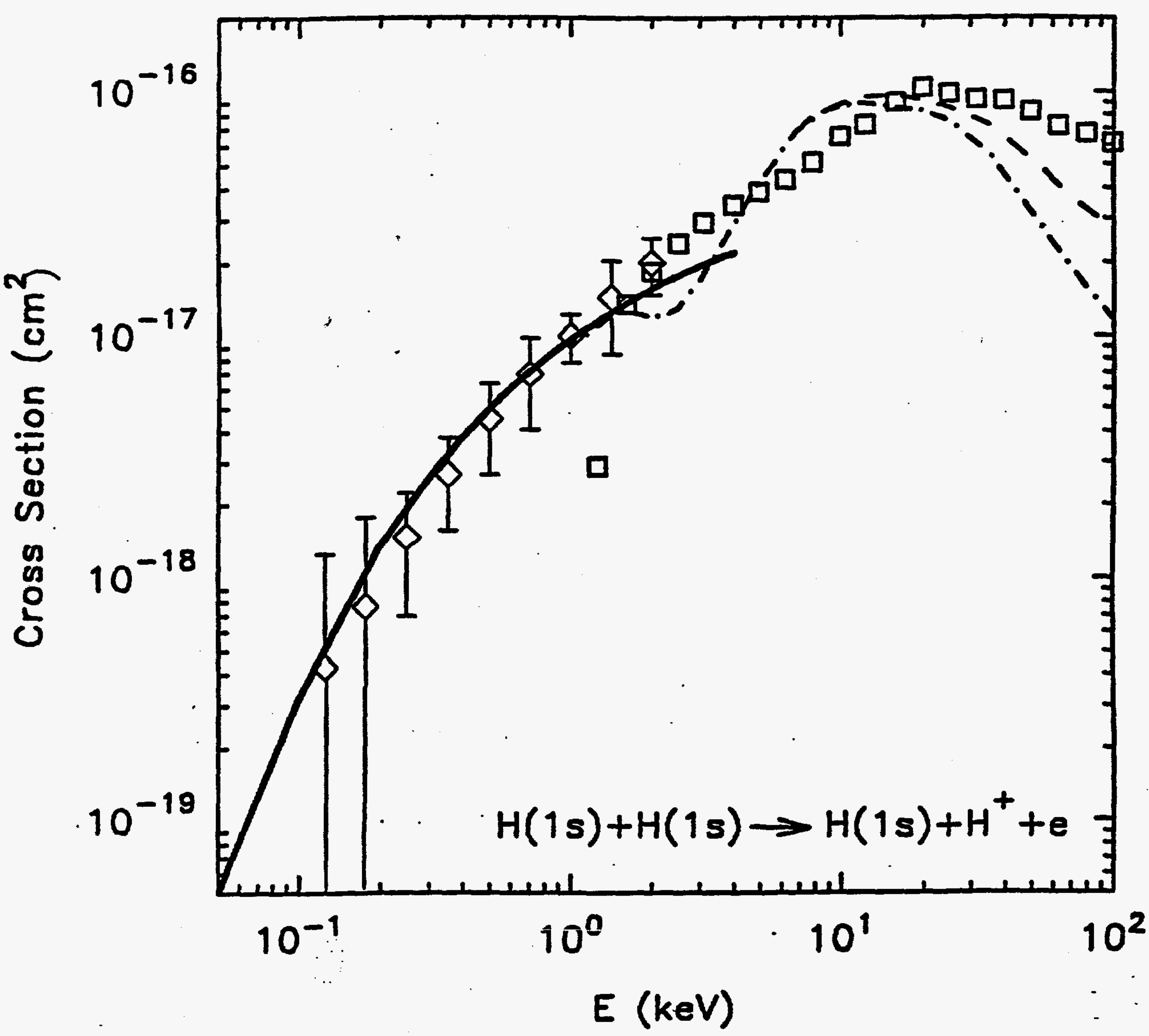
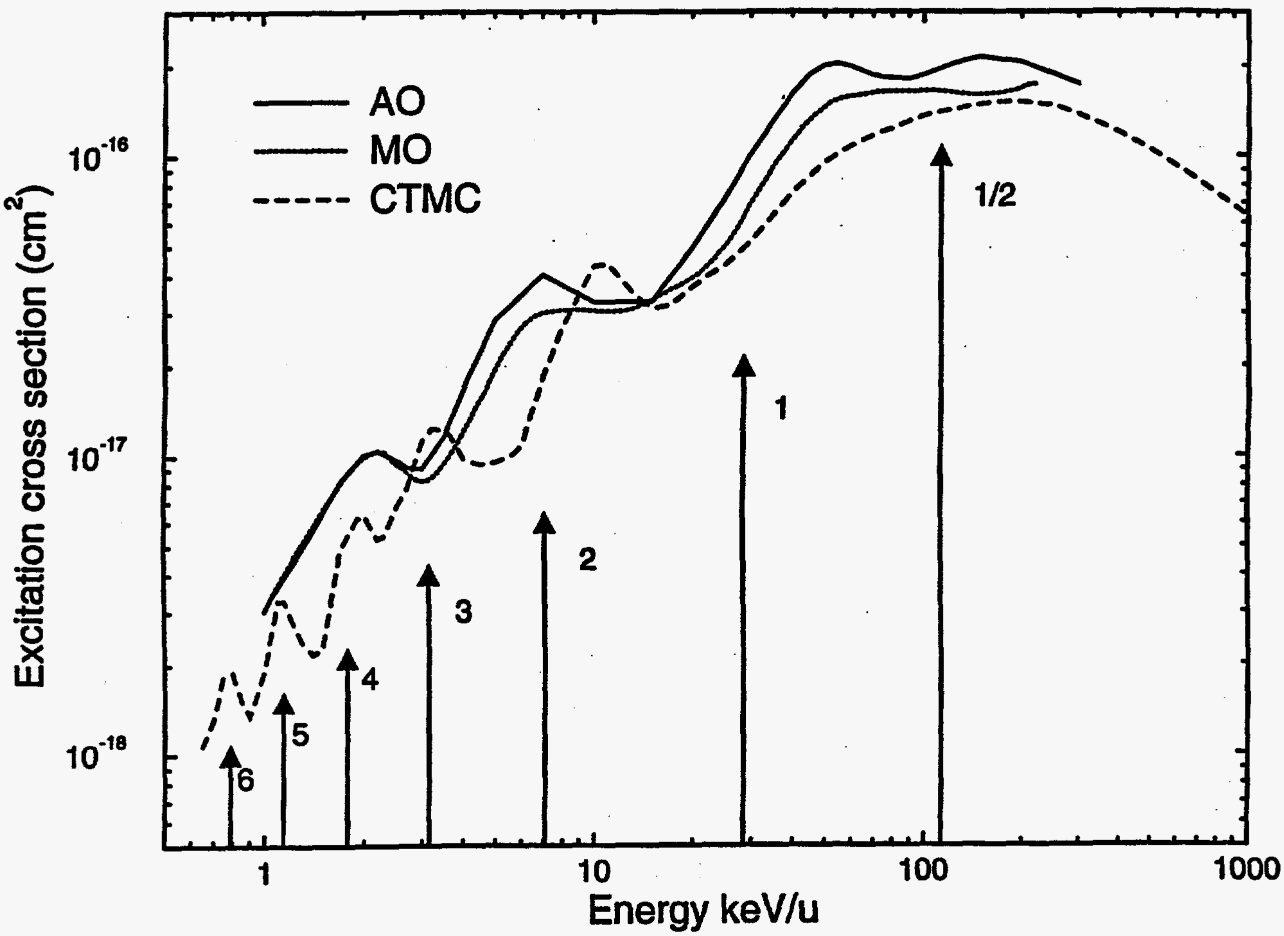


Figure 6. Excitation to the n=2 level of H by He^{2+} impact. Along with our CTMC result (dashed line), shown are atomic orbital (solid line, Fritsch *et al.*) and molecular orbital (dotted line, Errea *et al.*) results. Arrows indicate the peak positions predicted on the basis of a simple timing model presented in a forthcoming manuscript.



complex plane of internuclear separation. In brief, this method identifies the positions in the complex plane at which the promotion between electronic states (possibly the continuum) is strongly isolated, and thus can predict the probability of transitions. This recent work was the first in which diabatic promotion to the continuum in a two-center, two-electron system was shown. Excellent agreement with experiment was found regarding ionization in 50 to 1000 eV H + H collisions (see Figure 5).

4 Other inelastic collisions

As mentioned above, since beryllium is often used and proposed for plasma-facing components, its inelastic collisions with principle plasma species are important to quantitatively understand so that they maybe taken into account in plasma models. Furthermore, since charge exchange recombination spectroscopy has proven extremely useful in diagnosing the transport properties of the plasma and other characteristics, tabulations of the state-selective charge transfer cross section are often required by diagnostians. Thus, we have recently computed over a wide range of energies the excitation, ionization, and state-selective charge transfer cross sections for Be ions colliding with atomic and molecular hydrogen [12]. We have also carried out a similar study for neon ions [13] since this species may be puffed into the divertor in order to beneficially increase the radiated energy, thereby decreasing the power load directly on the divertor plates. In addition, frozen pellets of moderate-Z materials such as neon have been proposed as so-called "killer pellets" to quench the plasma quickly in the event of a disruption.

In these recent works we tabulate extensively the state-selective charge transfer cross section and compare our inelastic cross sections computed with the classical trajectory Monte Carlo (CTMC) technique with other available theoretical results and with experiment. By and large such other data does not exist. In addition to the rather routine tabulation of needed results, these works often provided surprises which proved quite interesting. For example, in both works we found oscillations of the excitation cross section at around 10 keV/u with the CTMC method which to our knowledge have never been seen before. We found that previous atomic orbital close coupling calculations also displayed this feature, but left the physical mechanism underlying its formation essentially undetermined. This has lead to much more detailed work to elucidate such a mechanism and is the subject of a manuscript in preparation. In Figure 6 we illustrate this oscillation for excitation in He^{2+} + H collisions where extensive atomic orbital calculations have been made by Fritsch *et al.* [14].

Acknowledgements

The authors gratefully acknowledge the support for this work by the U.S. D.O.E, Office of Fusion Energy Sciences in a grant to Oak Ridge National Laboratory, managed by Lockheed Martin Energy Research Corp. under contract number DE-AC05-96OR22464.

References

[1] R.K. Janev, in: *Review of Fundamental Processes and Applications of Atoms and Ions* (C.D. Lin, ed.), World Scientific, Singapore (1993).

[2] D. Reiter, in: *Atomic and Plasma-Material Interaction Processes in Controlled Thermonuclear Fusion* (R.K. Janev and H.W. Drawin, eds.), Elsevier Science Publishers (1993).

[3] D.R. Schultz, S.Yu. Ovchinnikov, and S.V. Passovets, *Elastic and Related Cross Sections for Low-Energy Collisions among Hydrogen and Helium Ions, Neutrals, and Isotopes*, in: *Atomic and Molecular Processes in Fusion Edge Plasmas*, edited by R.K. Janev (Plenum, New York, 1995) p. 279.

[4] P. Bachmann and H.J. Belitz, *Elastic Processes in Hydrogen-Helium Plasmas: Collision Data*, Max Planck Institut für Plamsaphysik Report IPP 8/2 (1993).

[5] G. Hunter and M. Kuriyan, Proc. Roy. Soc. (London) A **353**, 575 (1977).

[6] G. Hunter and M. Kuriyan, At. Data. Nucl. Data Tables **25**, 287 (1980).

[7] G. Hunter and M. Kuriyan, Proc. Roy. Soc. (London) A **358**, 321 (1977).

[8] R.R. Hodges and E.L. Breig, J. Geophysical Res. **95**, 7697 (1991).

[9] E.W. McDaniel, *Collision Phenomena in Ionized Gases*, John Wiley, New York (1964); *Atomic Collisions: Electron and Photon Projectiles*, John Wiley, New York (1989); *Atomic Collisions: Heavy Particle Projectiles*, John Wiley, New York (to be published).

[10] P. Krstić, D.R. Schultz, and G. Bent, Physica Scripta **T62**, 21 (1996).

[11] P. Krstić, G.Bent, and D.R. Schultz, Phys. Rev. Lett. **77**, 2428 (1996).

[12] D.R. Schultz, P.S. Krstić, and C.O. Reinhold, Physica Scripta **T62**, 69, (1996).

[13] D.R. Schultz and P.S. Krstić, Atomic and Plasma-Material Interaction Data for Fusion **6** (1996).

[14] W. Fritsch, R. Shingal, and C.-D. Lin, Phys. Rev. A **44**, 5686 (1991).