ASSOCIATIE EURATOM-FOM

FOM-INSTITUUT VOOR PLASMAFYSICA

RIJNHUIZEN — NIEUWEGEIN — NEDERLAND

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ABSTRACT

In this report a summary is given of the atomic processes which are relevant for the ionization balance and for the transport in a plasma consisting of hydrogen with a small admixture of helium.

Attention is paid mainly to processes in plasmas with temperatures below 100 eV and electron densities between 3×10^{13} and $3\times10^{14}\,cm^{-3}$. conditions which prevail in a so-called cold plasma blanket.

The species considered are electrons, protons, hydrogen atoms (ground state and excited), α-particles, He^{+}-ions (ground state and excited), and helium atoms (ground state and excited).

The discussed processes are charge exchange, ionization, recombination, (de-)excitation, and elastic scattering.

INTRODUCTION

One of the advantages claimed for a cold plasma blanket[1)] is the possibility to fuel the reacting core of a thermonuclear reactor and to exhaust the produced helium.

Of course, the behaviour of a small admixture of helium in a background plasma of hydrogen (H or D,T) must be known before a study of the exhaust problem is possible. This behaviour depends on the particle balance of the cold plasma blanket, i.e. on the ionization balance and on the transport processes.

Since the temperatures in the cold plasma blanket are low ($1 \div 100$ eV typically), also neutral species may be present. These may be used in experiments for diagnostic purposes[2)].

Thus, in order to gather the information required for a study of the behaviour of helium in a hydrogen background plasma, one has to analyse all processes in a mixture of e, H^+, H, He^{2+}, He^+ and He, where H, He and He^+ may be in excited states. As mentioned above, the emphasis is on temperatures less than 100 eV. Further restrictions are on the electron density (roughly 3×10^{13} - 3×10^{14} cm^{-3}) and on the total amount of helium (a few per cent of the total amount of hydrogen).

This report is a compilation of the information we use (or need) for our modelling of cold plasma blankets. Unless stated otherwise, cgs units are used.

CHARGE-EXCHANGE PROCESSES

Due to the low temperature, the energy of the ionic species will not be large enough to overcome the Coulomb repulsion, so charge exchange between ions will be impeded. Thus, only the interactions between neutral species and ions have to be considered.

Possible processes are:

a) $H + H^+ \rightleftarrows H^+ + H$

b) $H + He^+ \rightleftarrows H^+ + He$

c) $H + He^{2+} \rightarrow H^+ + He^+$

d) $He + He^+ \rightleftarrows He^+ + He$

e) $He + He^{2+} \rightarrow He^+ + He^+$

f) $He + He^{2+} \rightleftarrows He^{2+} + He$.

We shall now consider the importance of these processes:

a) $H + H^+ \rightleftarrows H^+ + H$.

The cross-section for this process is well-known: an analytic expression for low energies ($E \ll 34$ keV) is[3)]

$$\sigma = 6.94\times10^{-15}\ (1 - 0.155\ {}^{10}\log E_{eV})^2\ \text{cm}^2 . \qquad (1a)$$

The maxwellian rate coefficient can be expressed in a series expansion[3)] .

$$\ln \langle\sigma v\rangle = \sum_{i=0}^{8} A_i\ (\ln kT)^i . \qquad (1b)$$

For low energies a good approximation is simply $\langle\sigma v\rangle = \sigma(\langle v\rangle)\cdot\langle v\rangle$.

b) $H + He^+ \rightleftarrows H^+ + He + 11\ \text{eV}$.

This is an example of an asymmetric charge-exchange process, for which the so-called adiabatic criterion of Massey holds[4)]. At low impact energies the cross-section predicted by the approximation of Rapp and Francis[5,6)] is

$$\sigma = \frac{10.82\ \gamma^2 v^4}{\pi a_o^2\ \omega^4} \qquad (2a)$$

with $\gamma = \bar{E}_{ion}/13.6$ (= 1.4 for this process) and $\omega = |\Delta E|/\hbar$ (= $1.67\times10^{16}\ s^{-1}$ for this process). Here, $\bar{E}_{ion}$ is the average of the two ionization energies in eV and $|\Delta E|$ is the absolute difference between them.

For a relative velocity, v, this yields a cross-section of

$$\sigma = 3.1\times10^{-48}\ v^4\ \text{cm}^2 . \qquad (2b)$$

Experimental data of this cross-section are available only for high impact energies[3,7)]. The approximation of Rapp and Francis overestimates the $H^+ + He$ cross-section[3)] and underestimates the one for $He^+ + H$ (Ref. 7); it yields a maxwellian rate coefficient

$$\langle\sigma v\rangle = 6.7\times10^{-21}\ T_{eV}^2\ \text{cm}^3\ s^{-1} . \qquad (2c)$$

At very low energies, just above the energy defect ΔE of 11 eV, it is not clear how the cross-section of the process $H^+ + He$ behaves.
In the reverse process, of He^+ colliding with H, this energy is released; this may be of importance for the interaction between He^+ and a wall loaded with hydrogen.

Fortunately, the cross-section for the exchange process $H - H^+$ is many orders of magnitude larger and the protons are far more abundant, so the process $H - He^+$ is not important for the behaviour of the H-fluid.

Also the cross-section for resonant exchange between He and He^+ and between He and He^{2+} is so large (cf. d and f) that, in spite of the low He^+ and He^{2+} density, these processes are more important than the He - H^+ charge exchange.

c) $H + He^{2+} \rightarrow H^+ + He^+$.

This reaction will lead to extra recombination of α-particles, because the Coulomb force will impede the reverse reaction between the ions.

In this process, the excited states of the H-atom start to play a role, since the level with main quantum number, n, has the same ionization energy as the He^+ ion level with number 2n. Therefore, the process has a resonant character.

The cross-section for charge exchange between α-particles and excited H-atoms was measured using merging beams[8]. It increases with n and is almost independent of the energy below 100 eV. A useful expression is[9]

$$\sigma \approx 6.3\times10^{-16}\, n^4\ \mathrm{cm}^2 \ , \tag{3}$$

although this is questionable at low values of n.

As the population density of high levels increases as n^2 (assuming Partial Local Thermodynamic Equilibrium), the probability of charge exchange increases as n^6. Of course, due to the reduction of the ionization energy, the number of bound states is limited. The quantum number of the last bound state, n_{max}, depends on the lowering of the ionization energy, ΔE_∞, as[10]

$$n_{max} = \sqrt{\frac{Z^2 E_H}{\Delta E_\infty}} \ . \tag{4}$$

For ΔE_∞ several expressions can be used, either based upon Debye shielding or on nearest neighbour considerations[10].

In an actual plasma, levels with large quantum numbers are broadened so much that bound states overlap and are coupled to the continuum. It is not clear how the exchange cross-section behaves in that case.

Due to the resonant capture process, the recombination rate into the $He^+(2n)$ level is increased; this will, of course, lead to a larger population of this level. This results in a larger ionization rate and, as a consequence, the net recombination is less enhanced.

As the levels which are important for the charge exchange process are strongly tied to the continuum of α-particles and electrons, by collisional processes, the net increase in recombination is mainly due to contributions of low-lying levels, with a small charge-exchange cross-section. Here, the overpopulation of the ground state of hydrogen due to diffusion becomes important, as well as the deviations from the n^4-scaling law.

Estimates of the net extra recombination are given in Fig. 1. In these calculations it is assumed that the ground state of H is populated by a factor of 100 over the value in a homogeneous steady-state plasma (this becomes questionable for temperatures less than 3 eV). Two cases are shown: one based upon the the n^4-law also for the ground state (giving a net increase of about a factor of 2.5 in the temperature range between 10 and 100 eV; the second based also on the n^4-law for all excited levels, but with a zero cross-section for charge exchange with the ground state. The latter case is more in agreement with recent measurements[11] and theoretical predictions[12], at least for the ground state.

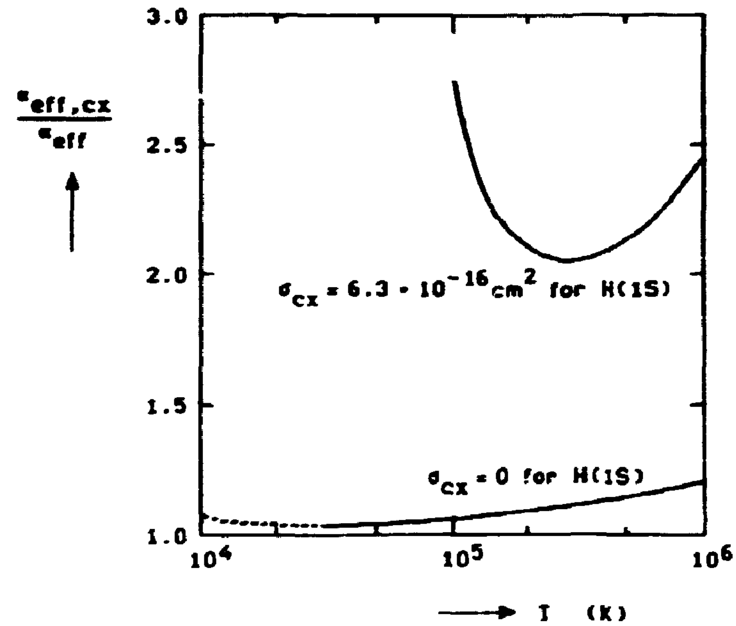

Fig. 1. The ratio of the net recombination rate coefficient for α-particles with and without the effects of charge exchange with H-atoms. Upper curve: cross-section according to Eq.(3) for all levels of H. Lower curve: cross-section according to Eq. (3) only for excited levels. The number density of ground state atoms is taken to be 100 times the value for a plasma in a homogeneous steady state. The electron density is 10^{14} cm^{-3}.

d) $He + He^+ \rightleftarrows He^+ + He$.

This is again a resonant process with a large cross-section[13]

$$\sigma \approx (5.1 - 0.3 \ln E_{rel,eV})^2 \; 10^{-16} \; cm^2 \; . \qquad (5)$$

e) $He + He^{2+} \rightarrow He^{+} + He^{+} + 30$ eV.

This is a reaction with an energy defect, which makes its occurrence less probable at low impact energies[14] (cf. b)). For energies below 1 keV, the cross-section is more than an order of magnitude smaller than the one of the resonant process $He + He^{2+} \rightleftarrows He^{2+} + He$ (cf. f)).

f) $He + He^{2+} \rightleftarrows He^{2+} + He$.

This resonant exchange of two electrons has again a weak energy dependence at low impact energies; from the data[15] the following cross-section at low energies may be obtained:

$$\sigma \approx 7\times10^{-16} E_{rel,eV}^{-0.15} \text{ cm}^2 \ . \qquad (6)$$

From the discussion of the charge-exchange processes we can conclude the following:

- the momentum balance of the H-atoms is, apart from elastic collisions, only influenced by charge exchange with H^{+};
- the momentum balance of the He-atoms is governed by charge exchange with the He^{+} and He^{2+} ions (unless, of course, their density is very low), apart from elastic contributions in He-H^{+} collisions which are discussed below;
- the ionization balance of the He^{+} - He^{2+} system is hardly affected by the 'charge-exchange recombination' $H + He^{2+} \rightarrow H^{+} + He^{+}$.

IONIZATION, RECOMBINATION AND (DE-)EXCITATION

A large number of collisional-radiative models are available for the ionization and excitation balance of neutral hydrogen, neutral helium and hydrogen-like ions.

Fujimoto[16] published an extensive model for neutral helium, based on rate coefficients presented in a separate report[17].

In order to use these models in combination with a transport code, a number of simplifications is required to reduce the computer time spent in the evaluation of the ionization balance. We introduced a number of simplifications in the code of Fujimoto viz.

- A reduction in the number of levels treated. A large electron density shifts the limit for Partial Local Thermodynamic Equilibrium (PLTE) to a level below the highest level Fujimoto treats separately. This reduces significantly the number of rate equations.

- Metastable levels have a short lifetime because they are easily excited by electrons. This implies that they require no special treatment, since interactions between atoms in metastable states can be neglected.
- Trapping of radiation does not occur because of the low helium density.

The use of this simplified model yields the net rate coefficients for ionization and recombination as presented in Figs. 2a and 2b. For data about the cross-sections for excitation and de-excitation we refer to Refs. 16 and 17.

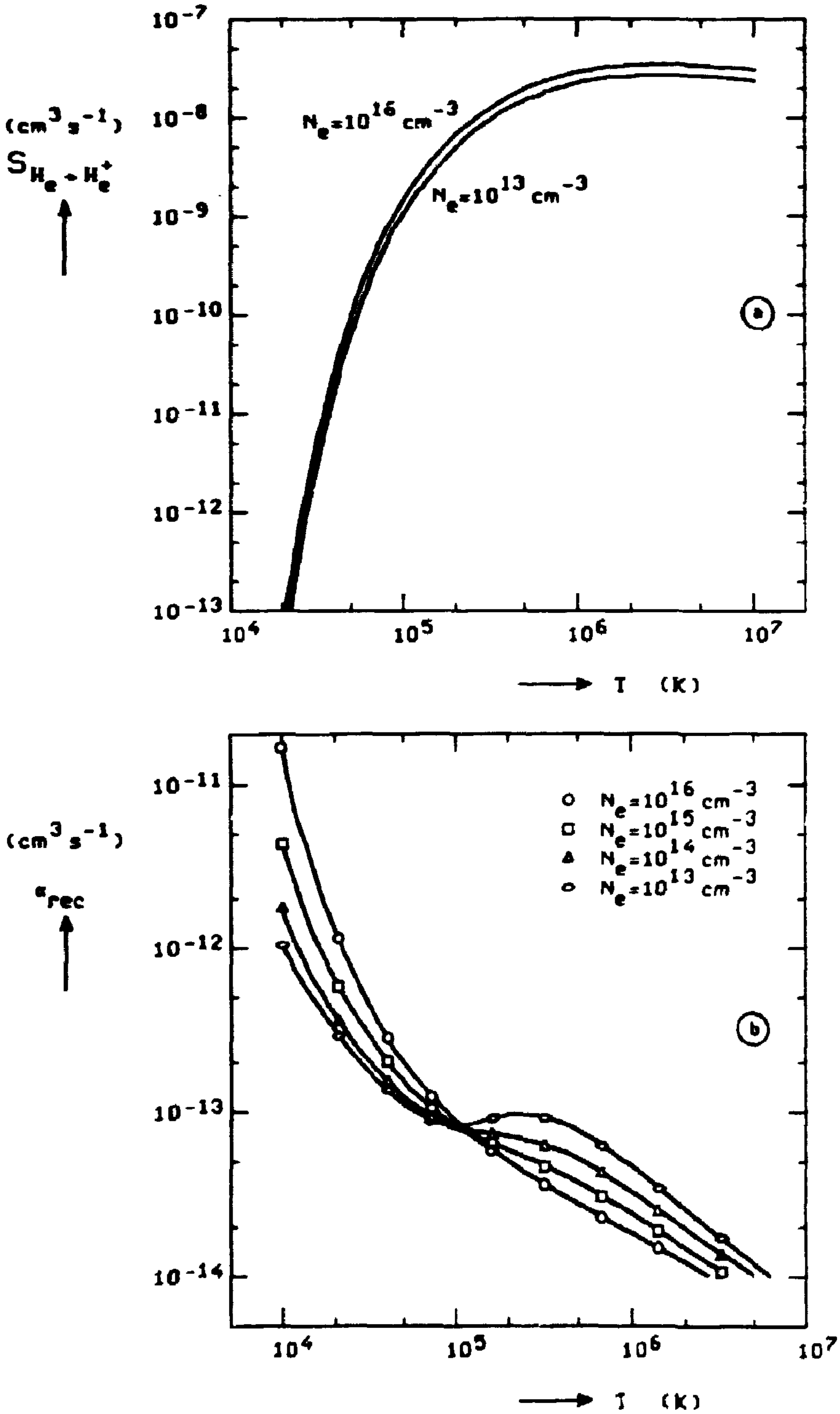

Fig. 2a,b.

The net ionization and recombination rate coefficient for neutral helium, as computed with the code of Fujimoto (Ref. 16).

For the H-atom we also have a simplified model available[18]. It has been adapted as to include also the range of electron densities between 10^{13} and 10^{14} cm^{-3}. The collisional-radiative model for hydrogen-like ions can be obtained from an appropriate scaling of the rate coefficients for the H-atom[19]. Apart from some minor changes it implies the use of the H-atom model at a reduced electron density $\eta = n_e/z^7$ and a reduced temperature $\theta = T/z^2$. Of course, in the case of He^+, the source of excited ions due to charge exchange with neutral hydrogen has to be inserted in the balance of the relevant levels. The corresponding sinks in the balance for the levels of hydrogen need not be considered, because there excitation by electrons is by far the dominant loss.

ELASTIC ION-NEUTRAL INTERACTIONS

The solution of the transport equations for neutral particles requires that elastic processes be considered as well. For pure hydrogen plasmas it is usually possible to neglect the elastic term because charge exchange and ionization play a dominant role for the H-atom. Only for temperatures below 1 eV this approximation loses its validity.

With the inclusion of a small contamination of helium, elastic collisions between He-atoms and protons become important for temperatures below approximately 15 eV, as we will show below. Firstly because the cross-section for resonant charge exchange with He^+ and He^{++} is about an order of magnitude less than the one for H with H^+ while, moreover, the abundance of the helium ions is expected to be much lower than that of protons (or, in thermonuclear plasmas, of D^+ and T^+). Secondly, the ionization rate for He is less than the rate for H at low ($\lesssim$ 50 eV) electron temperatures.

As far as momentum transfer is concerned, elastic interactions are characterized by the cross-section[20]

$$Q^{(1)}(g) = 2\pi \int_0^\infty (1-\cos\chi)\, b\, db \,, \tag{7}$$

where g is the relative initial velocity of approach between the colliding particles, b the impact parameter and χ the deflection angle, given by

$$\chi(g,b) = \pi - 2b \int_{r_m}^\infty \frac{dr/r^2}{\left(1 - \frac{b^2}{r^2} - \frac{2\varphi(r)}{\mu g^2}\right)^{\frac{1}{2}}} \,, \tag{8}$$

where μ is the reduced mass, r the radial coordinate, $\varphi(r)$ the particle interaction potential and r_m the distance of closest approach, which is obtained from the equation

$$1 - \frac{b^2}{r_m^2} - \frac{2\varphi(r_m)}{\mu g^2} = 0 \; . \qquad (9)$$

In order to make the cross-section $Q^{(1)}(g)$, as well as the other quantities, applicable for the widely used class of potentials, $\varphi(r) = \epsilon f(\frac{r}{\sigma})$, where ϵ is the strength of the potential, σ its characteristic range, and f a suitable function, it is convenient to define dimensionless quantities:

$$r^* = r/\sigma; \quad b^* = b/\sigma; \quad \varphi^* = \varphi/\epsilon; \quad g^* = g(\mu/2\epsilon)^{\frac{1}{2}} \; . \qquad (10)$$

The reduced cross-section $Q^{(1)*}$ is defined by dividing $Q^{(1)}$ by the 'rigid sphere' value $\pi\sigma^2$:

$$Q^{(1)*} = \frac{Q^{(1)}}{\pi\sigma^2} \; . \qquad (11)$$

In dimensionless form we find

$$\chi(g^*,b^*) = \pi - 2b^* \int_{r_m^*}^{\infty} \frac{dr^*/r^{*2}}{\left[1 - \left(\frac{b^*}{r^*}\right)^2 - \frac{\varphi^*(r^*)}{g^{*2}}\right]^{\frac{1}{2}}} \; , \qquad (12)$$

$$1 - \left(\frac{b^*}{r_m^*}\right)^2 - \frac{\varphi^*(r^*)}{g^{*2}} = 0 \; , \qquad (13)$$

$$Q^{(1)*}(g^*) = 2\int_0^{\infty} \left(1-\cos\chi(g^*,b^*)\right) b^* db^* \; , \qquad (14)$$

Evaluation of the above integrals for realistic potential functions requires numerical techniques. These deserve extra care because of the singularity in the integrand of Eq. (12). We shall not elaborate on the numerics here, but merely present results of calculations relevant for hydrogen/helium plasmas. Specific information pertaining to the methods employed is available on request.

Let us consider elastic interactions between H^+ on the one side and H or He on the other.

For H-H^+ we use the $2p\sigma_u$ potential of the molecular ion H_2^+:

$$\varphi_{2p\sigma_u}(r) = \frac{e^2}{a_o}\left\{\frac{1}{S(r)-1}\left[\frac{a_o}{r} - e^{-2r/a_o}\left(\frac{a_o}{r}+1\right) - e^{-r/a_o}\left(1+\frac{r}{a_o}\right)\right] + \frac{a_o}{r}\right\}, \qquad (15)$$

where $S(r) = \left[1 + \frac{r}{a_o} + \frac{1}{3}\left(\frac{r}{a_o}\right)^2\right]e^{-r/a_o}$.

Here, a_o = 0.529 Å is the Bohr radius and e^2/a_o = 1 Hartree = 27.211 eV.

The situation for He-H^+ is a bit complicated because no data covering the whole energy range of interest were available to us. Elastic scattering measurements were published by Weise et al.[21] for the energy range 3 to 20 eV and scattering angles of 3 to 33 degrees. These measurements are fitted well by a modified Morse potential

$$\varphi_M(r) = \varepsilon\left\{\exp\left(\frac{-2Cr_e}{\sigma}(1-r/r_e)\right) - 2\exp\left(\frac{-Cr_e}{\sigma}(1-r/r_e)\right)\right\}, \qquad (16)$$

with ε = 2.0 eV, σ = 0.485 Å, C = 1.18 and $r_e = \sigma(1+\ln 2/C)$ = 0.77 Å. Here, $-\varepsilon$ is the potential minimum, occurring at r_e.

Molecular orbital calculations performed by Michels[22] for the ground state $X^1\Sigma$ of the HeH^+ molecular ion, with the assumption that processes evolve adiabatically, are in good agreement with these results.

For what is referred to as the "intermediate energy range", 500 to 3000 eV, and scattering angles between 0.5 and 10 degrees, elastic cross-sections and scattering potentials were determined by Abignoli et al.[23]. At large internuclear distances, their results are close to Michels' ground state potential, but at smaller distances they differ, probably due to non-adiabatic effects not present at lower energies.

In principle, it is possible to calculate cross-sections $Q^{(1)*}$ as a function of energy g^{*2}, using the appropriate potential. There is no problem of interpretation over a large energy range because an energy $\frac{1}{2}\mu g^2$ = 30 eV and ε = 2.0 eV correspond to $g^{*2} = 7\ \mu$, whereas $\frac{1}{2}\mu g^2$ = 500 eV and ε = 60 eV (for the screened Coulomb function, Eq. (17)) give $g^{*2} = 4.2\ \mu$.

However, there is a practical difficulty in the evaluation of the integrand of Eq. (14) for the modified Morse potential. Like for any attractive potential, the integrand oscillates rapidly at certain impact parameters, reflecting the spiraling of the particles about one another; this phenomenon is known as orbiting. As the numerics for treating orbiting are quite involved, we shall use the adiabatic potential, described by the monotonous repulsive screened Coulomb function[23),

$$\varphi_{scr.C.}(r) = 2.2 \frac{e^2}{a_o} \frac{0.91/a_o}{r} e^{-r/0.91a_o} . \qquad (17)$$

As an a posteriori justification it was found that the cross-section for low energies, e.g. $g^{*2} = 0.20$, calculated by Lovell and Hirschfelder[24) for the modified Morse potential did not differ significantly from the one we found with Eq. (17) for the corresponding value $g^{*2} = 0.20 \times 2.0$ eV/(2.2×27.21 eV) $= 6.7 \times 10^{-3}$. It was not possible to compare the results precisely because Lovell and Hirschfelder's calculations did not cover a potential well as wide as C = 1.18 (cf. Eq. (16)), and an extrapolation from their data was necessary.

The reduced cross-sections we obtained with Eqs. (15) and (17) are plotted in Fig. 3. Note the steep decline of the elastic term towards higher energies.

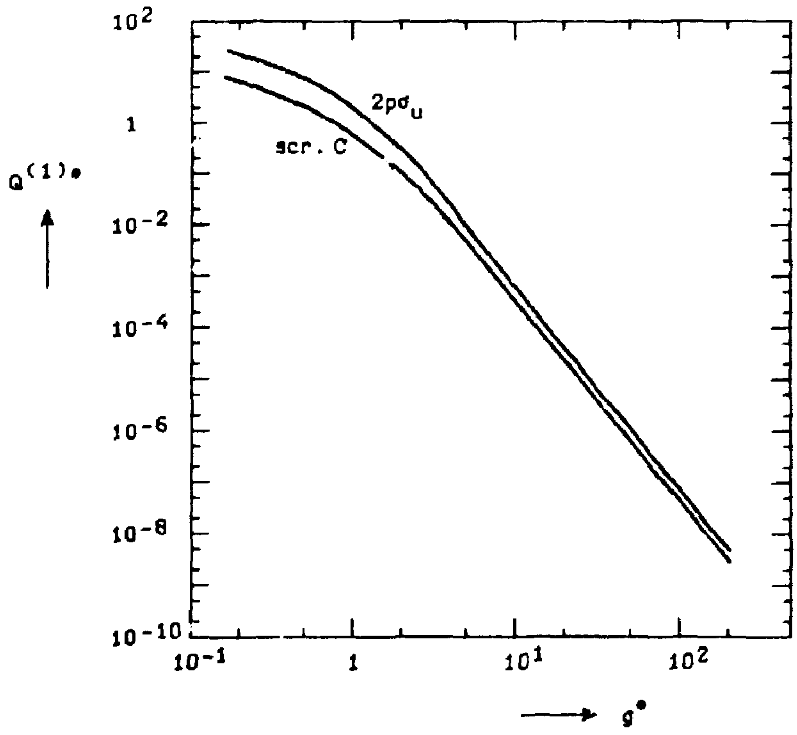

Fig. 3. The dimensionless cross-section as a function of the reduced relative speed for the screened Coulomb and $2p\sigma_u$ potentials.

It shows that at an energy of 1 eV, corresponding to $g^* = \sqrt{1/27.21} = 0.19$, the elastic cross-section for H on H^+ is

$$Q^{(1)}(1\ \text{eV}) = \pi a_0^2\, Q^{(1)*}(0.19) \simeq 1.93\times10^{-15}\ \text{cm}^2,$$

whereas

$$\sigma_{cx}(1\ \text{eV}) = 6.94\times10^{-15}\ \text{cm}^2.$$

Charge exchange is already important at 1 eV and becomes fastly dominant for higher energies. The latter also holds for ionization.

For helium atoms, the relative importance of ionization, scattering off protons and charge exchange with He^{+} and He^{++} is plotted as a function of relative energy in Fig. 4.

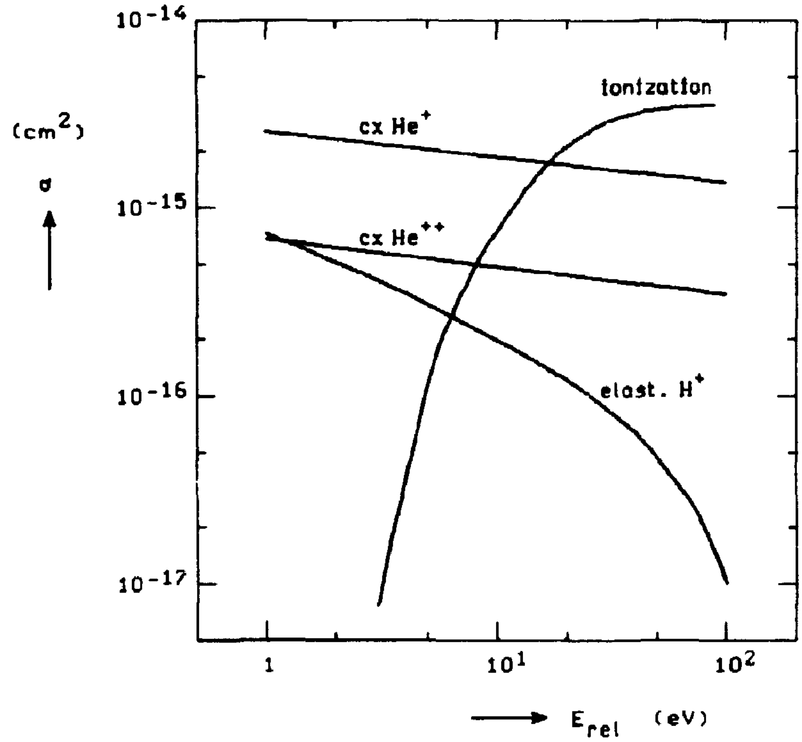

Fig. 4. The absolute cross-sections for He ionization (averaged over a Maxwellian electron distribution with $kT = E_{rel}$), He-He^{+} and He-He^{++} charge exchange and elastic scattering of He on protons (all single collisions) as a function of relative energy.

The charge exchange cross-sections are those from the preceding pages; the relative energy for elastic collisions is $E_{rel} = \varepsilon\, g^{*2}$ and the ionization cross-section is $\sigma_{ion} = \langle\sigma v\rangle_{ion}/v_{He}$, where $v_{He} = (2E_{rel}/m_{He})^{\frac{1}{2}}$, thus assuming that helium atoms and electrons have equal temperatures.

We conclude that for neutral helium it is necessary to include elastic scattering off protons for relative energies below approximately 15 eV.

It is confirmed by our calculations that, down to energies of 1 eV, ionization and charge exchange with protons are the dominant processes for hydrogen atoms; elastic interactions need not be taken into account.

For high densities, it is possible to circumvent the explicit use of the velocity-dependent cross-section. Momentum transfer, the quantity governing the diffusion coefficient of particles in a background gas or a plasma can then be treated as the friction force between two maxwellian distributions, which can be written in the form

$$- \vec{R}_{ab} = \frac{8}{3} (2\pi\mu kT)^{\frac{1}{2}} N_a N_b \sigma_{ab}^2 \Omega_{ab}^{(1,1)*} (\vec{v}_a - \vec{v}_b) \tag{18}$$

for particle densities N_a, N_b and drift velocities $\vec{v}_a$, $\vec{v}_b$. The dimensionless collision integral $\Omega^{(1,1)*}$ is a function of the reduced temperature,

$$\Omega^{(1,1)*}(T^*) = \frac{2}{T^{*3}} \int_0^\infty e^{-g^{*2}/T^*} g^{*5} Q^{(1)*}(g^*) dg^* , \tag{19}$$

where

$$T^* = kT/\varepsilon . \tag{20}$$

Equation (19) was evaluated for the two potentials used above; the results are plotted in Fig. 5.

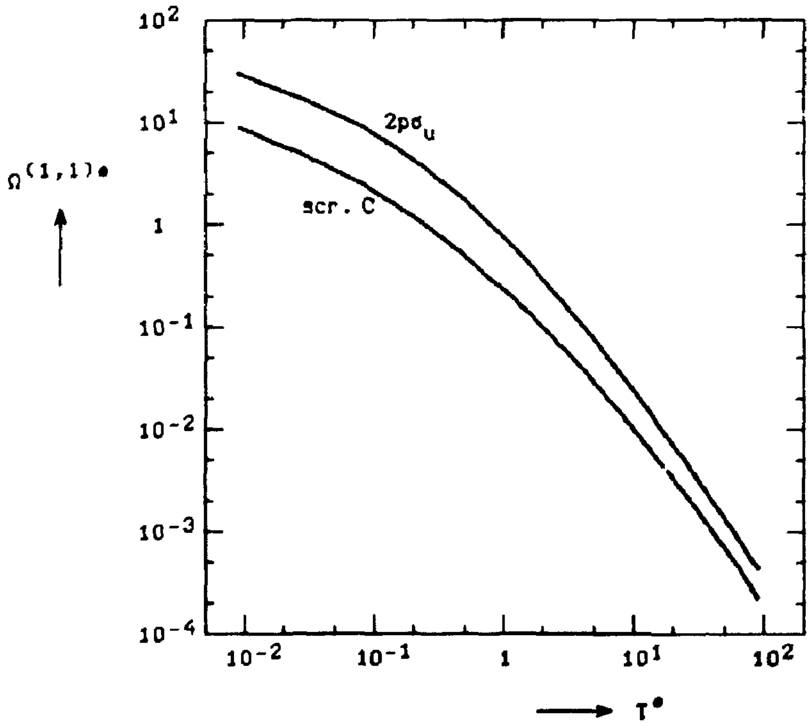

Fig. 5. The dimensionless collision integral, plotted against the reduced temperature, for the screened Coulomb and $2p\sigma_u$ potentials.

Upon defining friction coefficients f_{ab} by

$$- \vec{R}_{ab} = f_{ab} N_a N_b (\vec{v}_a - \vec{v}_b) , \tag{21}$$

we have

$$\begin{aligned} f_{HeH^+} &= 2.27\times10^{-34}\ T^{\frac{1}{2}}\ \Omega^{(1,1)*}_{scr.C.}\ (T/59.86)\ g\ cm^3s^{-1} \\ f_{HH^+} &= 2.15\ 10^{-34}\ T^{\frac{1}{2}}\ \Omega^{(1,1)*}_{2p\sigma_u}\ (T/27.21)\ g\ cm^3s^{-1} \end{aligned} \tag{22}$$

for T in electron volts.

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