

V. Collisional Processes

1. Classical collision theory

a) Scattering by a center of force

Consider a uniform beam of particles all of the same mass and energy incident upon a center of force. Characterize the beam by its incident intensity I [number $\text{cm}^{-2}\text{s}^{-1}$]: as the particle approaches the center of force it will be attracted or repelled (depending on the nature of the interaction) and will thus deviate from its initial straight-line trajectory. Far from the scattering center, as the force diminishes, the “orbit” once again approaches a straight line. The cross section for scattering in a particular direction Ω is:

$$\sigma(\Omega)d\Omega = \frac{\text{number of particles scattered into } d\Omega \text{ s}^{-1}}{\text{incident intensity}} \quad (5.1)$$

where $d\Omega$ = element of solid angle in direction Ω . For central forces, the cross section must be symmetrical around the axis of the incident beam:

$$d\Omega = 2\pi\sin\theta d\theta \quad (5.2)$$

where θ = angle between incident and scattered directions = scattering angle.

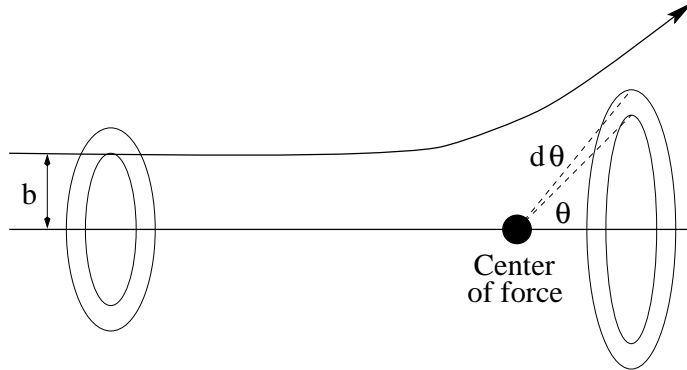


Figure 5.1– Scattering by a central force potential.

The energy and angular momentum of a particle determine its orbit in terms of the impact parameter b :

$$L = mv_0b = b(2mE)^{1/2} \quad (5.3)$$

where L is the angular momentum, v_0 the incident speed and m is the particle mass. The impact parameter is the perpendicular distance between the initial velocity vector and the center of force. Thus the number of particles scattering into $d\Omega$ about θ must equal the number of particles incident between b and $b + db$:

$$2\pi I b db = -2\pi\sigma(\theta) I \sin\theta d\theta \quad (5.4)$$

$$\text{or} \quad \sigma(\theta) = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right| . \quad (5.5)$$

If for a given θ several values of b contribute to the scattering, the cross section is the sum of all the contributions, or:

$$\sigma(\theta) = \sum_i \frac{b_i}{\sin\theta} \left| \frac{db_i}{d\theta} \right| . \quad (5.6)$$

The equations of motion of the scattering particle follow from the conservation of energy and angular momentum. Because the potential is central, the trajectory stays in a plane. Using polar coordinates r and θ , we obtain:

$$\vec{L} = \vec{p} \times \vec{r} = mr^2 \left(\frac{d\theta}{dt} \right) = b(2mE)^{1/2} \quad (5.7)$$

$$E = \frac{1}{2} \left(\frac{dr}{dt} \right)^2 + \frac{L^2}{2mr^2} + V(r) . \quad (5.8)$$

The quantity $L^2/(2mr^2)$ is called the centrifugal barrier, and the “effective potential” seen by the particle is therefore

$$V_{eff} = V(r) + \frac{L^2}{2mr^2} . \quad (5.9)$$

From (5.8), we obtain:

$$\frac{dr}{dt} = \sqrt{\frac{2}{m} [E - V(r)] - \frac{L^2}{m^2 r^2}} = \frac{dr}{d\theta} \frac{d\theta}{dt} . \quad (5.10)$$

Using $d\theta/dt = l/mr^2 = b(2mE)^{1/2}/mr^2$, equation (5.10) becomes

$$d\theta = \frac{bdr}{r^2 \sqrt{1 - \frac{V}{E} - \frac{b^2}{r^2}}} . \quad (5.11)$$

Integrating over the trajectory of the incident particle, we find

$$2 \int_{r_c}^{\infty} \frac{bdr}{r^2 \sqrt{1 - \frac{V}{E} - \frac{b^2}{r^2}}} = \int_{-\pi}^{\theta_d} d\theta = \theta_d + \pi , \quad (5.12)$$

where r_c is the distance of closest approach, and θ_d is the deflection angle:

$$\theta_d = 2 \int_{r_c}^{\infty} \frac{bdr}{r^2 \sqrt{1 - \frac{V}{E} - \frac{b^2}{r^2}}} - \pi . \quad (5.13)$$

The scattering angle θ_s is defined as the deflection angle, constrained between 0 and π :

$$\theta_s = \pm\theta_d \pm 2\pi m \quad \text{with } m \text{ an integer.} \quad (5.14)$$

The interaction potential between two atoms will typically have the form:

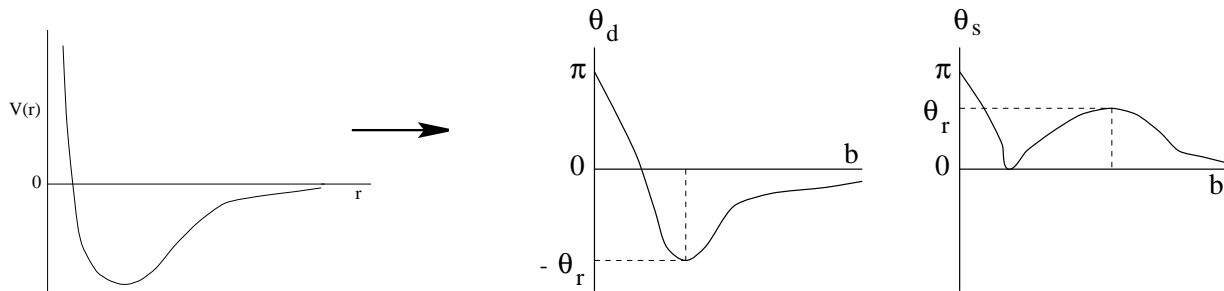


Figure 5.2– (Left) Typical interaction potential for the collision of two neutral atoms. **Figure 5.3**– (Right) θ_d and θ_s as functions of the impact parameter b .

At large distances, the potential is attractive, whereas at short internuclear distances, the potential is repulsive due to the core-core interaction. The shape of the deflection angle and the scattering angle as a function of impact parameter b look as illustrated in Figure 5.3. We see that for $\theta_s < \theta_r$, three different impact parameters contribute to the cross section. In a quantal calculation, there would be interference between the different contributions. In a classical calculation, there is no interference. Experimentally, interference effects are observed, demonstrating the failure of the classical calculations. Figure 5.4 illustrates the difference between the classical and quantal calculations.

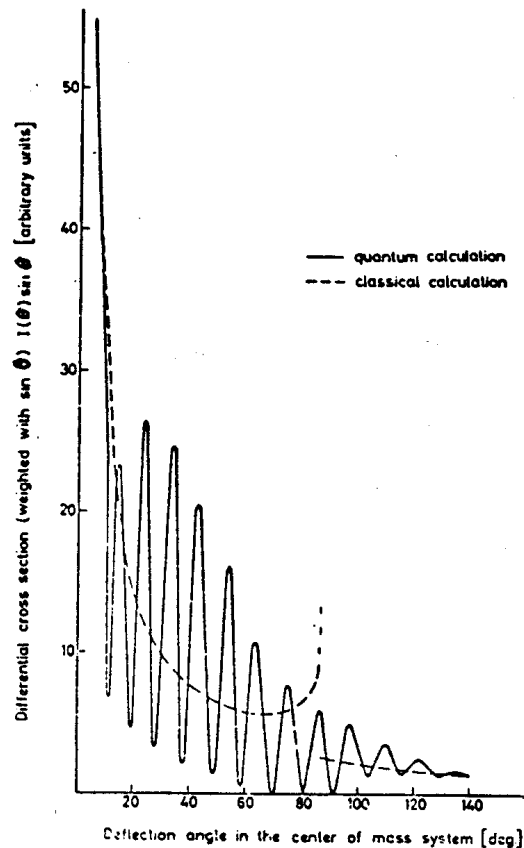


Figure 5.4– Differential cross section vs. scattering angle.

b) Rutherford formula

For the specific case of a Coulomb interaction, the potential is given by $Z_1 Z_2 e^2 / r \equiv \alpha / r$. The scattering angle then becomes:

$$\theta_s = \pi + 2 \arccos \left(\frac{\beta}{\sqrt{1 + \beta^2}} \right) \quad (5.15)$$

with $\beta = \alpha / 2bE$. The differential cross section is thus:

$$\sigma(\theta) = \left(\frac{\alpha}{4E} \right)^2 \frac{1}{\sin^4(\theta/2)} \quad (5.16)$$

which is the ‘‘Rutherford formula.’’ In astrophysical applications, the total cross section:

$$\sigma = \int \sigma(\Omega) d\Omega = 2\pi \int_0^\pi \sigma(\theta) \sin(\theta) d\theta \quad (5.17)$$

is more important than the differential cross section. In the case of pure Coulomb scattering, $\sigma \sim \infty$: this is a general property of all central potentials that fall off asymptotically at least as slowly as $1/r^2$. The total cross section will be finite if the scattering potential is steeper than this, or if it cuts off at some distance. In real cases, there will often be some physical reason for a cut-off.

2. Quantum theory

A full quantal treatment of the collision problem is necessary when considering

- (i) collisional excitation of low-lying atomic states to which the correspondence principle cannot be rigorously applied.
- (ii) low incident energies, at which the wave nature of the incident particle begins to manifest itself.

In the cases of astrophysical interest, these conditions are usually satisfied, with the possible exception of the high n Rydberg states of atoms. The full quantal treatment of scattering is discussed in many textbooks. The classic book is that by Mott and Massey: ‘‘Theory of Atomic Collisions’’ (1965). The textbook by Bransden: ‘‘Theory of Atomic Collisions’’ (1970) is often used.

The basic idea is always to try to represent the scattering between two particles by a central potential that incorporates all the physics of the interaction. In principle, the scattering of a free electron by an iron atom, say, should be considered a many-body problem in which the incident electron interacts with the attractive nucleus and with at least some of the repulsive atomic electrons. Such a problem becomes tractable, however, only if treated in terms of a potential that represents the time-dependent state of the combined electron-plus-atom system.

In terms of an idealized scattering experiment, we normally assume:

- (i) multiple scatterings can be neglected
- (ii) interactions between the incident particles are negligible (that is, a low density incident beam)
- (iii) each incident particle has a definite energy and momentum. Thus, due to the uncertainty principle, the particle is not well localized in space and time.

a) Cross section for elastic scattering

For a central potential, $V(r) \rightarrow 0$ as $r \rightarrow \infty$. Thus the Schrödinger equation for a beam of free particles ($V(r) = 0$) can be written:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - E\right)\Psi = 0 \quad (5.18)$$

or $(\nabla^2 + k^2)\Psi = 0 \quad (5.19)$

where

$$k^2 = 2mE/\hbar^2 \quad (5.20)$$

Equation (5.19) has the solution:

$$\Psi = e^{i\vec{k}\cdot\vec{r}} \quad (5.21)$$

In the presence of a scattering potential $V(r)$, the Schrödinger equation becomes:

$$\{\nabla^2 + k^2 - U(r)\}\Psi = 0 \quad (5.22)$$

where

$$U(r) = (2m/\hbar^2)V(r) \quad (5.23)$$

Physically, we expect the potential to introduce a scattered wave, spherically symmetric about the scattering center, whose amplitude is inversely proportional to r , that is, the asymptotic form of (5.22) is expected to be:

$$\Psi \propto e^{i\vec{k}\cdot\vec{r}} + \frac{e^{ikr}}{r} f(\theta) \quad (5.24)$$

where $f(\theta)$ is the “scattering amplitude.”

By comparing the number of particles per unit time entering $d\Omega$ in the direction θ to that of the incident flux, one can show that the differential cross section for elastic scattering:

$$\frac{d\sigma(\theta)}{d\Omega} = |f(\theta)|^2 \quad (5.25)$$

and the total cross section is

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = 2\pi \int_0^\pi |f(\theta)|^2 \sin\theta d\theta \quad (5.26)$$

The modification to (5.25) for inelastic scattering will be considered in §5.2.d.

b) Partial wave expansion

Owing to the spherical symmetry of the potential and the axial symmetry of the incident wave, the wave functions will be axially symmetric about the incident direction. Thus, the wave function depends only on r and θ ; $\Psi(\vec{r}) = \Psi(r, \theta)$, and can be expanded in a series of Legendre polynomials:

$$\Psi(r, \theta) = \sum_l r^{-1} f_l(r) P_l(\cos\theta) . \quad (5.27)$$

Each of the terms in (5.27) is an eigenfunction of the angular momentum operators L^2 and L_z . Substituting (5.27) into the Schrödinger equation (5.19), and using:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{1}{\hbar^2 r^2} L^2 \quad (5.28)$$

we obtain

$$\sum_{l=0}^{\infty} \frac{1}{r} P_l(\cos\theta) \left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - U(r) + k^2 \right] f_l(r) = 0 . \quad (5.29)$$

If we multiply (5.29) on both sides by $P_{l'}(\cos\theta)$ and integrate over $\cos\theta$ using

$$\int_{-1}^1 P_l(\cos\theta) P_{l'}(\cos\theta) d\cos\theta = \frac{2}{2l+1} \delta_{ll'} \quad (5.30)$$

we obtain an infinite set of equations:

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - U(r) + k^2 \right] f_l(r) = 0 . \quad (5.31)$$

Note that the quantity $U(r) + l(l+1)/r^2$ may be written as $(2m/\hbar^2)V_{eff}$. The classical impact parameter b is then seen to correspond to the quantity $(\hbar/mv)[l(l+1)]^{1/2} = [l(l+1)]^{1/2}/k$, except that in the wave treatment l has discrete values.

What are the physical solutions of Equation (5.31)? The first requirement is that the function $\psi(r, \theta)$ must remain finite when $r \rightarrow 0$. For potentials such that limit $r^2|V(r)| < \text{constant}$, the radial function $f_l(r)$ can be expanded:

$$f_l(r) = \sum_n a_n r^n . \quad (5.32)$$

At the origin, there are two solutions:

$$f_l(r) \sim r^{l+1} \quad \text{regular} \quad (5.33a)$$

$$f_l(r) \sim r^{-l} \quad \text{irregular} \quad (5.33b)$$

but only the first one, eq. (5.331), is physical. Note that the Coulomb potential is a special case which must be treated separately.

At large r , $U(r) \ll k^2$, so that we have to solve

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 \right] f_l(r) = 0 \quad . \quad (5.34)$$

The general real solution of this equation is a linear combination of the regular and irregular solutions, and can be written in terms of the spherical Bessel and Neumann functions $j_l(kr)$ and $n_l(kr)$:

$$f_l = A_l k r j_l(kr) + B_l k r n_l(kr) \quad . \quad (5.35)$$

For large kr , these functions become:

$$f_l \sim A_l \sin(kr - l\pi/2) - B_l \cos(kr - l\pi/2) \quad . \quad (5.36)$$

In the complete absence of a scattering potential ($V = 0$ everywhere), the boundary condition at the origin, $f_l(0) = 0$, would exclude the irregular solution, and we would have $B_l = 0$. Hence, the magnitude of B_l compared with A_l must be determined by solving the Schrödinger equation inside the scattering region, subject to the boundary condition (5.33a), and by joining the interior solution smoothly onto the exterior solution.

A very useful expression for the cross section can be derived by introducing the ratio B_l/A_l as a parameter:

$$B_l/A_l = -\tan\delta_l \quad , \quad (5.37)$$

where δ_l is a real angle which vanishes for all l if $V = 0$ everywhere. It is called the “scattering phase shift”, because we can write:

$$f_l(r) \sim \sin(kr - l\pi/2 + \delta_l) \quad . \quad (5.38)$$

Thus, δ_l measures the amount by which the phase of the radial function for angular momentum l differs from the no-scattering case ($\delta_l = 0$). Each phase shift is, of course, a function of the energy or k .

In order to compute the differential cross section, we must now relate expansion (5.27) to the general scattering formula (5.24). It can be shown that the first term of (5.24), the plan wave, can be expanded asymptotically as:

$$e^{i\vec{k}\cdot\vec{r}} \propto \sum_{l=0}^{\infty} (2l+1) i^l \frac{\sin(kr - l\pi/2)}{kr} P_l(\cos\theta) \quad . \quad (5.39)$$

The second part of (5.24), the scattered part, can also be expanded in terms of Legendre polynomials:

$$f(\theta) \frac{e^{ikr}}{r} \propto \left[\sum_{l=0}^{\infty} (2l+1) \frac{1}{k} T_l P_l(\cos\theta) \right] \frac{e^{ikr}}{r}$$

$$= \sum_{l=0}^{\infty} (2l+1) \frac{i^l}{kr} T_l P_l(\cos\theta) \{ \cos(kr - l\pi/2) + i \sin(kr - l\pi/2) \} \quad (5.40)$$

where T_l are the partial wave scattering amplitudes. The asymptotic form of $\Psi(r, \theta)$ thus becomes:

$$\Psi(r, \theta) \propto \sum_{l=0}^{\infty} (2l+1) \frac{i^l}{kr} P_l(\cos\theta) \left\{ \cos(kr - \frac{l\pi}{2}) + (1 + iT_l) \sin(kr - \frac{l\pi}{2}) \right\} \quad (5.41)$$

If we compare (5.41) to (5.27), using (5.36) we find:

$$k_l \equiv B_l/A_l = -\tan\delta_l = T_l/(1 + iT_l) \quad (5.42)$$

$$\text{or} \quad T_l = e^{i\delta_l} . \quad (5.43)$$

k_l is also called the “reaction” matrix element. Sometimes, one defines the S -matrix or “scattering” matrix element:

$$S_l = (2iT_l + 1) . \quad (5.44)$$

For elastic scattering, $|S_l(k)| = 1$, and $S_l = e^{2i\delta_l}$. Thus:

$$f(\theta) = \sum_{l=0}^{\infty} \frac{1}{ik} e^{i\delta_l} \sin\delta_l (2l+1) P_l(\cos\theta) \quad (5.45)$$

and

$$\frac{d\sigma}{d\Omega} = \frac{1}{k^2} \left| \sum_{l=0}^{\infty} \frac{1}{ik} e^{i\delta_l} \sin\delta_l (2l+1) P_l(\cos\theta) \right|^2 . \quad (5.46)$$

We see that in the quantum mechanical description, interference effects may occur between the contributions of the different values of the angular momentum to the cross section.

The total cross section is obtained by integrating (5.47), using (5.30)

$$\sigma = \sum_{l=0}^{\infty} \frac{4\pi}{k^2} (2l+1) \sin^2\delta_l . \quad (5.47)$$

This partial wave analysis of the cross section is only successful if the sum converges rapidly, that is, if the number of partial waves contributing to the cross section is not too large. Remember that each partial wave corresponds to a definite value of the angular momentum l . If the scattering potential is strongest at the origin and decreases in strength as r increases, then we expect the low angular momentum components, which classically correspond to *small* impact parameters and therefore close collisions, to scatter more intensely than the high angular momentum components. More specifically, if the range of the potential is a , only those particles will be scattered which have an impact parameter $b \approx [l(l+1)]^{1/2}/k < a \Rightarrow [l(l+1)]^{1/2} \leq ka$. In particular, when $ka \ll 1$, that is,

for low energies, light particles or short range potentials, only the $l=0$ partial wave will contribute significantly.

c) Example: scattering by a hard sphere

Let us look at an idealized example before going on to the more complicated cases of actual interest. Considering an infinitely repulsive potential for $r < a$; this gives an immediate boundary condition: $f_l(a) = 0$. At $r > a$, the radial function has the form (5.35):

$$f_l(r)/r \propto j_l(kr) - \tan\delta_l n_l(kr) . \quad (5.48)$$

Applying the boundary condition gives

$$\tan\delta_l = -j_l(ka)/n_l(ka) . \quad (5.49)$$

At $l = 0$, $j_0(ka)/n_0(ka) = \sin(ka)/\cos(ka) = \tan(ka) \Rightarrow \delta_0 = -ka$.

It can be shown that $\sigma_l \sim 0$ for $l > 0$ and $k \rightarrow 0$. Thus, for low energies $k \rightarrow 0$, $\sigma(k) \approx \sigma_0$, with

$$\sigma_0 = \frac{4\pi}{k^2} \sin^2(-ka) \approx 4\pi a^2 . \quad (5.50)$$

In other words, in the limit of zero energy, the total cross section is *four times* the classical result! At large energies, $ka \gg l$, it can be shown that:

$$\delta_l \approx -ka + l\pi/2 \quad (5.51)$$

which results in

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{l_{max}} (2l+1) \sin^2(-ka + l\pi/2) . \quad (5.52)$$

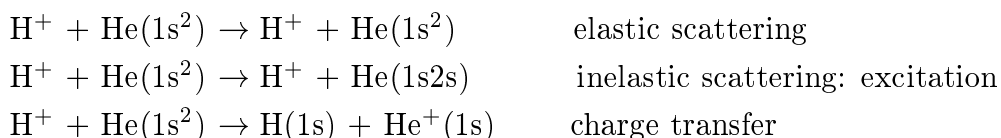
If we take $l_{max} = ka$, then this sum is approximately:

$$\sigma \approx 2\pi a^2 . \quad (5.53)$$

Thus, in the high-energy limit, the total cross section is *twice* the classical result.

d) Inelastic collisions

In general, there are several possible outcomes of a collision event. Consider, for example, the case of a proton-helium collision:



Each different initial or final state is called a “reaction channel”. Channels that are energetically allowed are called “open”; those for which the total energy of the collision system is less than the initial/final energy difference are called “closed”. Some ostensibly possible channels are not allowed because they do not satisfy conservation of spin, angular momentum, etc...

The cross section for these processes can be calculated along the same lines as for the elastic scattering. The total wave function for the incident particle can be represented by:

$$\phi_i = \frac{F_i(r)}{r} Y_{l_i m_i}(\hat{r}) \quad (5.55)$$

where $F_i(r)$ is the radial part of the function and $Y_{l_i m_i}(\hat{r})$ the angular part. We can then expand the total wave function Ψ in terms of the eigenfunctions of the target atom Φ_i (assuming that the particles are indistinguishable):

$$\Psi = \sum_i \Phi_i \phi_i \quad (5.56)$$

If we substitute (5.56) into the Schrödinger equation, we obtain a set of “coupled differential equations”:

$$\left\{ \frac{d^2}{dr^2} - \frac{l_i(l_i + 1)}{r^2} + k_i^2 \right\} F_i = \sum_j V_{ij} F_j \quad (5.57)$$

where $V_{ij} = \langle \Phi_i | V | \Phi_j \rangle$ is the potential operator.

The boundary conditions become for $r \rightarrow \infty$:

$$F_0 \sim \frac{1}{k_0} (e^{-ik_0 r} - e^{ik_0 r} S_{00}) \quad (5.58a)$$

$$F_i \sim \frac{1}{k_i} (-e^{ik_i r} S_{0i}), \quad i \neq 0, \quad (5.58b)$$

for 0 as the initial state. Finally, the cross section for excitation from state 0 to state f is given by:

$$\sigma_{f0} = \frac{\pi}{k_0^2} \cdot \frac{1}{g_0} \cdot \sum |T_{f0}|^2 \quad (5.59)$$

where T_{f0} is an element of the appropriately defined T matrix, and g_0 is the statistical weight of the initial state.

3. Electron-hydrogen scattering

Let us examine as a simple example the lowest order approximation to electron-hydrogen scattering with two open channels: $e + \text{H}(1s)$, $e + \text{H}(2s)$.

Consider scattering in the $l=0$ partial wave:

$$\Psi(r, \vec{x}) = \phi_{1s}(\vec{x}) r^{-1} f_1(r) + \phi_{2s}(\vec{x}) r^{-1} f_2(r) \quad (5.60)$$

where ϕ_i are the 1s and 2s eigenfunctions of the isolated hydrogen atoms. Neglect electron exchange for simplicity. In atomic units, this leads to a set of two coupled radial equations:

$$\frac{1}{2} \left(\frac{d^2}{dr^2} + k_i^2 \right) f_i(r) = \sum_{j=1}^2 V_{ij}(r) f_j(r) \quad (5.61)$$

where $k_2^2 = k_1^2 + 2(\epsilon_{1s}\epsilon_{2s}) = k_1^2 - 0.75$, and the matrix potential

$$V_{ij}(r) = \int d\vec{x} \phi_i(\vec{x}) \phi_j(\vec{x}) V(\vec{r}, \vec{x}) \quad (5.62)$$

incorporates the effect of the perturbation between the atom and the incident electron:

$$V(\vec{r}, \vec{x}) = \frac{1}{|\vec{r} - \vec{x}|} - \frac{1}{r} . \quad (5.63)$$

Taking $\phi_{1s}(r) = e^{-r}/\pi^{1/2}$ and $\phi_{2s}(r) = 2(2\pi)^{1/2}e^{-r/2}$, it can be shown that:

$$V_{11} = -(1 + 1/r)e^{-2r} \quad (5.64a)$$

$$V_{22} = 1/2 (r^2/4 + 5r + 2/r - 3)e^{-r} \quad (5.64b)$$

$$V_{12} = V_{21} = (8)^{1/2}/27 (6 + 3r - 8/r)e^{-3r/2} . \quad (5.64c)$$

By solving the above coupled equations numerically, one gets automatically all elements of the scattering matrix, and thus cross sections for both the elastic $1s \rightarrow 1s$ and the inelastic $1s \rightarrow 2s$ channels:

Table 5.1– e-H(1s) cross sections

Energy of incident e (eV)	σ_{1s-1s} (πa_0^2)	σ_{1s-2s} (πa_0^2)
11.5	2.52	0.286
13.5	2.12	0.204
19.4	1.42	0.102
30.4	0.828	0.045
54.0	0.394	0.0155

Note that the elastic cross sections are typically an order of magnitude larger than the inelastic cross sections.

Imagine now that we consider an energy slightly below the threshold for $1s$ - $2s$ excitation ($<10.2\text{eV}$ incident electron energy). The $1s$ - $2s$ channel is energetically closed, but its existence must still be acknowledged: the closed-channel wave function decreases exponentially like:

$$f_2(r) \sim e^{-|f_2|r} . \quad (5.65)$$

Mathematically, the reactance matrix k_{ij} is still a 2×2 matrix, but its elements k_{12} and k_{21} are now no longer real.

Improved treatments of e-H scattering must take into account several additional factors:

- (i) with electron spin, the total 2-electron wave functions have both singlet and triplet components

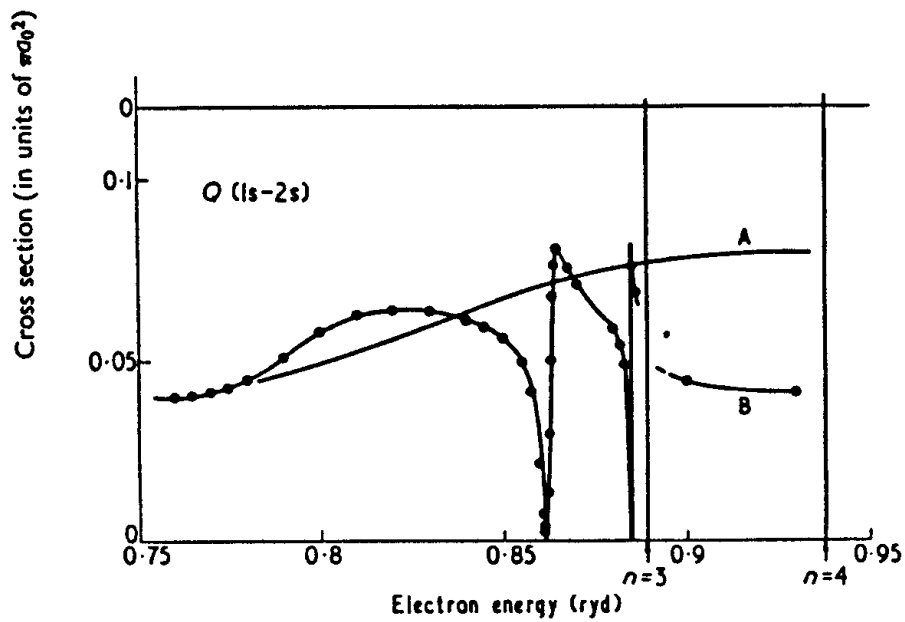


Figure 5.5— The 1S partial wave cross section $Q(1s-2s)$ calculated in the three state (curve A) and six-state (curve B) approximation.

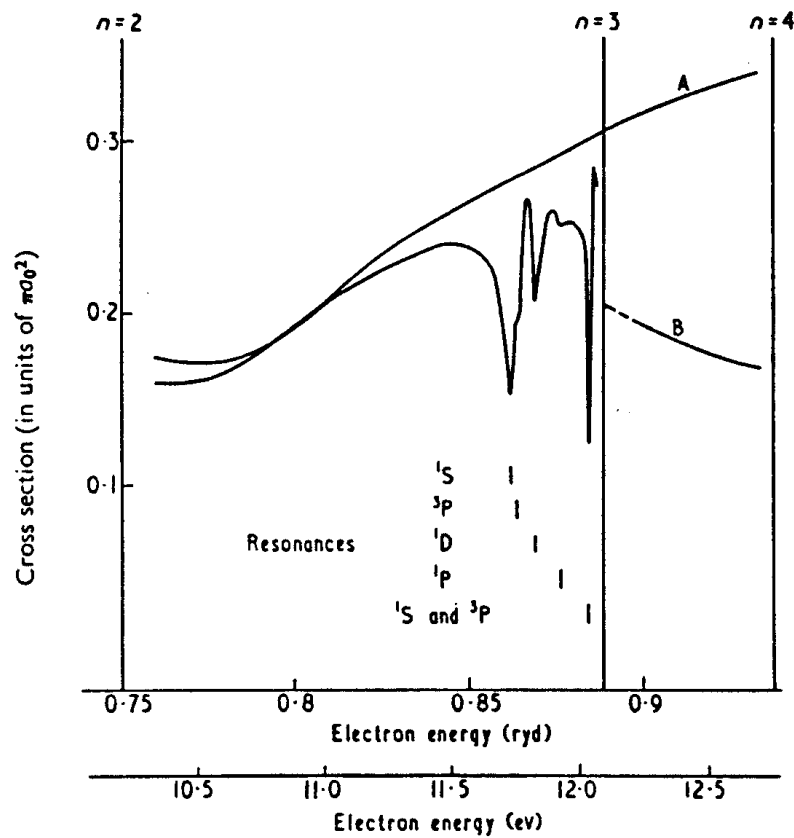


Figure 5.6— The total cross section $Q(1s-2s)$ calculated in the three state (curve A) and the six-state (curve B) approximation.

- (ii) electron exchange: the two electrons are not indistinguishable, so that (5.60) has to be anti-symmetrized.
- (iii) additional open and closed channels exist, such as 3s, 3p, ...

Even though this is the simplest atomic collision system, it was not until the mid-1960's that theoretical calculations were carried far enough to begin resolving discrepancies with experimental results. Indeed, it is fair to say that there is still disagreement between the available empirical data and theoretical calculations. (See, for example, S. A. Drake, 1983, *MNRAS* **205**, 151 and references therein.)

A detailed study of low-energy e-H scattering in the “close-coupling approximation” is that of Burke *et al.* (1967, *Proc. Phys. Soc.*, **92**, 319), in which the close-coupling expansion includes 1s, 2s, 2p, 3s, 3p, 3d terms. Figures 5.5 and 5.6 illustrate the results for the $l=0$ partial wave and the total cross sections, in the case that the expansion consists of 3 or 6 terms. Detailed structure occurs in the 6-state expansion cross sections which arises from bound levels of the H^- system. If the right hand side of (5.61) were neglected for $i \neq j$, the bound levels of H^- would be obtained. If coupling between the states is allowed, the bound states become “resonances” and the cross section will exhibit resonance structure.

e-H scattering

For many astrophysical applications, this structure has little direct importance because the physically significant property is the collisional excitation “rate coefficient” rather than the cross section as a function of electron energy. The rate coefficient is the thermal average of σ over a Maxwellian electron velocity distribution:

$$q = \int_0^{\infty} v\sigma(v)f(v)dv \quad (5.66)$$

with

$$f(v)dv = 4\pi^{1/2}\left(\frac{m}{2kT}\right)^{3/2}v^2e^{-mv^2/2kT}dv \quad (5.67)$$

The thermal averaging smooths over the resonance structure of the cross section. The e-H excitation rates are listed in Table 5.2 for a few temperatures.

Table 5.2– e-H excitation rates ($q(T)$ [cm^3s^{-1}])

T(K)	n = 1 → 2	1 → 3
5000	2.3(-18)	5.3(-21)
10000	2.4(-13)	5.2(-15)
20000	7.6(-11)	5.0(-12)

4. Collisional excitation of other species

The rate coefficients for e-H excitation are small at the lower T because the lowest threshold for excitation, $\Delta E_{12}=10.2\text{eV}$ corresponds to $\Delta E_{12}/k=118,000\text{K} \gg T$. However, as we have seen, common ions such as O^+ , O^{2+} , N^+ , ... have low-lying excited terms of the same configuration as the ground state (see also Figure 5.7). For example, the O^{++} 1D_2 level lies 2.5eV or $\Delta E/k \simeq 29,000\text{K}$ above the ground state. Moreover, because these are positively-charged ions, the “attractive” Coulomb force acting on the colliding electron

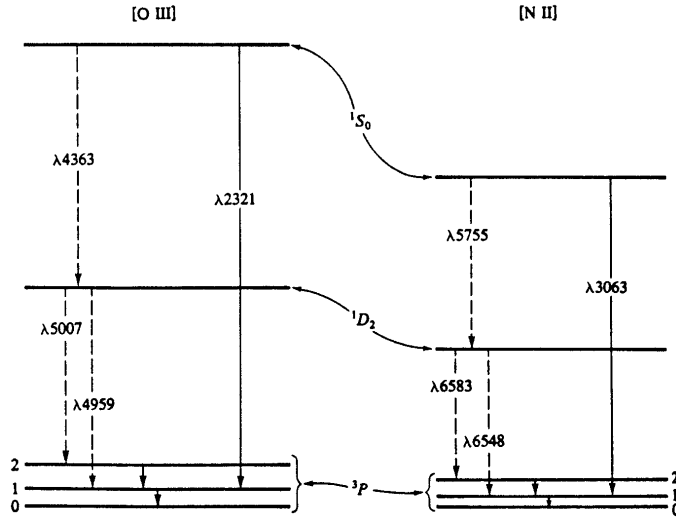


Figure 5.7– Energy level diagram for the lowest terms of O III and N II.

provides sort of a “focussing” effect that enhances the cross section. This focussing effect in fact causes the cross section to vary as:

$$\sigma(v) \propto v^{-2} \quad (5.68)$$

just above threshold. For this reason, it is often convenient to define a “collision strength” $\Omega(l, u)$ for a collisional transition $l \rightarrow u$, which is directly related to the excitation rate coefficient, but is usually nearly independent of T . To see how this works, consider the detailed balance between the upward and downward rates:

$$N_e N_l v_l \sigma_{lu}(v_l) f(v_l) dv_l = N_e N_u v_u \sigma_{ul}(v_u) f(v_u) dv_u \quad (5.69)$$

where v_l and v_u are related by:

$$mv_l^2/2 = mv_u^2/2 + \Delta E_{ul} \quad (5.70)$$

where ΔE_{ul} is the energy difference between the states. In thermal equilibrium (TE):

$$N_u/N_l = g_u/g_l e^{(-\Delta E_{ul}/kT)} \quad (5.71)$$

where g_u and g_l are the statistical weights. Combining (5.69) through (5.71), we find:

$$g_l v_l^2 \sigma_{lu}(v_l) = g_u v_u^2 \sigma_{ul}(v_u) . \quad (5.72)$$

The “collision strength” is defined for $mv^2/2 > \Delta E_{ul}$ by:

$$\sigma_{lu}(v) = \frac{\pi \hbar^2}{m^2 v_l^2} \cdot \frac{\Omega(l, u)}{g_l} , \quad (5.73)$$

so for electron-positive ion collisions, where $\sigma(v) \sim v^{-2}$ near threshold, $\Omega(l, u)$ is a slowly-varying function of v to first order. From the relation for detailed balance, the “downward” cross section is:

$$\sigma_{ul}(v) = \frac{\pi \hbar^2}{m^2 v_l^2} \cdot \frac{\Omega(l, u)}{g_u} , \quad (5.74)$$

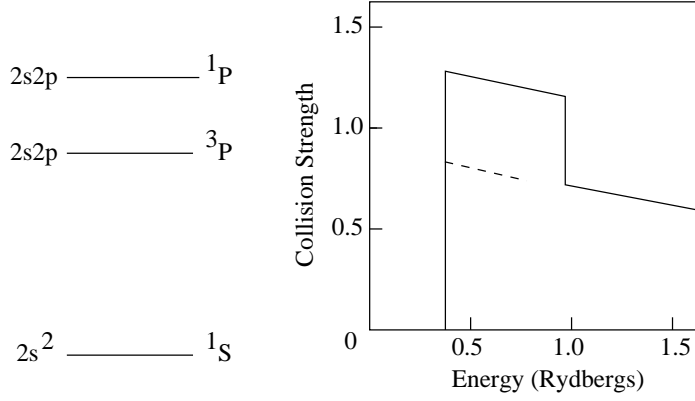


Figure 5.8– Energy variation of the $\Omega(^1S, ^3P)$ collision strength for C^{+2} . Full line: resonances included; broken line: coupling with 1P states neglected.

so the collision strengths are symmetrical in l, u . The relation between rate coefficient and collision strength is:

$$q_{ul} = \left(\frac{2\pi}{kT} \right)^{1/2} \cdot \frac{\hbar^2}{m^{3/2}} \cdot \frac{\Omega(u, l)}{g_u} \quad (5.75)$$

$$= \frac{8.629 \times 10^{-6}}{T^{1/2}} \cdot \frac{\Omega(u, l)}{g_u} \quad (5.76)$$

for de-excitation, if $\Omega(l, u)$ is constant.

Note that although Ω is in general slowly varying, it has superposed resonance contributions (see Figure 5.6) which vary rapidly with energy. As noted before, when the cross sections are integrated over a Maxwellian distribution, the effect of the exact positions of the resonances tends to be averaged out. Therefore, it is usually sufficient to use collision strengths averaged over the resonances;

$$\Omega = \int_0^\infty \Omega(E) e^{-E/kT} d(E/kT) \quad , \quad (5.77)$$

and often it is this averaged quantity that is listed at a typical temperature of 10,000 K. (See, for example, Osterbrock, Chap. 3). Nevertheless, resonances can have a substantial effect on the average results, as is shown below for the case of C^{2+} and O^{2+} . Note that with these definitions, Ω is of order unity for many transitions of interest. The excitation rate coefficient is related to the de-excitation rate coefficient (5.75) by:

$$q_{lu} = q_{ul} \left(\frac{g_u}{g_l} \right) e^{-\Delta E_{ul}/kT} \quad . \quad (5.78)$$

References:

A recent review of electron-impact collision strengths is that of Mendoza (1983, in “Planetary Nebulae” *IAU Symposium no. 103*, p.143). Useful summaries have also been given by Osterbrock, Ch. 3. One point to keep in mind is that we are largely dependent on

theoretical calculations for these atomic data because it is difficult to study forbidden-line excitation at typical laboratory pressures.

Note that for the excitation of neutral systems by electron impact, the cross sections are zero at threshold, and increase to a maximum generally located between two and three times the threshold energy. Cross sections for transitions involving a change in multiplicity fall rapidly at high energies.

5. electron-impact ionization

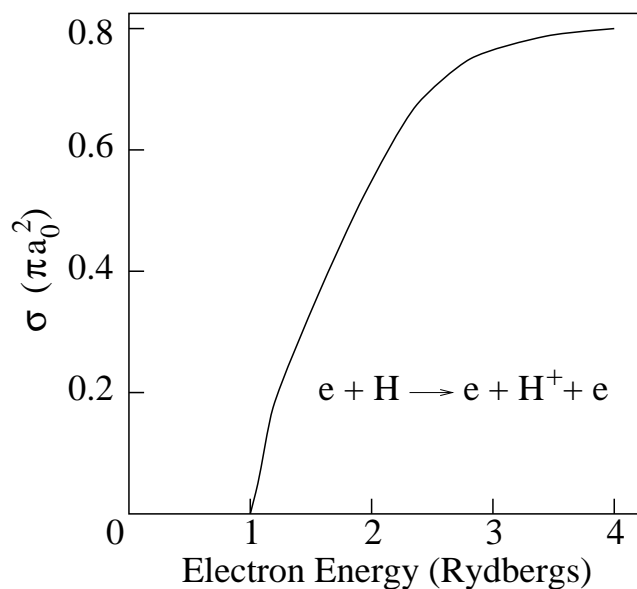
Collisions between electrons and atoms can also produce ionization, for example:



The cross section for this process is sketched in Figure 5.10. It has been measured near threshold by McGowan and Clarke 1968 (*Phys. Rev.* **167**, 43); see also Calloway *et al.* 1987 (*Phys. Rev. A* **36**, 2576). There is a widely used approximation formula for many e-impact ionization processes that gives a thermal rate coefficient for e + H:

$$q(T) = 5.85 \times 10^{-11} T^{1/2} e^{(-157,809/T)} \quad [\text{cm}^3\text{s}^{-1}] \quad (5.80)$$

For details, see Lotz 1967, *Ap. J. Suppl.* **14**, 207.

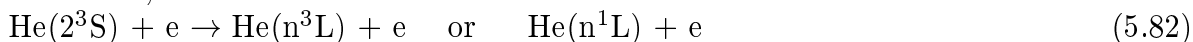


5.10– The electron-hydrogen impact ionization cross section.

Although e-impact ionization of ground-state He will be of interest only in very hot plasmas because of its very high ionization potential (24.6eV), recall that the He 2^3S state is highly metastable. This state lies only 4.8eV below the ionization limit. Accurate cross sections for



have been computed by Taylor *et al.* (1979, *J. Phys B*, 3093). Collisional excitation of metastable He,



can also play an important role in the formation of the He I emission line spectrum. At this point, it is interesting to compare the rates of the processes that remove population from He(2^3S):

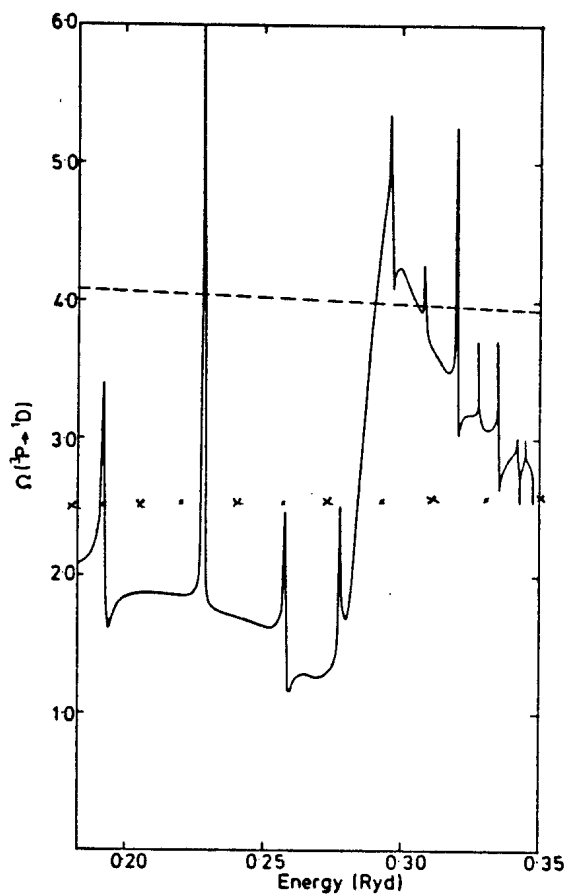


Figure 5.9a— The collision strength for the transition $1s^2 2s^2 2p^2 \ ^3P \rightarrow 1s^2 2s^2 2p^2 \ ^1D$ in O III as a function of energy. —, R -matrix with full CI wavefunctions; $\times \times \times$, distorted-wave results of Pindzola (1977); - - -; distorted-wave results of Mann (1980).

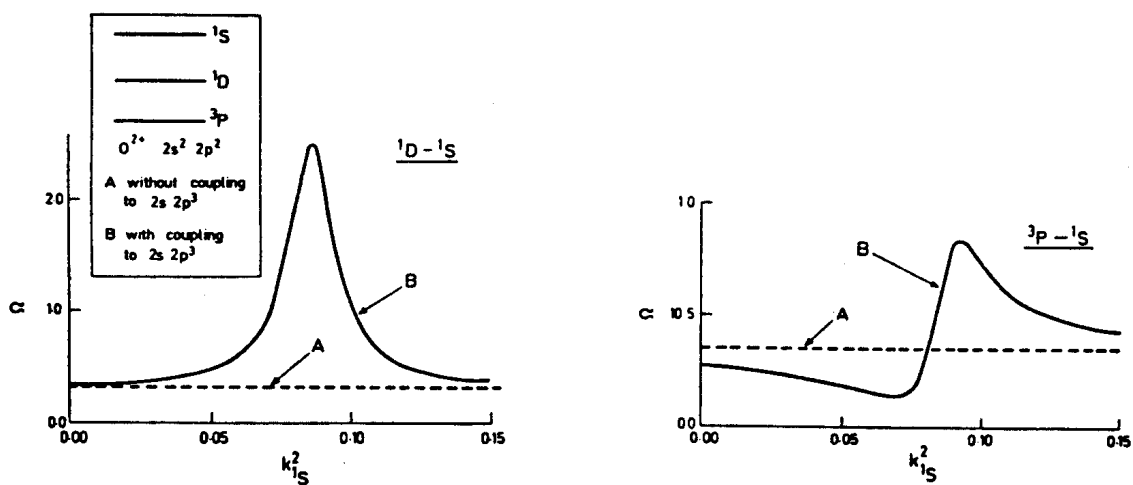


Figure 5.9b— Collision strengths for O^{++} with and without coupling between the $2s^2 2p^2$ and $2s 2p^3$ states.

- (i) forbidden radiative transition $2^3S - 1^1S$: $A_{tot}=1.27 \times 10^{-4} s^{-1}$.
(ii) collisional ionization: $e + He(2^3S) \rightarrow e + He^+ + e$
 $q(T) = 8.38 \times 10^{-10} T^{1/2} e^{(-55,338/T)} \approx 3.3 \times 10^{-10} cm^3 s^{-1}$ at $T=10^4$ K.
(iii) collisional excitation: e-impact at $T=10^4$ K:

$$\begin{aligned} 2^3S \rightarrow 2^3P &: q(T=10^4K) \approx 1.7 \times 10^{-7} cm^3 s^{-1} \\ 2^3S \rightarrow 2^1S &: q(T=10^4K) \approx 3 \times 10^{-8} cm^3 s^{-1} \\ 2^3S \rightarrow 2^1P &: q(T=10^4K) \approx 5 \times 10^{-9} cm^3 s^{-1} \\ 2^3S \rightarrow 1^1S &: q(T=10^4K) \approx 2.5 \times 10^{-9} cm^3 s^{-1} \end{aligned}$$

Most collisional excitations $2^3S \rightarrow 2^3P$ will tend to be followed by radiation back to the 2^3S state because $A(2^3P-2^3S) \approx 1 \times 10^7 s^{-1}$, while for the intersystem transition to the ground state $A(2^3P_1-1^1S_0) = 180 s^{-1}$. The same holds for the higher 3L states. Thus collisional excitation to the 2^3P and higher triplet states is not likely to lead to a net loss of population from $2^3S - 1^1S$ emission, for electron densities $n(e) \geq 3300 cm^{-3}$.

A useful summary of processes affecting the ionization and excitation of atoms in a plasma of hydrogen and helium is that of Gould and Thakur (1970, *Ann. Phys.* **61**, 351). Convenient analytic approximations to many of the relevant rate coefficients are given in Black (1981, *MNRAS* **97**, 553).

6. Charge-transfer processes

Charge-transfer processes of the type



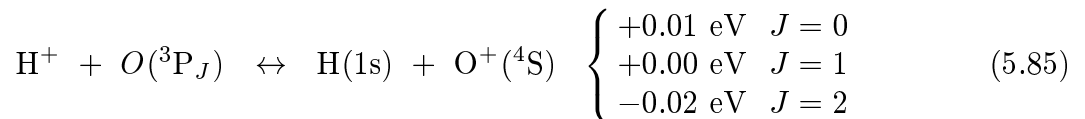
can play an important role in the ionization structure of a non-fully ionized plasma. The rate coefficients for charge-transfer often exceed $10^{-9} cm^3 s^{-1}$. Since radiative and dielectronic recombination have rate coefficients of order $10^{-12} cm^3 s^{-1}$, charge transfer is more effective when the fractional neutral content is larger than 10^{-3} . Such a situation occurs readily in cases that the ionizing source has a non-thermal spectrum, in which there are many more photons at the shortest wavelengths than at longer wavelengths. Since the heavy elements are more effective in absorbing high-frequency radiation (that is, far higher than 13.6 eV), they will be ionized, whereas few photons are available to ionize hydrogen at the longer wavelengths (nearer to 13.6 eV). Thus, non-thermal ionizing sources create plasmas in which multiply-charged ions co-exist with neutral hydrogen atoms.

We will look in some detail at the process of charge-transfer later in this course. Here, we will mention only some important examples. ‘‘Symmetric, resonant charge transfer’’ collisions such as



can have a large cross section. Because the reactants and products are symmetric, it does not change the ionization state of a plasma, however.

A very important astrophysical process is the ‘‘accidental resonant charge transfer’’ process between H^+ and O. The ionization potential of H is 13.598 eV, and that of O is 13.618 eV, so that, by accident, they nearly coincide. Thus, the process:



involves almost no change in internal energies. The cross sections for such processes can be large, even at low temperatures. This process in particular has been studied in detail by Chambaud *et al.* (1980, *J. Phys. B* **13**, 4205). At high temperatures ($T \approx 10^4$ K) it proceeds essentially at the collision frequency (that is, occurring on every collision) and the forward and reverse rates are related by:

$$g(\text{H}^+)g(\text{O})q_f \simeq g(\text{O}^+)g(\text{H})q_r \quad (5.86)$$

where $g(\text{H}^+)=1$, $g(\text{O})=9$, $g(\text{O}^+)=4$, $g(\text{H})=2$ are the ground state degeneracies or statistical weights, so that:

$$\frac{n(\text{O})}{n(\text{O}^+)} \simeq \frac{9}{8} \frac{n(\text{H})}{n(\text{H}^+)} \quad (5.87)$$

Most charge-transfer processes involve “asymmetric, non-resonant” charge transfer such as:



Charge transfer often leaves the product ion in a specific excited state. For example, reaction (5.88) leaves O^{2+} preferentially in the $2p3p \ ^1\text{P}$ state. This state relaxes by emission of photons, for example in the $2p3p \ ^1\text{P} - 2p3s \ ^1\text{P}$ transition at 5592\AA , resulting in a characteristic spectrum. The O III line at 5592\AA has been detected in many planetary nebulae (see for example, the spectrum of NGC 6741 in the first lecture of the course), Seyfert galaxies, etc... and provides a good measure of the importance of charge transfer, and, indirectly, of the neutral hydrogen fraction H/H^+ inside the highly-ionized region.

Note that these charge-transfer processes also affect the cascade resulting from the Bowen fluorescent excitation of O^{2+} . Table 5.3 presents results for a model of the planetary nebula NGC 7662 which includes both the Bowen mechanism and the charge-transfer excitation.

For singly-charged ions, charge transfer to H and to He is usually slow. For example, the rate coefficient for:



has been calculated to have a rate coefficient of only $1.0 \times 10^{-12} \text{cm}^3 \text{s}^{-1}$ at 10^4 K. Similarly, $\text{C}^+ + \text{H}$, and $\text{S}^+ + \text{H}$ charge transfer processes are slow. A notable exception is, of course, the accidental resonance charge transfer of $\text{O}^+ + \text{H}$.

On the other hand, charge transfer involving multiply-charged ions $M \geq 2$ is often rapid. Table 5.4 lists the rate coefficients at 10^4 K for some important ions. Except for C^{2+} , Ne^{2+} and S^{2+} , the rate coefficients are $10^{-9} \text{cm}^3 \text{s}^{-1}$ or larger. For the cases of Ne^{2+} and S^{2+} , charge-transfer can only proceed by a radiative process, for example:



Radiative charge transfer, however, is very slow and its influence on the ionization structure can be safely neglected. The fact that charge-transfer is much slower for Ne^{2+} than for O^{2+} provides a ready explanation of observations of emissions from Ne^{2+} and O^{2+} which appear to indicate an increase of in the $[\text{Ne}]/[\text{O}]$ abundance ratio at the perispheres of many nebulae. At the perispheres the neutral hydrogen fraction is just large enough that it rapidly removes O^{2+} , but not Ne^{2+} .

Table 5.3– Intensities for the triplet transitions $(2p3p) \ ^3S - (2p3s) \ ^3P^o$ and $(2p3s) \ ^3D - (2p3s) \ ^3P^o$ of O^{2+} in NGC 7662. The intensities used for the reference lines are $I(313.3) = 159$ and $I(559.2) = 0.18$.

		Measured I	I_b^*	I_c^*	I_b+I_c
3S	329.9 nm	<u>9+2</u>	4	0.03	4
	331.2	<u>12+3</u>	13	0.09	13
	334.1	<u>22+5</u>	22	0.15	22
3D	376.0	<u>7+2</u>	5.9	0.8	6.7
	375.5	<u>2+1</u>	0.8	0.6	1.4
	377.4	<u>0.4+0.2</u>	0.03	0.34	0.37
	375.7	<u>0.8+0.4</u>	0.04	0.44	0.48

(Note: I_b is the intensity arising from the Bowen mechanism; I_c the intensity from charge transfer.)

Table 5.4– Rate Coefficients for charge-transfer Recombination
 $X^{m+} + H \rightarrow X^{(m-1)+} + H^+$ at 10^4 K

Ion	k	Ion	k	Ion	k
C^{2+}	1.0(-12)	N^{2+}	8.6(-10)	O^{2+}	7.7(-10)
C^{3+}	3.6(-9)	N^{3+}	2.9(-9)	O^{3+}	8.6(-9)
C^{4+}	2.1(-9)	N^{4+}	3.0(-9)	Ne^{2+}	$\sim 1(-14)^*$
Si^{2+}	5.3(-9)	S^{2+}	$\sim 1(-14)^*$	Ne^{3+}	5.7(-9)

* These are approximate upper limits based on the expectation that radiative charge transfer is the most probable reaction channel.

References to charge-transfer processes of astrophysical interest:
 Shields, Dalgarno and Sternberg 1983, *Phys. Rev. A* **28**, 2137
 Heil, Butler and Dalgarno, 1983, *Phys. Rev. A* **27**, 2365
 Butler, Heil and dalgarno 1980, *Ap. J.* **241**, 442
 Butler and Dalgarno 1980, *Ap. J.* **241**, 838
 Dalgarno and Steinberg 1982, *Ap. J. Letters* **257**, L27
 Osterbrock 1983, *Ap. J.* **273**, L31
 McCarroll 1988, in “Rate coefficients in Astrochemistry”