Chapter 2 Collision Physics

Introduction

In order to describe the phenomena discussed in Chapter 1, an understanding of the transfer of energy between colliding atomic particles is needed. Such collisions are described by classical or semi-classical methods with the quantum mechanical effects, such as interference and diffraction, incorporated as corrections. These methods are employed when the wavelength associated with the collision is small compared to the dimensions of the system. This is the same basis for using geometric optics to approximate the passage of light through a medium. In the problem of interest, the incident “radiation” is a beam of particles and the medium is the field of a “target” atom or molecule. The wavelength of interest is \( h/p \), where \( h \) is Planck’s constant and \( p \) is the momentum of the particles. Comparing this wavelength to an atomic radius, e.g., the Bohr radius, \( a_0 \), a rough criterion for the usefulness of classical or semi-classical methods can be established: collision energies much greater than a Rydberg (27.2 eV) for incident electrons and much greater than hundredths of an eV for incident ions. For ions, atoms, or molecules this criterion is satisfied for the full energy range of interest in Chapter 1. However, scattering at small angles (diffraction) is always dominated by wave-mechanical effects, as are regions of interaction in which electronic transitions take place.

Before proceeding, certain cross sections will be defined. The total collision cross section is obtained from an experiment in which a beam of particles, \( A \), is incident on a target containing atoms, \( B \), and the change in intensity of the beam is monitored (Fig. 2.1). If the target is “thin”, that is, an incident particle is likely to make only a single collision, then the change in intensity, \( \Delta \Phi \), for a small change in thickness, \( \Delta x \), is

\[
\Delta \Phi = -\sigma n_B \Phi \Delta x,
\]

where \( n_B \) is the density of target atoms, \( B \), and \( \Phi \) is the measured intensity [particles/(cm\(^2\) s)]. In Eq. (2.1) \( \sigma \) is the cross section, with units of area, indicating the range of the interaction between the colliding particles. Such measurements show that the total cross section varies slowly with velocity, as shown in Fig. 2.2. That is, atoms have diffuse boundaries and the effective range of the interaction region changes with velocity. This dependence is quantum mechanical in nature, as the effective interaction range is determined by scattering at small angles.
Fig. 2.1. Beam experiment to obtain the scattering cross section of A by particles B. (R.E. Johnson 1982)

Fig. 2.2. He + He total scattering cross section vs. incident He energy: detector aperture size at 0°: A 0.57°; B 0.26°; C 0.11°; D 0.056°. Shows slow dependence on energy and the importance of scattering at small angles. (Savola et al. 1973)
Integrating Eq. (2.1), the intensity of unscattered particles vs thickness, x, for thick samples is

\[ \Phi = \Phi_0 e^{-n_0 \sigma x}. \] (2.2)

The quantity \( d\Phi/\Phi_0 = (n_0 \sigma) e^{-n_0 \sigma x} dx \) is the Poisson probability of the first collision occurring between \( x \) and \( x + dx \), and \((n_0 \sigma)^{-1}\) is the collisional mean free path.

Experiments in which the scattered particles are detected (Fig. 2.3) give more detailed information on atomic interactions. For a beam of atoms A incident on a target containing atoms B, the angular differential cross section, \((d\sigma/d\Omega)_A\), relates the number of incident particles per unit time scattered into a region of solid angle \( d\Omega \) to the incident flux. Similarly, \((d\sigma/d\Omega)_B\) applies to the target particles ejected into a region of solid angle. Collecting all particles A (or B) scattered into all solid angles is equivalent to integrating \((d\sigma/d\Omega)_A\) over all angles and gives the total scattering cross section \( \sigma \). In such experiments, discrimination may also be made between internal changes that have occurred (e.g., changes in mass, charge, energy, etc.). Therefore, the cross sections determined from these experiments indicate both the nature of the interaction between A and B and the probability of a change (transition) in either A or B.

In this chapter the nature of the cross section is first described, then the forces between atomic particles are discussed and are used to calculate cross sections and transition probabilities. Such calculations are divided into those methods useful for describing transitions in either fast or slow collisions. For incident ions and atoms collisions are fast or slow depending on whether the ratio of the collision time and the characteristic period of the target, \( \tau_c/\tau \), is less than or greater than one. The collision time can be written \( \tau_c \sim d/v \), where \( v \) is the relative speed and \( d \) is a characteristic dimension associated with A and B, e.g., \( d \approx a_0 \) for outer shell electrons. When describing ionization of outer shell electrons, the characteristic period is \( \sim 10^{-16} \) s, whereas it is \( \tau \sim 10^{-14} \) s for molecular vibrational motion and \( \tau \sim 10^{-13} \) s for rotational motion. Setting \( \tau_c \sim \tau \) these times translate into incident particle energies of the order 1 keV/amu, 0.1 eV/amu, and 0.001 eV/amu, where an amu is the atomic mass unit. It is useful to know that when the collision time is about the same size as the characteristic period, transitions are likely and the cross sections are “large” (i.e., of the order of the dimensions of the colliding particles). For much larger or much smaller collision times the cross sections decrease as described below. Many of the details of this discussion are given in the Appendix, as are a number of useful expressions.

**Impact Parameter Cross Sections**

The trajectory of an incident particle, A, interacting repulsively with an initially stationary target particle, B, is shown in Fig. 2.3. The quantity \( b \) in that figure
Fig. 2.3. Scattering of A by B. b is impact parameter; \( \vec{R} \) shows position of A with resp B; \( \alpha_R \) is orientation angle. \( \vec{v}_A = \vec{v} \) is the initial velocity and \( \vec{v}'_A \) and \( \vec{v}'_B \) are the final velo \( \theta_A \) is the scattering angle for A. The solid angle of acceptance indicated is \( 2\pi \sin \theta_A d\theta_A \).

indicates the closeness of approach and is referred to as the impact paran
It is the perpendicular distance between the incident velocity vector, \( \vec{v}_A \)
and the location of particle B (i.e., \( b = R \sin \alpha \) as \( z \to \infty \)). The impact paran
also indicates the angular momentum of the colliding particles (i.e., \(|M_A\vec{R} \times \vec{v}| = M_A v b\)) and, along with the relative velocity \( v \) (or ene
characterizes collisions between spherically symmetric particles. Therefore
probability of a collision is written \( P_c(b, v) \). If the incident and/or target pa
has a spin or is a molecule then initial orientations with respect to the coll
axis have to be specified, e.g., \( P_c(b, \phi, \Omega, v) \), where \( \phi \) is the azimuthal ang
approach and \( \Omega \) is an orientation angle. If all orientations occur then \( P_c \)
is the averaged probability.

Based on the description leading to Eq. (2.1), the interaction cross se
between A and B is

\[
\sigma(v) = 2\pi \int_0^\infty P_c(b, v) b \, db.
\]

That is, if A passes through the ring of area \( 2\pi b \, db \) about B (Fig. 2.3), i
be scattered from the beam with a probability \( P_c \), contributing to the cf
in intensity of the beam, \( \Delta I \). In classical mechanics, \( P_c \) is zero or one. Then
for a collision between two spheres of radius \( r_A \) and \( r_B \), \( P_c = 0 \) for \( b > r_A \)
and \( \sigma = \pi(r_A + r_B)^2 \). For interactions between atomic or molecular particle
forces are infinite in range but the diffraction effect causes the cross secti
be finite for most interactions (Appendix 2A), as in the measured values s
in Fig. 2.2. That is, \( P_c(b, v) \to 0 \) as \( b \to \infty \).
From Fig. 2.3 it is seen that, if the forces between the particles are independent of their orientations, then those particles passing through the ring of area \(2\pi b\,\text{db} \) will be scattered into some angular region \(2\pi \sin \theta_A\,\text{d}\theta_A\) with unit probability, \(P_c = 1\). The ratio gives the angular differential cross sections,

\[
\left( \frac{d\sigma}{d\Omega_A} \right) = \sigma(\theta_A) = \left| \frac{b\,\text{db}}{\sin \theta_A\,\text{d}\theta_A} \right|, \quad \left( \frac{d\sigma}{d\Omega_B} \right) = \sigma(\theta_B) = \left| \frac{b\,\text{db}}{\sin \theta_B\,\text{d}\theta_B} \right|,
\]

(2.4)

where the simplified notation for azimuthally symmetric cross sections, \(\sigma(\theta_A)\) is often used instead of \((d\sigma/d\Omega)_A\). Evaluation of these cross sections requires knowledge of the relationship between the angles and \(b\), determined from the forces.

For elastic collisions (no change in internal energy) the energy and momentum of each particle alter the collision is related to the incident energy and the scattering angle, which can be expressed either in the laboratory or in the center of mass (CM) system (Goldstein 1950). In Table 2.1 the relationships between laboratory and CM quantities are summarized for a moving particle \(A\) incident on a stationary particle \(B\). The CM deflection angle vs \(b\), \(\chi(b)\) (called the deflection function), gives a cross section

\[
\sigma(\chi) = \left| \frac{b\,\text{db}}{\sin \chi\,\text{d}\chi} \right|.
\]

(2.5)

The calculation of \(\chi(b)\), hence \(\sigma(\chi)\), is described in the following section and the transformations to the laboratory scattering cross sections discussed are given in Table 2.1. Because the collisional (elastic) energy transfer to particle \(B\), \(T\), is simply related to \(\chi\) (Table 2.1), it is often useful to consider the energy transfer cross section instead of \(\sigma(\chi)\),

\[
\frac{d\sigma}{dT} = \frac{4\pi}{\gamma E_A} \sigma(\chi),
\]

(2.6)

where the mass factor, \(\gamma\), is defined in Table 2.1. Throughout the text we will use \(d\sigma \rightarrow (d\sigma/dT)\,dT \rightarrow \sigma(\chi)2\pi \sin \chi\,\text{d}\chi \rightarrow 2\pi b\,\text{db}\) to represent an element of the elastic cross section \(\sigma(\chi)\).

In addition to a transfer of kinetic energy to \(B\), there is also a probability, \(P_{0\rightarrow f}(b, v)\), that one or both particles will experience a change in internal energy (a transition) where the subscripts indicate the initial (0) and final (f) states. Following Eq. (2.3), for these inelastic collisions

\[
\sigma_{0\rightarrow f}(v) = 2\pi \int_0^\infty P_{0\rightarrow f}(b, v) b\,\text{db}.
\]

(2.7)

The quantity \(P_{0\rightarrow f} \rightarrow 0\), as discussed earlier, for some \(b_{\max}\) for which the collision time \((\tau_E \approx b_{\max}/v)\) is of the order of the period of the electrons. (This is called the Bohr adiabatic cut-off, Appendix 2C.) Since each inelastic process is associated with an internal energy change, \(Q_{0\rightarrow f}\), the average inelastic energy
Table 2.1. Relationship between laboratory and CM variables

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity of CM</td>
<td>( \vec{V}_c = (M_A \vec{v}_A + M_B \vec{v}_B) / (M_A + M_B) \equiv \vec{R}_c )</td>
</tr>
<tr>
<td>Relative velocity in CM</td>
<td>( \vec{v} = (\vec{v}_A - \vec{v}_B) \equiv \vec{R} )</td>
</tr>
<tr>
<td>Total laboratory quantities</td>
<td>CM quantities</td>
</tr>
<tr>
<td>( M = M_A + M_B )</td>
<td>( m = M_A M_B / (M_A + M_B) ) : mass</td>
</tr>
<tr>
<td>( E_A + E_B = M \vec{V}_c^2 / 2 + E )</td>
<td>( E = m \vec{v}^2 / 2 ) : energy</td>
</tr>
<tr>
<td>( M_A \vec{v}_A + M_B \vec{v}_B = M \vec{V}_c )</td>
<td>( \vec{p} = 0 ) : momentum</td>
</tr>
<tr>
<td>( \vec{L}_A + \vec{L}_B = M \vec{R}_c \times \vec{V}_c + \vec{L} )</td>
<td>( \vec{L} = m \vec{R} \times \vec{v} ) : angular momentum</td>
</tr>
</tbody>
</table>

Transformations (for \( \nu_B \) initially zero and elastic collisions)

\[
\begin{align*}
\theta_B &= (\pi - \chi)/2 \\
\tan \theta_A &= \mu \sin \chi / (1 + \mu \cos \chi); \mu = M_B / M_A \\
T &= \gamma E_A \sin^2 (\chi/2); \gamma = 4 M_B M_A / (M_A + M_B)^2 \\
\frac{d\sigma}{d\Omega}_A &= \sigma(\chi) \left| \frac{d \cos \chi}{d \cos \theta_A} \right| = \sigma(\chi) \frac{(\mu^2 + 2 \mu \cos \chi + 1)^{3/2}}{\mu^2 |\mu + \cos \chi|} \\
\frac{d\sigma}{d\Omega}_B &= \sigma(\chi) \left| \frac{d \cos \chi}{d \cos \theta_B} \right| = \sigma(\chi) |4 \sin(\chi/2)| \\
\frac{d\sigma}{dT} &= \frac{4 \pi}{\gamma E_A} \sigma(\chi)
\end{align*}
\]

lost in the collision is

\[
Q(b) = \sum_f Q_{0 \rightarrow f} P_{0 \rightarrow f}(b,v).
\]

In Eq. 2.8 the sum of probabilities over all processes, including no internal energy change, is unity \([\Sigma P_{0 \rightarrow f} = P_0(b,v) = 1]\). The calculation of \( P_{0 \rightarrow f} \) is described shortly, and a useful estimate for \( Q(b) \) is given in Appendix 2C.

The above expressions can be used to define the average energy loss per unit path length for particle A traversing a material consisting of particles B, an important quantity in Chapter 3. This incident particle may be a cosmic ray particle traversing an interstellar cloud or an ion in the Jovian magnetosphere penetrating the icy surface of Europa. In the passage through a target gas or a solid, A loses energy both to electronic excitations and to momentum transfer to target nuclei B. Noting that \((n_B \sigma_{0 \rightarrow f})^{-1}\) is the mean-free path for the occurrence of an energy loss \(Q_{0 \rightarrow f}\), the averaged electronic energy loss per unit
path length in the target is
\[
\left( \frac{dE}{dx} \right)_e = n_B \sum_T Q_{0 \rightarrow r} \sigma_{0 \rightarrow r} = n_B 2\pi \int_0^\infty Q(b) b \, db.
\] (2.9)

Similarly, if \((n_B (d\sigma/dT) dT)^{-1}\) is the mean-free path for transferring an amount of kinetic energy between \(T\) and \(T + dT\) to a nucleus \(B\), then the averaged "elastic" collisional energy loss per unit path length is
\[
\left( \frac{dE}{dx} \right)_n = n_B \int_0^\infty T \left( \frac{d\sigma}{dT} \right) dT = n_B 2\pi \int_0^\infty T(b) b \, db.
\] (2.10)

Although the electronic and collisional energy losses occur concomitantly, they are generally treated separately and additively. Because they both depend on the material number density, the net energy loss is generally written
\[
\left( \frac{dE}{dx} \right) \approx n_B (S_e + S_n).
\] (2.11)

The quantity \((dE/dx)\) is referred to as the stopping power of the material, and the quantities \(S_e\) and \(S_n\) are the electronic and nuclear elastic (collisional) stopping cross sections. These are quantities determined by the single collision interaction of \(A\) with \(B\) and not properties of the target as a whole. For this reason they apply roughly to gases, liquids, and solids. Although they are generally measured for ions incident on neutrals, they can be applied to neutrals injected into a plasma. Results for \(S_e\) are tabulated (see Bibliography), and simple, generally useful expressions for \(S_n\) are available (Appendix 2B). In Fig. 2.4 we give such a result for hydrogen and oxygen ions incident on a medium containing H, O, or Si. At high energies most of the loss is to energy transfer to electrons, and at low energies it is to energy transfer to the target nucleus.

The nuclear stopping cross section, \(S_n\), is also related to the diffusion cross section or momentum transfer cross section, \(\sigma_d\) (Banks and Kocharts 1973; Johnson 1982). The change in the parallel component of momentum of a particle \(A\) due to a collision with \(B\) involving no electronic excitations is written
\[
(\Delta \vec{p}_A)_i = m v(1 - \cos \chi),
\]
where \(m\) is the reduced mass in Table 2.1. Therefore, the drag force on a particle \(A\) traversing a target containing particles \(B\) is the collision rate times this momentum loss,
\[
(\Delta \vec{F}_A)_i = \int (\Delta \vec{p}_A)_i v n_B (2\pi b db),
\] (2.12)

which we write as
\[
(\Delta \vec{F}_A)_i = n_B m v^2 \sigma_d,
\]
where
\[
\sigma_d = 2\pi \int_0^\infty [1 - \cos \chi(b)] b \, db = 2\pi \int_{-1}^1 (1 - \cos \chi) \sigma(\chi) d\cos \chi.
\] (2.13)

Using the expression for \(T\) from Table 2.1, \(S_n\) and \(\sigma_d\) are related by
\[
S_n = \frac{\gamma E_A}{2} \sigma_d.
\] (2.14)
Fig. 2.4. **a** The electronic and nuclear stopping cross sections, $S_e$ (*solid lines*) and $S_n$ (*dashed lines*), for H ions entering a medium containing H, O, or Si. **b** Same for O ions. Energy loss in a mixed atomic medium or molecular medium (e.g., H$_2$O, SiO$_2$) can be obtained by combining these (Bragg's rule). These are for the equilibrium charge state ($Z_{\text{eff}}$) in Eq. (2.41) but can be used roughly independent of charge. The "universal" $S_n$ in Appendix 2B is used. $S_e$ for ($\nu < Z_A^{2/3} \nu_0$), used Lindhard and Scharff (1961) [Eq. (2.40)]; for high $S_e$ (Bethe–Born), used Andersen and Ziegler tables (Bibliography)
That is, the drag force is related to the stopping power, i.e., \((\Delta F_A)_\parallel = (1 + M_B/M_A)(dE/dx)_n\). The electronic component adds to this. The elastic component of the force is also the force a streaming plasma applies to neutrals, which is of interest, for example, where the Jovian plasma torus intercepts the corona of Io. Because the factor \((1 - \cos \chi)\) goes to zero as \(\chi\) goes to zero, both \(S_n\) and \(\sigma_d\), unlike \(\sigma\), can be calculated classically (Appendix 2A). In order to give a feeling for the relationship between the quantities we have been discussing, the deflection function, energy transfer cross section, the \(S_n\) (\(\sigma_d\)) are given in Fig. 2.5 for a repulsive force which approximates the \(S^+ + O\) collision.

The cross sections have been defined without reference to the forces between the particles. These forces produce both the deflections and the transitions (inelastic processes). However, it has become customary to separate the

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**Fig. 2.5.** \(S^+ + O\) collision evaluated using “universal” potential (Appendix 2B) a Potential; b CM deflection function for \(E_s = 540\, \text{eV}\) and \(E_o = 0\), the average relative impact energy to Io. c Energy transfer and CM cross sections. d The nuclear (collisonal) stopping cross section and the diffusion cross section for a number of energies, \(E_s\).
discussion of these two effects. The deflections (elastic energy loss) are considered first and then, after a description of the forces, the inelastic effects are considered.

**Elastic Collisions**

In the CM system, the two colliding particles follow equivalent trajectories and the collision can be described as the scattering of a particle of reduced mass, \( m \), by a stationary center of force (B stationery and \( \theta_A \to \chi \) in Fig. 2.3). Therefore, the angular momentum, which is conserved, is

\[
L = mv\beta = mR^2\dot{\chi}_R. 
\]  
(2.15a)

Rearranging Eq. (2.15a) and integrating \( \dot{\chi} \) over time gives the CM scattering angle

\[
\chi(b) = \pi - \int_{-\infty}^{\infty} \dot{\chi}_R \, dt = \pi - v\beta \int_{-\infty}^{\infty} \frac{dt}{R^2}. 
\]  
(2.15b)

Assuming the interaction potential \( V(R) \) depends only on the separation \( R \), energy conservation is expressed as

\[
E = \frac{m\dot{R}^2}{2} + \frac{L^2}{2mR^2} + V(R). 
\]  
(2.16a)

Rearranging this gives a radial velocity,

\[
\dot{R} = \pm v[1 - b^2/R^2 - V/E]^{1/2}, 
\]  
(2.16b)

which goes to zero at the distance of closest approach \( R_0 \). Writing \( |dt| = |dR/\dot{R}| \), Eq. (2.15b) becomes

\[
\chi(b) = \pi - 2b \int_{R_0}^{\infty} \frac{dR}{R^2} [1 - b^2/R^2 - V/E]^{-1/2}. 
\]  
(2.17)

This expression can be integrated analytically for a few potentials of the form \( V(R) = A/R^n \) (Goldstein 1950) but otherwise is treated by the simple numerical procedure, given in Appendix 2B, used to obtain the results in Fig. 2.5b.

For fast incident ions [ratio \( V/E \) small in Eq. (2.17)], the deflections are generally small, and it is useful to replace the expression for \( \chi(b) \) by an impulse approximation. That is,

\[
\chi(b) \approx \frac{\int_{-\infty}^{\infty} F_{\perp} \, dt}{mv} = -\frac{d}{db} \left[ \frac{1}{2E} \int_{-\infty}^{\infty} VdZ \right], 
\]  
(2.18)

in which a straight line trajectory is assumed, i.e., \( R^2 = b^2 + Z^2 \), with \( Z = vt \) and \( R_0 = b \). For power law potentials \( V = C_n/R^n \)

\[
\chi(b) \approx a_n V(R_0)/E, 
\]  
(2.19)
where \(a_n\) is given in Appendix 2B. This shows explicitly that the deflection is determined primarily by the nature of the potential near the distance of closest approach of the colliding particles. Therefore, it is not necessary to know the potential accurately at all \(R\) in order to obtain an estimate of the deflection function as long as \(V/E \ll 1\). Since \(V\) is of the order of electron volts, this criterion is satisfied for a large number of astrophysical problems.

From Eq. (2.19) the quantity \(\chi E\) is seen to depend only on \(R_0\). Using Eq. (2.19) in Eq. (2.5) the modified cross section \(\chi \sin \chi \sigma(\chi)\), given in terms of \(\chi E\), is independent of the energy \(E\) for small angles. [In the lab frame use \(\theta_{\Lambda} \sin \theta_{\Lambda} \sigma(\theta_{\Lambda})\) in terms of \(\theta_{\Lambda} E_{\Lambda}\).] Therefore experimental measurements of angular differential cross sections can be directly converted into the useful power-law potentials which are applicable over limited ranges of \(R\). It is seen in Fig. 2.6 that \(n\) (Eq. 2.19) goes to unity as \(\chi E\) gets large (i.e., \(R_0 \to 0\)) as it should for the repulsive interaction between atoms. Also, as \(\chi E\) decreases (i.e., \(R_0\) increases) \(n\) increases; that is, the potential becomes steeper.

In Fig. 2.7 are schematic drawings of the deflection functions for a predominantly repulsive potential and a long-range attractive plus short-range repulsive potential. Based on Eq. (2.19) these follow the form of the potential. For the repulsive potential \(\chi\) is always positive, attaining a maximum value of \(\pi\) for head-on collisions \([b = 0, \text{Eq. (2.17)}]\). For the potential with a minimum

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**Fig. 2.6.** Angular differential cross section experiment for He\(^+\) + Ar and Ne\(^+\) + Ar at three values of \(E_\Lambda\), \(-\)-\(-\) \(25\ \text{keV}, \ -\ -\ -\) \(50\ \text{keV}, \ -\ -\ -\ -\ -\ -\ -\ -\) \(100\ \text{keV}\). Approximate power laws indicated by \(n\). (Fuls et al. 1957)
\( \chi \) is negative at large \( b \) but again reaches \( \pi \) at \( b = 0 \). Because the detector collects both negative and positive angles, it is seen in Fig. 2.7 that more than one value of the impact parameter contributes to scattering at a number of angles for such potentials. Since \( \chi \) also goes through a minimum, \( \chi_r \), at the impact parameter labeled \( b_r \), \( d\chi/db \) becomes zero, and the classical cross section in Eq. (2.5) becomes infinite. This large enhancement in the scattering probability is similar to the effect that produces rainbows in the scattering of light from water droplets; hence, \( \chi_r \) is called the rainbow angle. When \( \chi_r < \pi \) only one impact parameter contributes for \( \chi > \chi_r \). For angles \( \chi < \chi_r \) three impact parameters contribute with the same value of \( \cos \chi \) in Eq. (2.5). Using a Lenard-Jones form for the potential, \( V = C_{2n}/R^{2n} - C_n/R^n \), the rainbow angle is obtained from Eq. (2.19),

\[
\chi_r \approx \frac{-1}{4E} \left( \frac{a_n C_n}{a_{2n} C_{2n}} \right)^2 = -\frac{a_n^2 |V_{\text{min}}|}{a_{2n} E}.
\]

(2.20)

Therefore, knowledge of the depth of the potential, \( |V_{\text{min}}| \), gives the angle at which the cross section is strongly enhanced. For large \( E \) this angle is often negligibly small.

As the collision energy becomes small, \( \chi_r \) can become much larger than \( \pi \), so that the two particles may orbit each other before separating. In fact, for very small velocities there is a particular impact parameter for which the particles orbit continuously (i.e., \( d^2R/dt^2 = 0 \) at \( dR/dt = 0 \)). Using the attractive part of potential above along with Eq. (2.16b), this impact parameter is

\[
b_0 \approx \left( \frac{n C_n}{2 E} \right)^{1/n} \left( \frac{n - 2}{n} \right)^{(n-2)/2n}.
\]

(2.21)

Therefore, for \( b < b_0 \), the interaction times can be long because the particles orbit, whereas for \( b > b_0 \), the particles simply scatter. Because the long interaction times...
enhance the likelihood of low probability processes, $b_0$ is very useful for estimating inelastic ion-molecule cross sections for astrophysics (McDaniel et al. 1970).

Near the rainbow angle (or when orbiting occurs) a number of impact parameters contribute to the scattered flux at a given observation angle; hence, interference phenomena occur and classical cross section estimates of $\sigma(\chi)$ are not valid. If the angular resolution is not large, the simple addition of the contributions to the scattered flux from each impact parameter gives an adequate representation of the cross section. That is,

$$\sigma(\chi) \approx \sum \frac{b \, db}{\sin \chi \, d\chi_{|b=b_i}}$$  \hspace{1cm} (2.22)

where $b_i$ are all those impact parameters giving the same value of $\cos \chi$ [i.e., $\chi \to \pm (\chi + 2\pi q)$, $q$ an integer]. In Appendix 2A, we briefly review the wave-mechanical description of the elastic scattering cross section. The results have parallels in light scattering, a subject familiar to the astronomy community. In the following section we describe the nature of the interaction potential $V(R)$.

Interaction Potentials

The primary force determining the behavior of colliding atoms or molecules is the Coulomb interaction. This acts between each of the constituent electrons and nuclei of the colliding particles and, therefore, the description of the interaction between such particles would appear to be straightforward. However, the Pauli principle must be applied, and each of the constituents moves relative to the center of mass of its parent atom or molecule. As this motion is superimposed on the overall collisional motion, the description of a collision can be complex even for the simplest atoms. Rather than solve the complete many-body system, the interaction potential between the atomic centers is averaged over the motion of the electrons. This separation of the motion of the electrons and nuclei, based on their huge differences in mass, is referred to as the Born–Oppenheimer separation (Torrens 1972; Johnson 1982).

Since the behavior of the electrons during a collision will depend on the relative motion of the nuclei, interaction potentials are generally calculated in two limiting cases (Bates 1962; Massey 1979). If the collision of two atoms is fast relative to the motion of the electrons ($v \gg v_e$), then the electronic distribution is static during the collision, except for abrupt changes or transitions, which occur when the particles are at their closest approach. These transitions reflect the ability of an atom to absorb (emit) energy when exposed to the time-varying field of a moving particle (Appendix 2C) in the same way that atoms absorb or emit photons. Before and after the transition, the potentials are determined from the separate atomic charge distributions.
In the opposite extreme (slow collisions, \( v \ll v_e \)) the electrons adjust continuously and smoothly to the nuclear motion, returning to their initial state at the end of the collision. This is an adiabatic process, as the electrons do not gain or lose energy. That is, even though the molecules may be deflected and change kinetic energy, their initial electronic state does change, i.e., it is an "elastic" collision. During the collision the electron distribution evolves from one in which electrons are attached to separate centers into a distribution at small separations in which the electrons are shared by the two centers, a covalent distribution. Therefore, for every possible initial state for each atom there is a corresponding adiabatic potential, resulting in a complex potential diagram like that shown in Fig. 2.8. Such potentials also determine the ability of the two particles to form a molecule.

For collisions which are nearly adiabatic the nuclear motion can induce a transition between states. This is often described as a "transition between potential curves," because these curves indicate the energy levels of the system at each \( R \). Such transitions generally occur at well-defined internuclear separations at which the atomic character of the wave function gives way to the molecular, covalent character (Olson 1980).

Since the electrons in different shells have very different velocities, the separation into fast and slow collisions allows the orbitals to be treated separately. For instance, when a collision is fast with respect to the outer-shell electrons, it may be adiabatic with respect to the inner-shell electrons. Therefore, the inner-shell electrons return to their initial state only screening the interaction between the nuclei and, hence, play a passive role in the collision. As a point of reference, it is useful to remember that a nucleus with a speed equivalent to an electron in the ground state of a hydrogen atom (2.19 \( \times 10^8 \) cm/s) has an energy of about 25 keV/amu. Therefore, a 25 keV He\(^+\) or even a 100 keV O\(^+\) colliding with an H or O atom is considered a slow collision. In addition, the orbital speed of an electron in the target atom scales to the speed of an electron in a ground state of hydrogen using the effective nuclear charge, \( Z' \) (Clementi and Roetti 1974), which accounts for screening of nucleus.

Interaction potentials between two atoms, such as those in Fig. 2.8, can be written as a sum of the nuclear repulsion and the averaged electronic energy, \( \varepsilon_j(R) \),

\[
V_j(r) = \frac{Z_A Z_B e^2}{R} + [\varepsilon_j(R) - \varepsilon_j^0].
\] (2.23)

In this expression \( j \) labels the electronic state, \( Z_A \) and \( Z_B \) are the nuclear charges, and \( \varepsilon_j^0 \) is the value of the electronic energy, \( \varepsilon_j(R) \), as \( R \to \infty \). Each state, \( j \), is associated with a pair of atomic states at large \( R \) as indicated in Fig. 2.8. In the electrostatic limit (\( v \gg v_e \)) the electronic energy, \( \varepsilon_j \), is sum of the electronic energies of the separated atoms, \( (\varepsilon_A^0 + \varepsilon_B^0) = \varepsilon_j^0 \), and the averaged interaction of the electrons on each atom with the electrons and nucleus of the other atom,
Fig. 2.8. Adiabatic potential energy curves vs. internuclear separation. R, for O⁺ + O, O + O and, O + O⁻. (Gilmore 1964)
which we write \( V_j^e \). That is
\[
V_j(R) \approx \frac{Z_A Z_B e^2}{R} + V_j^e
\]
with \( V_j^e \) written as
\[
V_j^e(R) = -Z_B e^2 \int \frac{\rho_{A_j}(\vec{r}_A)}{|R - \vec{r}_A|} d^3r_A - Z_A e^2 \int \frac{\rho_{B_j}(\vec{r}_B)}{|R + \vec{r}_B|} d^3r_B
\]
\[
+ e^2 \int \frac{\rho_{A_j}(\vec{r}_A) \rho_{B_j}(\vec{r}_B)}{|R - \vec{r}_A + \vec{r}_B|} d^3r_A d\vec{r}_B.
\]
(2.24)

Here the \( \rho_{A_j} \) and \( \rho_{B_j} \) are the atomic densities for the electrons on atoms A and B. The evaluation of \( V_j^e \) is treated in texts on electrostatics (Jackson 1963).

In the adiabatic limit \( (v \ll v_e) \), \( \varepsilon_j(R) \) in Eq. (2.23) is calculated at each \( R \) from the electronic wave function or an approximation to it (Bates 1962). Because the deflection function is determined primarily by a narrow region of \( R \) for each \( b \) (or \( \chi \)), [viz: Eq. (2.19)], the behavior of \( V_j(R) \) for various regions of \( R \) is described below.

**Short-Range Potentials**

For close collisions \( (R \ll r_A, r_B \text{ where } r_A \text{ and } r_B \text{ are the atomic radii}) \) nuclear repulsion dominates. The electrons screen this repulsive interaction, giving an effective potential
\[
V_j(R) = \frac{Z_A Z_B e^2}{R} \Phi(R/\tilde{a}),
\]
(2.25)

where \( \tilde{a} \) is the screening length and \( \Phi \) the screening function. Considerable effort has been expended determining \( \Phi \) and \( \tilde{a} \) for many-electron atoms and, therefore, experimental results should be used when possible. For fast collisions, the electrostatic calculation in Eq. (2.24) can give a reasonable estimate. Even simpler, \( \Phi \) is often approximated as \( \exp(-R/\tilde{a}) \) in scattering calculations (Everhart et al. 1955). Since the electrons in different shells have different screening lengths, a better approximation for a bare ion on a light atom is to assume the \( i \)th shell has a screening constant determined by the electron removal (ionization) energy \( I_i, a_i \sim a_0 (I_0/I_i)^{1/2} \), where \( I_0 \) and \( a_0 \) are the ground-state, hydrogen atom ionization potential and radius. Then, \( Z_B \Phi \sim \Sigma N_i \exp(-r/a_i) \) where \( N_i \) is the number of electrons in the \( i \)th shell.

For collisions between larger \((Z > 10)\) atoms, the screening is often estimated by Thomas–Fermi (electron-gas) approximation in the Appendix 2B (Torrens 1972). Expressions for \( \Phi \), the energy transfer cross section, \( d\sigma/dT \), and the nuclear stopping cross section, \( S_n \), have been given by Lindhard et al. (1968) (Appendix 2B). Even though such static potentials are intended for close collisions, universal semi-empirical functions based on this have been obtained which roughly
describe elastic collisions in the repulsive regime even down to very low energies. These are also given in Appendix 2B, and a useful screening constant for organizing the many data sets (Ziegler et al. 1985) is

\[ \hat{a} = 0.885 \, a_0 / (Z_A^{0.23} + Z_B^{0.23}) \]  

(2.26)

Long-Range Interactions

For slow collisions even small disturbances can lead to deflections; therefore the interaction potential at large separations \( R \gg r_A, r_B \) is of interest. The electronic distributions of each of the colliding particles are slightly distorted by the presence of the other so that the long-range interaction potential is written in powers of \( R \),

\[ V_j(R) = \sum C_n / R^n. \]  

(2.27)

Generally, only the largest term (lowest power of \( n \)) is kept and, therefore the power-law expression for cross section, Eq. (2.19), can be used. The lead terms in Eq. (2.27) can be obtained from the electrostatic interaction in Eq. (2.24) by expanding the denominators in powers of \( R \). For ion-ion collisions the lead term in Eq. (2.27) is \( n = 1 \), \( C_1 = Z_A Z_B e^2 \), which is the Coulomb interaction with \( Z_A \rightarrow Z_A - N_A \) (the net ionic charge). For ion collisions with a neutral molecule having a dipole moment \( \mu_B \) (e.g., a water molecule) the lead term is \( n = 2 \), \( C_2 = -Z_A \mu_B e \cos \theta \), where \( \cos \theta \) is the angle between the internuclear axis and the dipole moment. If the neutral molecule does not have a dipole moment (e.g., \( O_2, N_2 \)) the ion-quadrupole interaction dominates \( (n = 3) \). For two colliding neutral molecules having dipole moments, the dipole-dipole interaction \((n = 3)\) dominates, and so on.

For colliding atomic particles the electrostatic multipole-moments of the charge distribution are zero and for some molecules (e.g., \( H_2 \)) the moments are small. However, the field of the other particle distorts the charge distribution inducing such moments. The lead-term for ion-neutrals is the ion-induced dipole interaction \((n = 4)\), \( C_4 = -\kappa_B (Z_A e)^2 / 2 \), where \( \kappa_B \) is the polarizability of the neutral particle B. For collisions between two neutrals there is no average field at B due to A or vice versa, but instantaneous fluctuations in charge density on either atom lead to short-lived fields. In this case the lead term is the (induced-dipole)-(induced-dipole) interaction, the well-known van der Waals interaction used to describe the behavior of realistic gases. This interaction \((n = 6)\) is attractive [i.e., \( C_6 \) negative in Eq. (2.27)], and coefficients have been obtained from experiment. In Table 2.2 we give values for the dipole moments and the polarizabilities for a number of atoms and molecules in their ground states. These coefficients depend on the initial state and, therefore, differ considerably for collisions with an excited atom or molecule.
Table 2.2. Interaction parameters$^a$

<table>
<thead>
<tr>
<th></th>
<th>$\alpha_0(a_0^3)$</th>
<th>$(\mu_0/e)(a_0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>4.50</td>
<td>—</td>
</tr>
<tr>
<td>He</td>
<td>1.38</td>
<td>—</td>
</tr>
<tr>
<td>C</td>
<td>11.9</td>
<td>—</td>
</tr>
<tr>
<td>N</td>
<td>7.5</td>
<td>—</td>
</tr>
<tr>
<td>O</td>
<td>5.4</td>
<td>—</td>
</tr>
<tr>
<td>S</td>
<td>19.5</td>
<td>—</td>
</tr>
<tr>
<td>H$_2$</td>
<td>5.41</td>
<td>0</td>
</tr>
<tr>
<td>N$_2$</td>
<td>11.7</td>
<td>0</td>
</tr>
<tr>
<td>CO</td>
<td>13.2</td>
<td>0.05</td>
</tr>
<tr>
<td>O$_2$</td>
<td>10.7</td>
<td>0</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>9.8</td>
<td>0.72</td>
</tr>
<tr>
<td>H$_2$S</td>
<td>26.</td>
<td>0.38</td>
</tr>
<tr>
<td>NH$_3$</td>
<td>14.6</td>
<td>0.58</td>
</tr>
<tr>
<td>CH$_4$</td>
<td>17.5</td>
<td>0</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>19.6</td>
<td>0</td>
</tr>
<tr>
<td>SO$_2$</td>
<td>26.</td>
<td>0.64</td>
</tr>
</tbody>
</table>

$^a$van der Waals coefficients can be estimated from the polarizabilities of the interacting atoms or molecules $C^\ddagger \approx (3/2)a_0\alpha_0(\Gamma_A\Gamma_B/(\Gamma_A+\Gamma_B))$ where $\Gamma_A$ and $\Gamma_B$ are average dipole transition energies (for ground state species a reasonable estimate is obtained using the ionization energy).

Intermediate-Range Potentials and Charge Exchange

When R is the order of the atomic radii ($r_A$, $r_B$), the electron clouds on the two interacting particles overlap. In this region the distortion of the charge clouds on each center becomes too large to treat as simply a perturbative polarization of the separated electronic distributions.

The overlap of charge on the two centers allows for the possibility of charge-exchange collisions (e.g., $H^+ + O_2 \rightarrow H + O_2^+$). For such collisions the potentials before and after can be drastically different, as seen in Fig. 2.9 for $S^2^+ + O \rightarrow S^+ + O^+$, a process of considerable interest in the Io plasma torus. Depending on the final states of $O^+$ and $S^+$, the initial and final state potential energy curves may cross. Therefore, electron transfer between $S^2^+$ and $O$ can occur, with little change in the total electronic energy, at the crossing points. This transfer gradually results in a net change in the final electronic energy when the particles separate from each other. The likelihood of charge exchange occurring at the crossing point is proportional to the size of the overlap of the charge distributions of the electron on each center (Rapp and Francis 1962).

For intermediate R the covalent (electron exchange) interaction can be examined by considering the $H^+ + H$ (i.e., $H_2^+$) system. For this colliding pair the electron transfer $H^+ + H \rightarrow H + H^+$ occurs without a net change in internal energy. The two identical states at large R ($H + H^+$ and $H^+ + H$) mix at smaller R because of electron sharing, forming both attractive and repulsive potentials.
Fig. 2.9. Potential curves vs. internuclear separation, \( R \), at intermediate and large \( R \). Collisions between ions have repulsive potentials \( (e^2/R) \) at large \( R \); between the ion and neutral an attractive polarization potential, \( -(Z_A - N)^2 \alpha e^2/2R^4 \): for this case \((Z_A - N)\) nuclear charge minus number of electrons is 2. Shows curve crossings for the \( S^{3+} + O \to S^+ + O^+ \) collision. \( \alpha \) for O from Table 2.2.

These are seen in Fig. 2.10 and can be understood by considering the wave function at large \( R \). If the wave functions placing the electron on centers A and B in identical states of the hydrogen atom are \( \phi_A \) and \( \phi_B \), then the linear combinations appropriate to the \( H_2^+ \) molecule are \( \psi_{g,u} \approx (\phi_A \pm \phi_B)/\sqrt{2} \). The labels \( g \) and \( u \) refer to symmetric and antisymmetric (gerade and ungerade) states of \( H_2^+ \) (Herzberg 1950). The forms of these wave functions are such that the electronic binding energy decreases in the \( u \) state, as the electron is excluded from the region \( R/2 \), while the reverse is true for the \( g \) state. Therefore, in the scattering of protons by hydrogen, half the collisions will be along the repulsive potential \( (u) \) and half along the attractive potential \( (g) \). The difference in energy between these states is the exchange energy which determines the behavior of charge-exchange collisions. The exchange energy decreases with increasing \( R \) like the overlap of wave functions for the electron on A and on B, which decays like \( \exp(-R/a_0) \) for \( R > a_0 \). Because the covalent interaction decays exponentially, it is eventually dominated at very large \( R \) by the long-range, power-law potentials discussed earlier.

Molecular orbital potentials for \( H_2^+ \) can also be constructed for each excited
state of H as well as for one electron in the field of two identical nuclei and other electrons. In Fig. 2.11 we give a diagram showing the general behavior of these one electron, molecular orbital binding energies, \( \varepsilon_i(R) \) (Herzberg 1950). This quantity does not include the nuclear repulsive term in Eq. (2.23), so we can follow its behavior down to \( R = 0 \). The diagram in Fig. 2.11 correlates the one electron states of the separated centers (\( R \to \infty \)) with those of the united atom (\( R \to 0 \)) indicating how the electronic binding energy changes with \( R \). The states are labeled by their symmetry (\( g \) or \( u \)) under inversion and by the component of electronic angular momentum along the internuclear axis (\( |M_1| = 0, 1, 2, \ldots \), called \( \sigma, \pi, \delta, \ldots \)).

To obtain total interaction potentials for a particular pair of atoms, the net binding energy of each electron, determined from the correlation diagram and the Pauli principle, is combined with the nuclear repulsive potential in Eq. (2.23). One finds that two hydrogen atoms (\( \text{H}_2 \)) interact via a singlet state \( (\sigma_g 1s)^2 \Sigma_g^+ \), which is attractive at intermediate \( R \), and a triplet state \( (\sigma_g 1s)(\sigma_g 1s) \Sigma_g^+ \), which is repulsive. Therefore, in describing collisions between two \( \text{H} \) atoms, 3/4 are repulsive and 1/4 attractive. Two helium atoms (\( \text{He}_2 \)) interact via a \( (\sigma_g 1s)^2 (\sigma_u 1s)^2 \Sigma_g^+ \) ground repulsive state. The lowest state for two oxygen atoms is \( (\sigma_g 1s)^2 (\sigma_g 2p)^2 (\pi_g 2p)^4 (\pi_g 2p)^4 (\sigma_g 2s)^2 \Sigma_g^+ \). In Fig. 2.8 the \( \Sigma, \Pi, \Delta, \ldots \) represent the net angular momentum along the internuclear axis. These states are doubly degenerate (i.e., the angular momentum vector can be pointed either way) except for the \( \Sigma \) states which are, therefore, also labeled (+ or -) according to their behavior under reflection about a plane containing the nuclei.

The molecular orbital diagrams are extremely useful for determining which transitions are likely to occur. Following the molecular orbital states at large \( R \) into small \( R \) will result in a number of curve crossings, as seen in the potential
Fig. 2.11. Correlation diagram for one electron on two identical centers with effective charge $Z_A$.

diagram for certain states of He$_2^{2+}$ in Fig. 2.12. In a fully adiabatic process, for which the electrons totally adjust to one another, crossings are avoided for states of the same total symmetry. Therefore, the crossings in the molecular orbital diagram indicate at which R the character of the wave function is changing (i.e., the transition regions for slow collisions). The $(\sigma_u 1s)^2 \Sigma_g^+$ state of He$_2^{2+}$ is seen to make a series of crossings as both of the electrons are promoted to (2p) electrons in the united atom limit. Therefore, half of the collisions for He$_2^{2+}$ on He will proceed along an attractive $\Sigma_u^+$ for which transitions are unlikely at low velocities and half along a strongly repulsive $\Sigma_g^+$ state for which transitions are very likely to occur if the distance of closest approach is small enough. Such electron promotion occurs in all colliding systems as there are two atomic orbital states at large R for every atomic orbital state at small R (Fig. 2.10), as pointed out by Fano and Liethen (1965).
Molecular orbital diagrams are also constructed for an electron in the field of two positive centers having different effective charges $Z'_A$ and $Z'_B$. The importance of promotion and the covalency of the interactions depends on the similarity of these charges. For instance, for a proton interacting with a nitrogen atom ($\text{NH}^+$ potential) the ground state potentials at intermediate $R$ are well described by a single electron shared by an $\text{N}^+$ core and a proton. These have binding energies $I_N = 14.5\text{ eV}$ and $I_H = 13.6\text{ eV}$ giving effective charges $Z' = \sqrt{1/13.6}\text{ eV}$ which are similar ($Z'_N = 1.03$, $Z'_H = 1$). Therefore, the lowest $\Sigma$ state potentials of $\text{NH}^+$ resemble those of $\text{H}_2^+$ in Fig. 2.10 at intermediate $R$, except
there is a small energy difference as $R \to \infty$. The similarity is even stronger for $H^+ + O$ for which the ionization potentials are very close in value. The covalent nature of such states results in an exchange interaction like that for $H_2^+$, written as

$$
\Delta \epsilon \approx A \exp(-R/\bar{a}),
$$

(2.28)

where the effective radius is $\bar{a} = a_o/(Z_A' + Z_B')$. Smirnov (1964) evaluates $A$.

This confusion of potentials presents a problem. For example, even though the $O^+ + O$ ($O_2^+$ system) has a lowest lying attractive (bound) state, $^2\Pi_g$, the collision of an oxygen ion with an oxygen atom involves seven different potential curves each with a different multiplicity (Fig. 2.8). In a detailed calculation these potentials are not averaged; rather the elastic collision cross sections for each potential are averaged [viz. Eqs. (2.22) and 2A.8]] (Yee and Dalgarno 1987). However, when calculating integrated quantities such as $S_\sigma$ [Eq. (2.11)] a net repulsive potential is often used at intermediate $R$. Based on the electron exchange interaction discussed above, the form, $V = A e^{-r/\bar{a}}$, referred to as a Born–Mayer potential, is used in particle penetration calculations and is essentially an extension of the short-range repulsive interaction [Eq. (2.25)]. The "universal" potential (Appendix 2B) has also proven useful for describing the average repulsive energy transfer cross sections at intermediate and short range for many electron systems.

**Inelastic Collisions**

When the interacting particles are moving, as in a collision, then the forces described in the preceding sections become dynamic and the time-dependent fields produce changes in the internal state of the molecule. The motion of each of the constituent particles of the molecules can be characterized by a period $\tau$ and a mean radial extent from the center of mass $r$ ($\sim \bar{a}$). The interaction with a passing particle of velocity $v$ at a distance $b$ from the center of a target atom or molecule is said to be adiabatic if $\tau_c > \tau$, where $\tau_c$ is the larger of $b/v$ and $r/v$. For such collisions, electronic transitions are unlikely ($b_{\text{max}} \approx v/\omega$, where $\omega = 2\pi/\tau$ is referred to as the Bohr adiabatic cut-off). For $\tau_c < \tau$, the interaction times are short and again transitions are unlikely. Therefore, inelastic cross sections generally go through a broad maximum when $\tau_c \approx \tau$, as discussed in the introduction to this chapter. The collision time gives an uncertainty in the energy during the collision of $\Delta E \approx h/\tau_c$, i.e., a width to the state. Therefore, the maximum in the cross section occurs when $\Delta E$ equals the excitation energy $h\omega$. This is referred to as the Massey criterion.

Many of the approximations used to describe such transitions incorporate only the initial and final states. Such models can be divided into two categories: strong interactions, for which the evolution of the electronic states during the collision is important (e.g., curve crossing transitions); and weak interactions,
for which the initial charge distribution can be considered static. This parallels the division used above to calculate the interaction potentials. The first case applies to velocities comparable to or smaller than the speeds of the constituent particles of the target and is generally associated with the intermediate range interactions. The second case corresponds to large velocities. If, in addition, the collision is a distant collision, \((b \gg r)\) small momentum transfer, the target atom or molecule must be viewed as a whole and the constituent particles are often treated as bound oscillators of frequency \(\omega\). These oscillators are then excited by the time-dependent field of the passing particle (Appendix 2C). On the other hand, for close collisions, \((b \ll r)\) large momentum transfer, the incident particle can be thought of as interacting with each of the constituents of the target molecule separately. This is referred to as the binary-encounter limit.

In the following we first calculate the large momentum transfer (close collision) contribution to the inelastic energy-loss cross section, and then the Bethe–Born approximation for the two contributions. Following this strong interactions at intermediate range such as charge exchange are considered.

**Binary-Encounter Approximation**

In the often-used binary-encounter approximation (BEA), the incident particle is assumed to make a close collision with only one of the constituents of the target molecule. Therefore, the stopping power [Eqs. (2.10) and (2.11)] can be approximated as a sum of contributions from each of the target molecule constituents, electrons and nuclei,

\[
S = S_e + S_n \approx \sum N_j \int Q d\sigma_j(Q) + \sum_k \int T d\sigma_k(T).
\]

(2.29)

The cross section \(d\sigma_j(Q)\) is the elastic energy transfer cross section to the electrons in orbit \(j\) with population \(N_j\) and \(d\sigma_k(T)\) is the energy transfer cross section to nucleus \(k\) in the target molecule. For a close collision between charged particles

\[
d\sigma_k(T) = 2\pi \frac{(Z_A Z_k e^2)^2}{M_k v^2} \frac{dT}{T^2}.
\]

(2.30)

Using Eq. (2.30) in Eq. (2.29) the nuclear stopping cross section [Eq. (2.12b)] is

\[
S_n \approx \sum_k 2\pi \frac{(Z_A Z_k e^2)^2}{M_k v^2} \ln(\gamma_k E_A / T_k),
\]

(2.31a)

where \(\gamma_k E_A\) is the maximum energy transfer to nucleus \(k\) and \(T_k\) is a “minimum” energy transfer due to the screening by the other constituent particles (Appendix 2B). This is the general form for \(S_n\) (see Fig. 2.4).

\(S_n\) can be rewritten so that energy transferred to the center of mass of the target molecule and that energy transferred to vibrational and rotational excitation of the molecule are separated. That is, energy transfer is assumed to
occur predominantly in close collisions of the ion with one of the atoms of mass \( M_k \) in the molecule of total mass \( M \). The deflection of the incident particle is determined by this binary collision and the direction of motion of the center of mass of the target molecule is along the direction of the impulse to \( M_k \). Of the total energy transfer \( T \), an amount \( (M_k/M)T \) goes into motion of the center of mass and the remainder, \((1 - M_k/M)T\), goes into relative motion of the components. If the latter energy is greater than the dissociation energy for \( M_k \), the molecule is likely to dissociate, but if it is less, then it all goes into vibration and/or rotation of the molecule. For a diatomic molecule, if \( \phi \) is the angle between the direction of the impulse given to \( M_1 \) and the orientation of the axis between \( M_1 \) and \( M_2 \), then \( T_{\text{vib}} = (M_2/M)T \cos^2 \phi \) and \( T_{\text{rot}} = (M_2/M)T \sin^2 \phi \). For random orientation one-third of the internal energy goes into vibration and two-thirds into rotation, consistent with the number of modes available. The binary collision model breaks down if the important energy transfers occur with the impact parameter comparable to the bond lengths.

Whereas the BEA can be used to calculate the total energy transfer to nuclei in molecules or solids, it describes only the high momentum transfer collisions of an ion with the electrons. Since the energy transfer cross section to the electrons on B can also be described by the coulomb interaction between each electron and the incident ion A, \( d\sigma_j(Q) \) has the same form as \( d\sigma_k(T) \) in Eq. (2.29) with \( T \rightarrow Q, \gamma E_A \rightarrow 2m_e v^2, Z_B \rightarrow 1 \), and \( M_k \rightarrow m_e \) in Eq. (2.30). The quantity \( S_e \) then also follows from Eq. (2.31a),

\[
S_e \approx N \sum_{j} \frac{2\pi (Z_A e^2)^2}{m_e v^2} \ln \left( \frac{2m_e v^2}{I_j} \right), \tag{2.31b}
\]

where \( I_j \) is the ionization potential of the \( j \) electrons. It is seen that both \( S_e \) and \( S_n \) vary as \( (\ln E_A)/E_A \) at high energies. The large difference in magnitudes between \( S_e \) and \( S_n \) exhibited in Fig. 2.4 are due to the difference in mass of the particle receiving the energy transfer, \( M_k \) or \( m_e \) in Eq. (2.31a) and (2.31b).

**Bethe–Born**

The calculation of the energy loss to the electrons also requires a description of the binding conditions, often estimated by treating the electrons as classical oscillators (Appendix 2C). The appropriate quantum mechanical calculation at high velocities is to use the first Born approximation (Bethe and Jackiw 1968). In the Bethe estimate the large and small momentum transfers (close and distant collisions) can be separated (Appendix 2D). The large momentum transfers are equivalent to the BEA estimate, and the small momentum transfers are equivalent to photon-like dipole excitations of the target by the time-dependent field of the passing particle. Remarkably, in determining \( S_e \), the forms for these two contributions are identical so that the final expression is not sensitive to the separation between close and distant collisions. The expression often used for an
incident ion of charge \( Z_A \) is

\[
S_c \equiv \sum \int (Q_{0 \rightarrow f} \, d\sigma_{0 \rightarrow f} \approx \frac{4\pi(Z_Ae^2)^2}{m_v^2Z_B} \left[ \ln \frac{2m_vv^2}{I} - 1 - C/Z_B \right]
\]  

(Inokuti et al. 1981). Here \( Q_{0 \rightarrow f} = e_f^0 - e_0^0 \), \( \bar{I} \) is called an average ionization potential, and \( C \) is a factor associated with the shell structure of the target atom or molecule giving a small correction to the expression. Values of \( \bar{I} \) and \( C \) have been extracted from experiment and are tabulated (see Bibliography). The expression in Eq. (2.32) for \( S_c \) is about twice the BEA result in Eq. (2.31b), indicating that for incident ions distant and close collisions contribute equally at high velocities. As the velocity decreases, close encounters are eventually required to produce an excitation, so the BEA applies using an appropriate interaction potential (Johnson and Gooray 1977). The quantity \( (2m_vv^2/\bar{I}) \) in Eq. (2.32) is often given as a ratio of impact parameters \( (b_{\text{max}}/b_{\text{min}}) \) (Appendix 2C).

The Bethe–Born method can also be used to estimate the total ionization cross section \( \sigma_i \) (Inokuti 1971) and the straggling cross section \( S_{e}^{(2)} \), a quantity we will discuss in the following chapter. The lead terms at large \( v \) are

\[
\sigma_i = \sum \int d\sigma_{0 \rightarrow f} \approx \frac{4\pi(Z_Ae^2)^2}{m_v^2Z_B} \ln \frac{2m_vv^2}{3\hbar^2} 
\]  

(2.33a)

where \( f \) implies all final states leading to an ionization and \( \bar{r}^2 \) is the mean-squared radius of the initial state, which is tabulated for most atomic species, and

\[
S_{e}^{(2)} = \sum \int (Q_{0 \rightarrow f} \, d\sigma_{0 \rightarrow f} \approx 4\pi (Z_Ae^2)^2Z_B.
\]  

(2.33b)

\( S_{e}^{(2)} \), which weighs large energy changes heavily, is given by the BEA calculation at high velocities as close collisions dominate, and is approximately a constant. On the other hand, the ionization cross section, \( \sigma_i \), which, unlike \( S_c \) and \( S_{e}^{(2)} \), is not weighted by the energy transfers, is determined primarily by the dipole excitations (Appendix 2D). Because of this, \( \sigma_i \) has a high energy dependence which parallels that of the stopping cross section, i.e., \( (\ln E_A)/E_A \), as seen in Fig. 2.13a. This has the very useful consequence that the ionization rate in a gas or solid due to a fast incident ion is roughly proportional to \( S_c \). For fast (neutral-atom)–(neutral-atom) collisions the dipole excitations are small contributors and BEA gives reasonable estimates.

Cross sections for incident electron ionization (Fig. 2.13a) have the same high energy dependence as those for incident protons at the same value of \( v \). On the other hand, at low incident velocities an energy threshold is seen for electron impact ionization. For these same \( v \) the ions have considerable energy and the cross sections decrease more slowly. As the ionization cross sections described have a smooth dependence on \( v \), semi-empirical expressions (Table 2.3) have been developed based on the forms given above (Green and McNeal 1971). The electron impact cross sections are also approximated by such expressions.
Fig. 2.13. a Solid lines ionization cross sections for H$^+$ on H, H$_2$O (data from Table 2.3) and for e on H and H$_2$O plotted at same velocity. Dashed lines charge exchange cross sections. Note the H$^+$ + H$_2$O $\rightarrow$ H + H$_2$O$^+$ cross section goes to zero at lower ion energies (e.g., Fig. 2.15) due to the difference in ionization energies. b Rate constant for ionization of H$_3$O by electrons vs. electron temperature [E = kT] using ionization cross section in a. (Johnson et al. 1989a)
Table 2.3. Parameters for ionization of species by H+. (Rudd et al. 1985a,b)*

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>0.28</td>
<td>1.15</td>
<td>0.44</td>
<td>0.907</td>
</tr>
<tr>
<td>He</td>
<td>0.49</td>
<td>0.62</td>
<td>0.13</td>
<td>1.52</td>
</tr>
<tr>
<td>Ne</td>
<td>1.63</td>
<td>0.73</td>
<td>0.31</td>
<td>1.14</td>
</tr>
<tr>
<td>Ar</td>
<td>3.85</td>
<td>1.98</td>
<td>1.89</td>
<td>0.89</td>
</tr>
<tr>
<td>Kr</td>
<td>5.67</td>
<td>5.50</td>
<td>2.42</td>
<td>0.65</td>
</tr>
<tr>
<td>Xe</td>
<td>7.33</td>
<td>11.1</td>
<td>4.12</td>
<td>0.41</td>
</tr>
<tr>
<td>H₂</td>
<td>0.71</td>
<td>1.63</td>
<td>0.51</td>
<td>1.24</td>
</tr>
<tr>
<td>N₂</td>
<td>3.82</td>
<td>2.78</td>
<td>1.80</td>
<td>0.70</td>
</tr>
<tr>
<td>O₂</td>
<td>4.77</td>
<td>0.00</td>
<td>1.76</td>
<td>0.93</td>
</tr>
<tr>
<td>CO</td>
<td>3.67</td>
<td>2.79</td>
<td>2.08</td>
<td>1.05</td>
</tr>
<tr>
<td>CO₂</td>
<td>6.55</td>
<td>0.00</td>
<td>3.74</td>
<td>1.16</td>
</tr>
<tr>
<td>H₂O</td>
<td>2.98</td>
<td>4.42</td>
<td>1.48</td>
<td>0.75</td>
</tr>
<tr>
<td>NH₃</td>
<td>4.01</td>
<td>0.00</td>
<td>1.73</td>
<td>1.02</td>
</tr>
<tr>
<td>CH₄</td>
<td>4.55</td>
<td>2.07</td>
<td>2.54</td>
<td>1.08</td>
</tr>
</tbody>
</table>

*σ₀ = (σ₀⁻¹ + σₙ⁻¹)⁻¹; σᵣ = 4πa₀²Cx; σₙ = 4πa₀²[A ln(1 + x) + B]/x; x = (Eₐ/25 keV).

(Jackman et al. 1977) and averaged over a speed distribution given by the plasma temperature. These rate constants (kᵢ = σᵢv, e.g., Fig. 2.13b) are used to determine the ionization rate of neutrals ejected into a plasma in Chapter 4.

**Two-State Models: Charge Exchange**

For collision velocities comparable to or smaller than the speed of the constituents of the target molecules (v < vₐ), the details of the interaction potentials can control the transition probabilities. When the coupling between neighboring states is strong, a number of models are used to calculate these probabilities based on the impact parameter cross section in Eq. (2.7) and the transition probabilities in Appendix 2D. A requirement for strong coupling in this velocity range is that the energy difference between the states at some point in the collision, εᵣ(R) − ε₀(R), is small compared to the uncertainty in the energy of the states during the collision: ΔE ≈ h/(ΔRₓ/v), where ΔRₓ is the extent of the transition region. For two strongly interacting states the transition probabilities and the angular differential cross sections exhibit interference and are oscillatory in velocity and angle. Here we consider the integrated cross sections.

Approximate models for the two-state impact parameter cross section in Eq. (2.7) can be written in the form

\[
σ₀→r ≈ P₀→r(πbₓ²)
\]

(Appendix 2D). Here bₓ is that impact parameter giving the onset for a transition, and \( P₀→r \) is the averaged transition probability for impact parameters less than bₓ.

For symmetric-resonant charge exchange (e.g., H⁺ + H → H + H⁺ or
O$_2^+ + O_2 \rightarrow O_2^+ + O_2^+$ the average probability of a transition (exchange) is 1/2, as the initial and final states are identical (i.e., Q$_{0\rightarrow f} = e_i^0 - e_f^0 = 0$). This is described in Appendix 2D. As the time for exchanging an electron is $\tau_x \approx h/\Delta \varepsilon$, where $\Delta \varepsilon$ is the exchange energy in Eq. (2.28), then at some large value of $b_x$, $\tau_x > \tau_\varepsilon$ so that the transition probability goes to zero. Since $\Delta \varepsilon(R)$ increases exponentially with decreasing $R$, that impact parameter at which charge exchange begins is

$$b_x = b_{ct} \approx \tilde{a}[B(v) - \ln v]. \quad (2.35)$$

Here $B$ is a slowly varying function of $v$ [see Eq. (2D.12)] and $\tilde{a}$ is the screening constant in Eq. (2.28). Using $b_{ct}$ in Eq. (2.34), it is seen that the charge exchange cross section increases slowly with decreasing velocity at intermediate velocities. At high velocities ($v > v_\varepsilon$) the exchange of an electron from a stationary atom to a fast ion requires a significant change in the momentum of the electron. Therefore, $\tilde{P}_{0\rightarrow f}$ goes to zero rapidly ($\sim v^{-12}$ for H$^+ + H$). The net cross section over many orders of magnitude in $E_\lambda$ is shown in Fig. 2.13a and is compared to ionization cross sections. It is seen that at large energies ionization dominates in a plasma whereas at low energies charge exchange dominates.

At very low velocities the interaction potential at large $R$ can control the collision. An ion and neutral (< 10's eV) can orbit because of the long-range polarization potential: $n = 4$ (McDaniel et al. 1970). From Eq. (2.21) the orbiting occurs at an impact parameter $b_0 \propto v^{-1/2}$, which varies faster than $b_{ct}$ in Eq. (2.35) and eventually exceeds $b_{ct}$ as $v \to 0$. Therefore, the cross section grows as $v^{-1}$ at very low velocity. For ion–ion charge exchange (e.g., S$^2^+ + S^+ \rightarrow S^+ + S^2^+$) the repulsive force dominates at low energies so that the cross section goes to zero (see Fig. 2.16c).

Charge exchange between nonsymmetric systems (e.g., S$^+ + O$ in the Io plasma torus or H$^+ + O$ in the Saturnian magnetospheric plasma) requires a net change in the electronic energy, albeit a small change. Such cross sections will exhibit a maximum, as discussed earlier. For large velocities, when the uncertainty in the energy $\Delta E$ is much greater than the state separation, $Q_{0\rightarrow f}$, the cross section behaves like the symmetric resonant cross section (e.g., $b_x$ given by Eq. (2.35) and $\tilde{P}_{0\rightarrow f} \approx 1/2$; see H$^+ + H_2O$ in Fig. 2.13a). At velocities for which $\Delta E$ is comparable to or smaller than $Q_{0\rightarrow f}$, the “transition” generally occurs in a narrow range of internuclear separations $\Delta R_x$ about a particular value, $R_x$, and the transition probability is a rapidly varying function of $v$. These transitions are treated according to whether the potentials cross (Fig. 2.9) or do not cross (Olson 1980).

For the curve crossing case, $b_x$ in Eq. (2.34) is set equal to the crossing point, $R_x$. For impact parameters less than $b_x$ the colliding particles pass through the point $R_x$ twice, on the approach and exit (Fig. 2.14). At each passage the average transition probability is $p_{0f}$. After the collision a change in state will have taken place if a transition occurred on the first passage but not the second $[p_{0f}(1 - p_{0f})]$ and vice versa $[(1 - p_{0f})p_{0f}]$. Therefore, $\tilde{P}_{0f} = 2p_{0f}(1 - p_{0f})$, and Eq. (2.34)
becomes
\[ \sigma_{0f}^{LZS} \approx 2p_{0f}(1 - p_{0f})\pi R_s^2. \] (2.36)

The Landau–Zener–Stueckleberg expression for \( p_{0f} \) is
\[ p_{0f} \approx 1 - \exp\left(-\frac{\tau_c}{\tau}\right). \] (2.37)

Here \( \tau_c \) is the collision time, the time spent in the interaction region \( |\Delta R_e/(dR/dt)| \), and \( \tau \) the electron exchange time \( |\pi\Delta\varepsilon(R)/\hbar|^{-1} \). These are evaluated at \( R = R_s \) with \( \Delta\varepsilon(R) \) as in Eq. (2.28) and \( \Delta R_e \approx |2\Delta\varepsilon(R)/[d\varepsilon_e - \varepsilon_0]/dR| \), where \( \varepsilon_e \) and \( \varepsilon_0 \) are the electronic energies of the states (e.g., \( S^2^+ + O = S^+ + O^+ \) in Fig. 2.9). Extensive measurements have been made for doubly charged ions on neutrals, for which Olson et al. (1971) fit a form for \( \Delta\varepsilon \) [see Eq. (2.28)] for use with Eq. (2.37),
\[ \Delta\varepsilon(R) \approx (I_A I_B)^{1/2}(R/\bar{a}) \exp\left(-0.86R/\bar{a}\right) \]
\[ \bar{a} = a_0(Z'_A + Z'_B)^{-1} \text{ with } Z' = (I/13.6eV)^{1/2}. \] (2.38)

Such forms have been used to estimate cross sections for the Io plasma torus (Johnson and Strobel 1982; Brown et al. 1983b; McGrath and Johnson 1989) and they join to the symmetric-resonant-like result [i.e., Eq. (2.35)] at high velocities.

For the noncrossing case an effective transition region, \( R_s \), exists at the separation for which the interaction, \( \Delta\varepsilon(R) \), is approximately half the spacing between states \( |\varepsilon_f(R) - \varepsilon_0(R)| \). Demkov (1964) gives an expression for the transition probability
\[ \tilde{P}_{0\rightarrow f} \approx (1/2) \text{sech}^2\left\{ (\pi\bar{a}/2\hbar)[\varepsilon_f(R) - \varepsilon_0(R)]/\tilde{R}|_{R_s}\right\}. \] (2.39)

with \( \bar{a} \) as given above. In evaluating \( \tilde{P}_{0\rightarrow f} \) in Eq. (2.39) the energy difference \( [\varepsilon_f(R) - \varepsilon_0(R)] \) is often set equal to the initial energy difference and \( |dR/dt| \approx v \), giving an extremely simple expression for \( \tilde{P}_{0\rightarrow f} \), requiring only the electron binding energies. Applying Eq. (2.34), \( b_x \approx R_s \) and, again, the low-velocity results join smoothly onto the symmetric-resonant-like result at high velocities where the energy difference \( Q_{0\rightarrow f} \) becomes unimportant. Figure 2.15 from Rapp and Francis
Fig. 2.15. Symmetric resonant charge exchange cross section vs. ion velocity for incident H$^+$ on H, solid line (Eq. 2.35). For H$^+$ + A $\rightarrow$ H + A$^+$ with $Q_{0 \rightarrow f}$ given, dashed lines. This estimate from Rapp and Francis (1962) is close to the Demkov (1964) form in Eq. (2.39).

(1962) shows the relationship between the symmetric and nonsymmetric charge exchange for differing $Q_{0 \rightarrow f}$.

The expressions above have been developed for transfer of a single $s$ electron but are often used more generally. For other cases the matrix elements may have prefactors determined by the spin and orbital angular momentum of the states (Matic et al. 1980; McGrath and Johnson 1989). The expressions above can still give rough estimates if $\bar{P}_{0 \rightarrow f}$ is multiplied by the fraction of states associated with the incident ion and atom which have the same molecular identification as the exiting ion and atom states. For one electron transfer in which net spin is conserved (the so-called Wigner-Witmar rule), these factors and estimates of $\Delta \varepsilon$ have been used in the impact parameter equations to calculate the cross sections in Fig. 2.16 and estimates of sulfur and oxygen charge transfer cross sections in the Io torus are given in Table 2.4.

At very low velocities, when orbiting occurs, the cross sections for both the crossing and noncrossing cases may again increase if the transitions are exothermic. That is, even though the transition probability is small for any one pass through the transition region, after many passes the accumulative effect can lead to a significant probability for a change in the electronic state. At very low speeds this can occur only if internal energy is released. This principle is extensively used by chemists to estimate low-temperature reactions rates. The cross section for such reactions (e.g., ion-molecule reactions, Langevin cross section) is obtained by setting $b_a$ in Eq. (2.34) to the orbiting radius, $b_0$, Eq. (2.21), as described earlier (McDaniel et al. 1970). The value of $\bar{P}_{0 \rightarrow f}$ is then estimated
statistically for those final states available energetically. As a rough estimate, for \( N \) available final states, \( \bar{P}_{0 \rightarrow f} \sim N^{-1} \) for each possible transition.

Although we have primarily discussed charge-exchange collisions and only collisions involving ions and atoms, these procedures also apply to molecular collisions and to all varieties of internal changes including molecular reactions. However, the approximations given here and in Appendix 2 should be used only as a guide when more accurate results are not available.
Fig. 2.16. Calculated charge exchange cross sections vs. ion energy, $E_A$, for the Io plasma torus ions in their ground state. a Charge exchange of Na$^+$ with Na, K, and S as indicated. Data: (+, [] Na$^+$ + Na, (x) Na$^+$ + K; (+) Smirnov (1964) approximation. b Sulfur/oxygen charge exchange: resonant and nonresonant processes. c S$^+$ + S$^{2+}$ symmetric resonant cross section with repulsive barrier; S$^{2+}$ + O and O$^{2+}$ + S$^{2+}$ are curve crossings. (McGrath and Johnson 1989)

Table 2.4. Charge exchange cross sections at Io ($v = 60$ km/s)

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$\sigma$(Å$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1. O$^+$ + O → O + O$^+$</td>
<td>22</td>
</tr>
<tr>
<td>R2. O$^+$ + S → O + S$^+$</td>
<td>5</td>
</tr>
<tr>
<td>R3. S$^+$ + S → S + S$^+$</td>
<td>40</td>
</tr>
<tr>
<td>R4. S$^+$ + O → S$^+$ + O$^+$</td>
<td>0.1</td>
</tr>
<tr>
<td>R5. S$^{2+}$ + S → S + S$^{2+}$</td>
<td>13</td>
</tr>
<tr>
<td></td>
<td>→ S$^+$ + S$^+$</td>
</tr>
<tr>
<td>R6. S$^{2+}$ + O → S$^+$ + O$^+$</td>
<td>3.8</td>
</tr>
<tr>
<td>R7. O$^{2+}$ + O → O + O$^{2+}$</td>
<td>9</td>
</tr>
<tr>
<td></td>
<td>→ O$^+$ + O$^+$</td>
</tr>
<tr>
<td>R8. O$^{2+}$ + S → O$^+$ + S$^+$</td>
<td>$\sim 40$</td>
</tr>
<tr>
<td></td>
<td>→ O$^+$ + e + S$^{2+}$</td>
</tr>
<tr>
<td>R9. O$^{2+}$ + S → O$^+$ + S$^{2+}$</td>
<td>2.3</td>
</tr>
<tr>
<td>R10. O$^{2+}$ + S$^{2+}$ → O$^+$ + S$^{3+}$</td>
<td>1.3</td>
</tr>
<tr>
<td>R11. S$^{3+}$ + O → S$^{2+}$ + O$^+$</td>
<td>32</td>
</tr>
<tr>
<td></td>
<td>S$^+$ + O$^{2+}$</td>
</tr>
<tr>
<td>R12. S$^{3+}$ + S → S$^{2+}$ + S$^+$</td>
<td>22</td>
</tr>
<tr>
<td></td>
<td>S$^+$ + S$^{2+}$</td>
</tr>
<tr>
<td>R13. S$^{3+}$ + S$^+$ → S$^{2+}$ + S$^{2+}$</td>
<td>0.5</td>
</tr>
</tbody>
</table>

*Some of the Io plasma torus charge-exchange cross sections from McGrath and Johnson (1989). A number of these are estimated using techniques discussed here and in Johnson and Strobel (1982).
Stopping Cross Section: Summary

In the above we have considered the individual collisional processes which will determine the behavior of a fast particle penetrating a gas, liquid, or solid. Here we examine the relative importance of the events described for determining the overall energy loss rate of the fast particle. In Fig. 2.17 the total stopping cross section, \( S \equiv n_b^{-1} (dE/dx) \) [see Eq. (2.11)], and the separate contributions to \( S \) are shown for protons losing energy to \( \text{H}_2\text{O} \).

First, the molecular effects are small, so that the stopping cross section for \( \text{H}_2\text{O} \) is very nearly a sum of 2H's and an O from Fig. 2.4. The most important difference would be that the ionization potential is lower for \( \text{H}_2\text{O} \). Second, it is seen that the separate contributions, \( S_e \) and \( S_n \), dominate the total stopping in very different velocity regions, as discussed earlier. At high velocities \( S_e \) and \( S_n \) both decay as \( (\ln E_A)/E_A \) but their magnitudes differ by the ratio of the mass of the electron to that of the nucleus. That is, even though in a close collision an ion transfers energy more efficiently to a nucleus, cross sections are dominated by the large impact parameters, for which energy is transferred more efficiently to the lighter electrons [Eqs. (2.31a) and (2.31b)].

At high velocities ionization is the dominant process with, roughly, a 10% contribution from excitations but charge exchange dominates \( S_e \) at lower velocities (see Fig. 2.13a). Energy loss due to charge exchange is a two-step process differing, therefore, from the other contributions which are single collision. That is, on traversing a gas, ions capture an electron and later are

---

**Fig. 2.17.** Stopping cross section of \( \text{H}_2\text{O} \) vs. proton energy. Contribution from various processes (*lines*) as labeled; experiment (*points*). (Miller and Green 1973)
ionized again. The capture and loss at low velocities can be described in the solid state as a drag force on the ion in which the electron cloud is distorted (polarized) by the passing ion increasing the electron density in the vicinity of the ion (i.e., the covalent effect discussed earlier). The drag force produced is such that \((dE/dx) \propto v\). Lindhard and Scharff (1961) give an expression for the \(S_e\) at low \(v (v < Z_A^{2/3} v_0)\) based on the Thomas-Fermi model of the atom,

\[
S_e \approx \xi_e 8\pi e^2 a_0 \frac{Z_A Z_B}{Z} \frac{v}{v_0} = \xi_e \frac{Z_A Z_B}{Z} \frac{v}{v_0} (1.92 \times 10^{-14} \text{ eV cm}^2).
\]

(2.40)

In this expression \(v_0\) is the velocity of an electron on the hydrogen atom \((2.19 \times 10^8 \text{ cm/s})\), \(Z\) is the average charge \([Z^{1/3} = (Z_A^{2/3} + Z_B^{2/3})^{1/2}]\) used in the Thomas-Fermi screening length (Appendix 2B) and \(\xi_e \approx Z_A^{1/6}\).

Because the values of the stopping cross section, \(S\), given in data tables are measurements, the charge exchange cycle is always included. This also means that the tabulated values of \(S\) are not necessarily those for the ion initially incident on a solid or on a gaseous envelope of an object, it may be larger or smaller (Crawford 1989). Imagining the incident ion to be in a variety of charge states during its passage through even a relatively thin material, these stopping cross sections are referred to as equilibrium-charge-state stopping cross sections. Average charge states for ions exiting a sample are given in Fig. 2.18. We see that ions become neutralized at low velocities and fully stripped at high velocities. The thickness of material at which the equilibrium charge state is achieved is determined by the

![Graph showing \(Z_{eff}/Z_A\) vs. reduced velocity \(\chi\).](image)

**Fig. 2.18.** \(Z_{eff}/Z_A\) vs. velocity in scaled units (see Eq. 2.41) for a variety of ions on carbon. \(Z_{eff}\) is the effective average charge state of ions exiting a thin solid. It is independent of the incident ion charge state if the material is sufficiently thick. (Shima et al. 1985)
atomic density of the material and the average charge capture, $\sigma_{ct}$, and loss, $\sigma_l$, cross sections i.e., $[(\sigma_{ct} + \sigma_l)/n_b \sigma_{ct} \sigma_l]$. This thickness corresponds to hundreds of monolayers of material at high velocity ($v \gg v_e$) and 10's of monolayers at intermediate velocities ($v \approx v_e$).

A number of semi-empirical expressions for the effective equilibrium charge state, $Z_{\text{eff}}$, have been given. For example (Shima et al. 1985),

$$ Z_{\text{eff}} \approx Z_A \left(1 + X^{-1.06}\right)^{-0.6}, \quad X \equiv 3.86 \sqrt{E_A/M_A/Z_A^{0.45}} \tag{2.41} $$

with $E_A$ in MeV and $M_A$ in amu. At large velocities, estimates of $S_e$ are made using $Z_{\text{eff}}$ in place of $Z_A$ in Bethe–Born expression for a bare incident ion in Eq. (2.32).

In fact, as $I$ in Eq. (2.32) depends primarily on the target properties, heavy ion values of $S_e$ and $\sigma_l$ can be estimated from measured proton values by multiplying by $(Z_{\text{eff}})^2$.

At very high velocities relativistic effects associated with the electron density in the target alter the form for $S_e$ in Eq. (2.32) although ionization is still the dominant energy loss process. Ignoring $C$, the term in brackets is replaced by $\ln[(2m_e v^2/\sqrt{[1 - (v/c)^2]^2} - (v/c)^2)]$. As $v \rightarrow c$ the ln term increases so that $S_e$ increases, as seen in Fig. 2.19, because of emission of radiation (Bremmstrahlung). Calling $\beta = v/c$, a useful form for the electronic stopping power of an ion, $Z_A$, is (Turner 1986)

$$ \frac{dE}{dx}_e = 5.10 \times 10^{-19} \text{eV cm}^2 \text{Z}_{\text{eff}}^2 Z_B n_B [G(\beta) + \ln(I_0/I)]/\beta^2 \tag{2.42} $$

where $I_0 (= 13.59 \text{eV})$ is the ionization energy of the hydrogen atom. In Eq. (2.42) $Z_B n_B$ is the total electron density of the material. Because the electron density is roughly proportional to the mass density for heavy elements, results are often presented as $\rho_B^{-1}(dE/dx)_e (= S_e/M_B)$ as in Fig. 2.19. To estimate $I$ in eV ($\approx 19$, $Z_B = 1; \approx 11.2 + 11.7 Z_B, 2 \leq Z_B \leq 13; \approx 52.8 + 8.71 Z_B, Z_B > 13$). For a molecular medium the $(dE/dx)_e$ can be added for each atomic constituent (called Bragg’s rule). This is equivalent to calculating a new effective $I$ (ln I = $\Sigma Z_i$ ln $I_i/\Sigma Z_i$, where $Z_i$ and $I_i$ are the nuclear charge and I for each atomic constituent: for H$_2$O $I \approx 74.6 \text{eV}$). In the condensed state the effective I in Eq. (2.42) is about 20% larger.

In addition, at very high velocity the material density modifies the G above. Note that although $(dE/dx)_e$ becomes small at high velocities, it is because the energy loss events are less probable. Each event is energetic, however, resulting in ionizations.

At high energies (many MeV), nuclear reactions can also be induced. For example, in the close collision of a GeV proton with a nucleus, a proton or neutron can be ejected by a direct collision. Since the mean free path for nuclear inelastic collisions by GeV protons in many materials is $\approx 100 \text{gm/cm}^2$ with the proton giving up approximately half of its energy this contribution to the mass stopping is $\approx 5 \text{MeV cm}^2/\text{gm}$. This is comparable in size to the radiation losses. Because the incident proton experiences an impulse, the resulting deflections also
limit its penetration into the material. The ejected species carry off some of the energy and the "damaged" nucleus may decay (e.g., emit a γ-ray, α-particle, etc.) releasing additional energy. Except for the binding energy of the ejected nucleon, the energy lost by the incident proton is mostly converted into ionization of the target. Because a variety of nuclear processes can be induced, this component is harder to quantify in a simple way (Ryan and Draganic 1986).

Appendix to Chapter 2

A Wave Mechanics: Elastic Scattering

In wave mechanics the scattering of the particle is replaced by scattering of a wave. In the CM system (see Table 2.1) the differences from and similarities to the quantities considered in the text are shown below. The beam of particles incident on a target is replaced by a plane wave, $\exp(i\mathbf{K}\cdot\mathbf{R} - \omega t)$, where $K = 2\pi/\lambda$, $\lambda$ the wavelength, $\hbar K$ gives the momentum, and $\hbar \omega = \hbar^2 K^2/2m$ is the energy. When this incident wave is scattered, as in light scattering, the outgoing wave at very large distances from the scattering center has the general form

$$\left[ \exp(i\mathbf{K}\cdot\mathbf{R}) + f(\chi) \frac{e^{iKR}}{R} \right] e^{-i\omega t}.$$  (2A.1)
The plane wave is the unscattered portion and the second term is the scattered part. The magnitude of the wave scattered into an angular region about \( \chi \) is given by \( |f(\chi)|^2/R^2 \) where \( f(\chi) \) is referred to as the scattering amplitude and \( R \) is the distance from the scattering center. Therefore, the differential cross section (probability of scattering into a unit solid angle about \( \chi \)) is

\[
\sigma(\chi) = |f(\chi)|^2.
\]

That is, the scattering problem reduces to solving the Schröedinger equation subject to the boundary condition at large \( R \) given by Eq. (2A.1).

To draw analogies with the classical calculation of cross section, it is customary to express the plane wave in terms of multiple moments,

\[
\exp(i\mathbf{K} \cdot \mathbf{R}) = \sum_{\ell = 0}^{\infty} i^{\ell} (2\ell + 1) P_\ell(\cos \chi) j_\ell(KR).
\]

The \( j_\ell(KR) \) are the spherical Bessel functions which have the asymptotic form \( j_\ell(KR) \rightarrow \sin(KR - \ell\pi/2)KR \). The \( P_\ell \) are the Legendre polynomials, where \( \ell \) labels the various moments (\( \ell = 0 \), spherical; \( \ell = 1 \), dipole; \( \ell = 2 \) quadrupole; . . . ) and is the angular momentum index \( [L^2 = \ell(\ell + 1)\hbar^2] \). Therefore, \( \ell \) replaces the impact parameter

\[
b \rightarrow \sqrt{\ell(\ell + 1)\hbar/mv} \approx (\ell + 1/2)K^{-1}.
\]

Upon intersecting a scattering center each spherical wave, \( j_\ell \), experiences a phase shift \( (\eta_\ell) \) becoming \( \sin(KR - \ell\pi/2 + \eta_\ell)/KR \) in the asymptotic region. Substituting Eq. (2A.3) and the asymptotic forms for \( j_\ell \) into the radial part of Eq. (2A.1)

\[
f(\chi) = \frac{1}{2K} \sum_{\ell = 0}^{\infty} (2\ell + 1) [\exp(2i\eta_\ell) - 1] P_\ell(\cos \chi).
\]

Substituting this expression for \( f(\chi) \) into Eq. (2A.2), the scattering cross section can be reduced to the determination of the phase shifts. A useful semi-classical estimate for the phase shift has a form like that in light scattering. Since \( \hbar K = h/\lambda \) is a momentum, the phase shift is related to the accumulated change in the wavelength (momentum) due to the presence of the target atom,

\[
\eta_\ell \approx \eta(b) = 2h \int_{R_0}^{\infty} p(R)dR - \int_{b}^{\infty} p_0(R)dR \approx \frac{1}{2h\nu} \int_{-\infty}^{\infty} V(R)dZ.
\]

The radial momentum \( p(R) = m\dot{R} \) is obtained from Eq. (2.16b), and \( p_0(R) \) is the same quantity in the absence of the potential, \( V(R) = 0 \). Therefore, the phase shift is due to the interaction potential which acts like a refracting medium.

The total cross section, obtained using Eq. (2A.5) and by integrating over angle in Eq. (2A.2), becomes

\[
\sigma = 2\pi \int_{-1}^{1} |f(\chi)|^2 d\cos \chi
\]
\[ \frac{8\pi}{K^2} \sum_{\ell=0}^{\infty} (\ell + 1/2) \sin^2 \eta_{\ell} \approx 2\pi \int_{0}^{\infty} 4 \sin^2 \eta(b) b \mathrm{d}b. \] (2A.7)

It is seen that the expression for \( \sigma \) is in the form of the impact parameter cross section in Eq. (2.3) if the collision probability is \( P(\ell) \approx 4 \sin^2 \eta(b) \). At large impact parameters (or \( \ell \)) the phase shift \( \eta(b) \) and the scattering probability go to zero and, therefore, the cross section can be finite. However, because of diffraction, the “probability” \( P(\ell) \) above has an average value of 2 at small \( b \) and not unity as in the classical model, clearly showing that \( \sigma \) is a nonclassical quantity.

In evaluating the sum in Eq. (2A.5) and substituting into Eq. (2A.2) constructive interference occurs at those impact parameters which produce classical scattering into the angular region \( \chi \) as determined by Eq. (2.17). Therefore, the classical trajectories are like the light rays in geometrical optics. In this spirit the angular differential cross section can be approximated as a sum of contributing amplitudes and their corresponding phases

\[ \sigma(\chi) \approx | \sum \{ \sigma[\chi(b)] \}^{1/2} \exp[i \alpha(b)] |^2. \] (2A.8)

This replaces the expression in Eq. (2.22), where \( \sigma[\chi(b)] \) is the classical value \( \frac{b}{\sin \chi} \frac{\mathrm{d}b}{\mathrm{d}\chi} \bigg|_{b=b_0} \), and exhibits interference between contributions to scattering into angle \( \chi \) from different impact parameters. The net phase factor \( \alpha(b) \) is \( \alpha(b) = A/\hbar \pm \pi/4 + \varepsilon \), where \( \varepsilon \) is a constant, and \( A = [2\hbar \eta(b) - L \chi] \) is the difference in the classical action between an undeflected particle and a scattered particle. Therefore, for the sum in Eq. (2A.5), the regions of constructive interference are those for which the difference in this classical action is a minimum \( \partial A / \partial b = 0 \), i.e., the classical trajectories. Now \( \chi \) and \( \eta(b) \) are related by

\[ \chi = \frac{2}{K} \frac{d\eta(b)}{db}. \] (2A.9)

This is equivalent to the expression for \( \chi(b) \) in Eq. (2.17) using the form for \( \eta(b) \) given in Eq. (2A.6). Therefore, if only one region of impact parameter contributes in Eq. (2A.8), the semiclassical result for \( \sigma(\chi) \) is identical to the classical result. When more than one region contributes at a given scattering angle, as in the rainbow scattering described earlier, \( \sigma(\chi) \) is oscillatory. When \( (V/E \ll 1) \) then the classical deflection estimate in Eq. (2.18) is obtained.

Using Eq. (2A.6) in Eq. (2A.5) for \( \eta_{\ell} \) and an approximation to \( P(\ell) \cos \chi \) in which \( \ell \) (i.e., \( b \)) is a continuous variable, a wave mechanics estimate of \( f(\chi) \) which is valid for small \( V/E \) can be obtained

\[ f(\chi) \approx \frac{m}{2\pi \hbar^2} \int \mathrm{d}^3 R \, V(R) e^{\Delta \beta \cdot \vec{R}/\hbar}, \] (2A.10)

The scattering amplitude is seen to be a Fourier transform of the interaction potential, which is the frequently used first Born approximation for elastic collisions (Appendix 2B).

For wavelengths small compared to the dimensions of the particles \( (K^{-1} \ll \Delta) \),
the integral in Eq. (2A.7) can be estimated: the Massey–Mohr approximation to \( \sigma \) in Appendix 2B. For power law potentials with \( n > 2 \), \( \sigma \) is finite and the cross section decreases monotonically with increasing energy as shown in Fig. 2.2. A similar evaluation of the diffusion cross section, \( \sigma_d \) (or \( S_n \)) produces the same form as the classical expression [Eq. (2.13)] at small wavelengths, because of the exclusion of scattering at \( \chi = 0 \). Therefore, classical expressions for the diffusion cross and the nuclear stopping cross section are accurate over a broad range of incident ion energies, allowing their use for ion penetration of gases and solids.

When the wavelength is large compared to the dimensions of the particles (\( K^{-1} \gg d \)), then only the lowest \( \ell \) values contribute in Eq. (2A.5). At very low energies often only the first term is needed.

\[
\sigma(\chi) = |\tilde{f}(\chi)|^2 \approx \frac{1}{K^2} \sin^2 \eta_0. \tag{2A.11}
\]

This expression represents the same region of impact parameter as above. However, because the wavelength is large, an increase of \( \ell \) from zero to one in Eq. (2A.4) makes \( b \approx K^{-1/2} \gg d \), the size of the colliding particles. In this limit it is seen that the differential cross section is independent of angle for any potential, a result obtained classically only for the collision of spheres. Because of its simplicity, such an isotropic scattering cross section is often used for low energy collisions, even when the large wavelength criterion does not rigorously apply. The integrated cross section in Eq. (2A.7) becomes \( \sigma \approx (4\pi/K^2) \sin^2 \eta_0 \) for this case, which is also equal to the diffusion cross section, \( \sigma_d \), for large wavelengths. At long wavelengths, \( \eta_0 \rightarrow \text{const} \cdot K \) and \( \sin^2 \eta_0 \propto K^2 \), so that \( \sigma \) and \( \sigma_d \) are independent of \( E_A \) and \( S_n \propto E_A \) (Appendix 2B).

B Elastic Collision Expressions: Summary

Some expressions are summarized for the classical and wave mechanical elastic collision quantities discussed in the text and Appendix 2A (Johnson 1987).

\[
\chi(b) = \pi - 2b \int_{r_0}^{\infty} \frac{dR}{R^2} \left( 1 - \frac{b^2}{R^2} - \frac{V}{E} \right)^{-1/2} \approx -\frac{1}{2E} \frac{d}{db} \int_{-\infty}^{\infty} V(R) dZ
\]

\[
\eta(b) = \frac{p_0}{h} \left[ \int_{r_0}^{\infty} \left( 1 - \frac{b^2}{R^2} - \frac{V}{E} \right)^{1/2} dR - \int_{b}^{\infty} \left( 1 - \frac{b^2}{R^2} \right)^{1/2} dR \right], \quad p_0 = mv
\]

\[
\approx -\frac{1}{2hv} \int_{-\infty}^{\infty} V(R) dZ
\]

\[
L_{\chi}(b) = (2hb) \frac{\partial \eta(b)}{\partial b}, \quad L = p_0 b
\]
\[ \sigma(\chi) = \frac{\gamma E_A}{4\pi} \frac{d\sigma}{dT} \text{ (B initially stopped)}, \quad S_n = \frac{\gamma E_A}{2} \sigma_d \]

**Impulse Estimates \((V/E \ll 1)\)**

For potentials of the form \(V = C_n/R^n\),

\[ \chi(b) \approx a_n V(b)/E, \quad a_n = \pi^{1/2} \Gamma\left(\frac{n + 1}{2}\right)/\Gamma\left(\frac{n}{2}\right) \xrightarrow{n \to \infty} \left(\frac{n}{2}\right)^{1/2} \]

\[ \eta(b) \approx \frac{-L \chi(b)}{2\hbar(n - 1)} \]

\([\Gamma(x + 1) = x\Gamma(x), \quad \Gamma(1) = 1, \quad \Gamma(1/2) = \pi^{1/2}; \quad \text{gamma function – tabulated}]\]

\[ T \approx (a_n V(b))^2/(M_B v^2/2) \]

\[ \frac{d\sigma}{dT} \approx \frac{\pi}{n} A_n^2 (\gamma E_A)^{1/n} T^{1 + 1/n}, \quad A_n = \left(\frac{2M_A}{M_A + M_B} a_n C_n\right)^{1/n} \]

\[ S_n \approx \frac{\pi}{n - 1} A_n^2 (\gamma E_A)^{1 - 2/n}, \quad n > 2. \]

For the potential \(V = (Z_A Z_B e^2) \exp(-\beta R)/R\)

\[ \chi(b) \approx \frac{(Z_A Z_B e^2)\beta}{E} K_1(\beta b) \xrightarrow{b \to \infty} \left(\frac{\pi\beta}{2}\right)^{1/2} \frac{V(b)}{E} \]

\[ \eta(b) \approx -\frac{(Z_A Z_B e^2)}{\hbar v} K_0(\beta b) \xrightarrow{b \to \infty} -\frac{L \chi(b)}{2\hbar(\beta b)} \]

\((K_n \text{ are the modified Bessel Functions – tabulated}).\)

**Massey-Mohr**

This gives an estimate to the total elastic collision cross section when the tail of the potential can be fitted to a power potential \(C_n/R^n\). \(\beta\) is obtained by setting \(|\eta(b)| \approx 1/2 \) (R.E. Johnson 1982),

\[ \sigma \approx 2\pi \overline{b}^2 \left[1 + \frac{1}{2n - 4}\right], \quad \overline{b} \approx \left|\frac{2a_n C_n}{(n - 1)\hbar v}\right|^{1/(n - 1)}, \quad n > 2, \]

\(a_n\) given above.

**Born Approximation** [Eq. (2A.10)]

For the potential \(V = (Z_A Z_B e^2) \exp(-\beta R)/R\),

\[ \frac{d\sigma}{dT} \approx \frac{\pi A_n^2 (\gamma E_A)(T + T_0)^2}{2M_B}, \quad A = \left(\frac{2M_A}{M_A + M_B} Z_A Z_B e^2\right), \quad T_0 = \left(\frac{\hbar \beta}{2M_B}\right)^2 \]

\[ \sigma \approx \frac{\pi A_n^2}{T_0} (\gamma E_A + T_0) \]
\[
S_n \approx \frac{\pi A^2}{(\gamma E_A)} \left[ \ln \left( \frac{\gamma E_A}{T_0} + 1 \right) - \frac{\gamma E_A}{(\gamma E_A + T_0)} \right]
\]

**Thomas Fermi (Lindhard)**

These are historically important forms used in the literature on particle penetration.

Scaling quantities:

- length: \( a_{\text{TF}} = 0.8853a_0/(Z_A^{2/3} + Z_B^{2/3})^{1/2} \)
- energy: \( \varepsilon = (\gamma E_A)a_{\text{TF}}/2A, \) (A as above)
- energy transfer: \( t = \varepsilon^2 T/(\gamma E_A) \)

\[
\frac{d\sigma}{dt} \approx \pi a_{\text{TF}}^2 \xi/4t^{4/3}[1 + \xi^{2/3}t^{4/9}]^{3/2}, \xi \approx 2.62
\]

\[
S_n \approx \frac{9\pi}{2} \frac{A^2}{(\gamma E_A)} \left\{ \ln \left[ B + (1 + B^2)^{1/2} \right] - B/(1 + B^2)^{1/2} \right\}, \quad B = \xi^{1/3} \varepsilon^{4/9}
\]

**Lenz-Jensen Potential**

Gives a better low energy dependence for \( S_n \) than does the Thomas Fermi form above. The potential in Eq. (2.25) is

\[
V = \frac{Z_A Z_B}{R} e^2 \Phi(R/a_{\text{TF}})
\]

\[
\Phi = (1 + b_1 y + b_2 y^2 + b_3 y^3 + b_4 y^4)e^{-y}
\]

\[
y = (9.67R/a_{\text{TF}})^{1/2}
\]

\[
b_1 = 1, \quad b_2 = 0.3344, \quad b_3 = 0.0485, \quad b_4 = 0.002647
\]

**Universal Potential**

This potential and the corresponding stopping cross section are the most recent improvement in scaling and fitting to laboratory data for atomic collisions (Ziegler et al. 1985). It is close to the Lenz-Jensen potential, but provides a somewhat better fit and should be used in most cases for describing the average repulsive interaction.

**Scaling Quantities**

- length: \( a_U = 0.8853a_0/(Z_A^{0.23} + Z_B^{0.23}) \)
- energy: \( \varepsilon = (\gamma E_A)a_U/2A, \) (A as above)
- energy transfer: \( t = \varepsilon^2 T/(\gamma E_A) \)

The potential in Eq. (2.25) is

\[
V(R) = \frac{Z_A Z_B e^2}{R} \Phi(R/a_U)
\]
$\Phi(y) = 0.181 \exp(-3.2x) + 0.5099 \exp(-0.9423x)$
$+ 0.2802 \exp(-0.4029x) + 0.02817 \exp(-0.2016x)$

$S_n = 2\pi \frac{A^2}{\gamma E_A} \left[ 2\varepsilon S_n(\varepsilon) \right]$  

$I_n(\varepsilon)$ is the "reduced" stopping cross section

$\left[ 2\varepsilon S_n(\varepsilon) \right] = \begin{cases} \ln \varepsilon, & \varepsilon > 30 \\ \ln(1 + 1.138\varepsilon)/(1 + 0.0132\varepsilon^{-0.787} + 0.196\varepsilon^{0.5}), & \varepsilon < 30 \end{cases}$

$\frac{d\sigma}{dt} = \frac{\pi a^2 g(t^{1/2})}{t^{3/2}} f(\varepsilon) = \frac{d}{d\varepsilon} \left[ \varepsilon S_n(\varepsilon) \right]$  

**Quadrature**

In order to integrate the deflection function and, hence, obtain differential cross sections for any potential, a simple quadrature is often used.

$g(x) = \frac{b}{R_0} \left[ \frac{1 - x^2}{1 - (b/R_0)^2 x^2 - (V(R_0/x)/E)} \right]^{1/2}$  

$\chi(b) \approx \pi \left[ 1 - \frac{1}{m} \sum_{i=1}^{m} g(x_i) \right], \quad x_i = \cos \left[ (2i - 1)\pi/4m \right]$  

$\eta(b) \approx \frac{2L}{\hbar} \left[ \frac{\pi}{(2m + 1)} \sum_{j=1}^{m} \sin^2 \left( \frac{j\pi}{2m + 1} \right) (g(x_j)^{-1} - 1) \right], \quad x_j = \cos \left( \frac{j\pi}{2m + 1} \right)$  

$m$ is the number of terms used in the calculation.

**C Classical Oscillator**

Treating the electrons on an atom or molecule as classical oscillators gives the energy loss forms discussed in the text. For distant collisions, low momentum transfer, the bound electrons are excited by the time varying field of the passing particle (Jackson 1963). The motion of an electron oscillating in a field $\overline{E}_j(t)$ is

$m_e \ddot{x}_j + \Gamma_j \dot{x}_j + m_e \omega_j^2 x_j = - e \overline{E}_j(t)$  \hspace{1cm} (2C.1)

where $\omega_j$ is the binding frequency and $\Gamma_j$ is a damping constant. Writing the energy transfer to the electron as $Q_j(b) = \int_{-\infty}^{\infty} \overline{\dot{F}}_j(-e\overline{E}_j(t))dt$, it is straightforward to show that, as $\Gamma_j \to 0$,

$Q_j(b) \to \frac{\pi}{m_e} |e\overline{E}_j(\omega_j)|^2$  \hspace{1cm} (2C.2)

where $\overline{E}_j(\omega)$ is the Fourier transform of $\overline{E}_j(t)$.  

Describing \( \bar{E}_j \) in Eq. (2C.1) as the field associated with a screened Coulomb potential, \( V = \left( \frac{Z_A e^2}{R} \right) e^{-\beta R} \) and assuming straight line trajectories, \( (R^2 \approx b^2 + v^2 t^2) \), the energy transfer becomes

\[
Q_j(b) = \frac{2(Z_A e^2)^2}{m_e v^2} \frac{1}{b^2} \left[ (\beta'_j b)^2 K_1(\beta'_j b) + \left( \frac{\omega_j b}{v} \right)^2 K_0(\beta'_j b) \right],
\]

(2C.3)

where \( (\beta'_j)^2 = (\beta'_j)^2 + (\omega_j/v)^2 \) and \( K_1 \) and \( K_0 \) are modified Bessel functions. This energy transfer goes through a maximum and behaves asymptotically at high and low velocities as

\[
Q_j(b) \rightarrow \frac{2(Z_A e^2)^2}{m_e v^2} \frac{1}{b^2} \left[ (\beta'b)^2 K_1(\beta'b) \text{ for } \beta' \neq 0; \omega_j b/v \ll 1. \right]
\]

\[
\pi \left( \frac{\omega_j b}{v} \right) \exp(-2\omega_j b/v) \text{ for } \omega_j b/v \gg 1.
\]

(2C.4)

In these expressions the screening of the collision is a result of both the screening in the potential, via \( \beta' = \frac{a}{1 - \frac{1}{v}} \) in Eq. (2.25), and dynamic screening due to the motion of the electron, via \( \omega_j \). The limit \( (\omega_j b/v \gg 1) \) is the adiabatic limit discussed in the text giving an effective \( b_{\text{max}} \approx v/\omega_j \), the Bohr adiabatic radius. Writing the electronic stopping power as in Eqs. (2.9) and (2.29)

\[
S_e = \sum_j N_j 2\pi \int_{b_{\text{min}}}^{\infty} Q_j(b) b \, db,
\]

(2C.5)

where \( N_j \) is the number of electrons of frequency \( \omega_j \). Substituting Eq. (2C.3) into Eq. (2C.5), the expression for \( S_e \) is exactly integrable and depends on the lower limit. Setting \( b_{\text{min}} \) equal to the wavelength in the center of mass of the electron-incident-ion system \( (\hbar/m_e v) \), then

\[
S_e \approx 4\pi \frac{(Z_A e^2)^2}{m_e v^2} \sum_j N_j \left[ \ln \left( \frac{1.123 m_e v}{\beta'_j \hbar} \right) - (1/2) \left( \frac{\beta'_j}{\beta'_j} \right)^2 \right].
\]

(2C.6)

When the direct screening is dominant (i.e., \( \beta'_j \rightarrow \beta' \) when \( v \) is large), then the screening constant determines the effective low-energy cut-off,

\[
S_e \approx 2\pi \frac{(Z_A e^2)^2}{m_e v^2} \frac{Z_B}{\hbar} \left[ \ln \left( \frac{2m_e v^2}{Q_{\text{min}}} \right) - 1 \right] \text{; } Q_{\text{min}} \approx 1.59 \left( \beta' \hbar \right)^2/m_e
\]

(2C.7a)

as for collisions of neutrals. On the other hand when \( \beta' = 0 \) (i.e., no direct screening, only dynamic screening) then

\[
S_e \approx 4\pi \frac{(Z_A e^2)^2}{m_e v^2} \sum_j N_j \left[ \ln \left( \frac{2m_e v^2}{\hbar \omega_j} \right) - 0.577 \right].
\]

(2C.7b)

This has the same form as the Bethe–Born result in Eq. (2.32)

**D Wave Mechanics: Inelastic Collisions**

The important Born scattering amplitude for a transition from an initial state (0) to a final state (f) is given by
\[
f^{(1)}(\chi) = -\frac{m}{2\hbar^2} \int e^{-i\hat{K}_f \cdot \vec{R}} V_{f_0}(R) e^{i\hat{K}_0 \cdot \vec{R}} \, d^3R.
\]

This leads to a cross section having a form like that in Eq. (2A.2)

\[
\sigma_{0 \rightarrow f}^{(1)}(\chi) = \frac{K_f}{K_0} |f_{0 \rightarrow f}^{(1)}|^2,
\]

where \( \hbar K_f \) and \( \hbar K_0 \) are the final and initial momentum and \( \cos \chi = \hat{K}_f \cdot \hat{K}_0 \).

In Eq. (2D.1), \( V_{f_0}(R) \) is the interaction potential averaged over the final and initial states involved in the transition given as incoming and outgoing plane waves. For the Born approximation for elastic scattering, the final and initial electronic states are the same, hence, the potential is that for the initial state, \( \phi(R) \), and \( \exp \left[ i(\hat{K}_0 - \hat{K}_f) \cdot \vec{R} \right] = \exp(-i\Delta \vec{p} \cdot \vec{R}/\hbar) \), yielding the results in Eq. (2A.10).

For a fast collision of an incident ion with a neutral (e.g., Bethe and Jackiw 1968; Inokuti et al. 1981) Bethe approximated the cross section above as

\[
d\sigma_{0 \rightarrow f}^{(1)} \approx \frac{2\pi(Z_A e^2)^2}{m_e v^2} \frac{dQ}{Q^2} Z_B |M_{0f}(Q)|^2,
\]

where \( M_{0f}(Q) \) is the matrix element of the ion interaction with an electron on the atom. This is often written in terms of

\[
F_{0f}(Q) = \left[ (\tilde{\varepsilon}_f - \varepsilon_0)/Q \right] \cdot Z_B |M_{0 \rightarrow f}(Q)|^2,
\]

where \( F_{0f}(Q) \) is called the generalized oscillator strength of the electrons on the atom (e.g., by analogy with model in Appendix 2C) and \( Q = \Delta p^2/2m_e \). Here \( \Delta p \) is not the momentum transfer to a single electron, as in the BEA method, but to the atomic system \( B \) as a whole. Hence, even for very small momentum transfers those electronic transitions which require significant internal energy changes can occur, albeit with small probability. The generalized oscillator strength has the property that

\[
\sum_f F_{0f}(Q) = Z_B.
\]

Therefore, the \emph{average} effect of all the electronic transitions is like the BEA.

For large \( Q \), Bethe showed that

\[
|M_{0 \rightarrow f}(Q)|^2 \approx \begin{cases} 0, & \varepsilon_f^0 - \varepsilon_0^0 \neq Q \\ 1, & \varepsilon_f^0 - \varepsilon_0^0 = Q \end{cases}
\]

giving the classical BEA result discussed earlier. This means that the momentum transferred to \( B \) is, with high probability, equal to that transferred to a single electron raising it to an excited state. At low \( Q \), on the other hand, \( F_{0f}(Q) \) is approximately the \emph{dipole} oscillator strength which determines the polarizability of an atom. Using these expressions to calculate the stopping power, one finds the remarkable result that the form of the stopping power is the same at high and low
Q. Therefore, the total, given in Eq. (2.32), is about twice the BEA result in Eq. (2.31b).

For the impact parameter formulation of the cross section in Eq. (2.7) the calculation of the transition probability is straightforward. The wave equation is treated as a time-dependent equation due to the motion of the nuclei, i.e., \( \vec{R}(t) \), and one often uses the straight line trajectory \( [R^2(t) \approx v^2 t^2 + b^2] \). When only two states are involved, the wave function is written as

\[
\psi(t) \approx C_0(t) \psi_0 + C_f(t) \psi_f,
\]

where \( \psi_0 \) and \( \psi_f \) correspond to the separate states associated with \( \varepsilon_0^0 \) and \( \varepsilon_f^0 \) described earlier and the \( C \) are coefficients which give the likelihood of being in either state as a function of time. Now the wave equations, \( i\hbar \partial \psi / \partial t = H \psi \), can be reduced to two coupled equations for the coefficients,

\[
\begin{align*}
\hbar & \frac{\partial C_0}{\partial t} = C_0 \varepsilon_0^0 + C_f V_{f0} \\
\hbar & \frac{\partial C_f}{\partial t} = C_0 V_{f0} + C_f \varepsilon_f^0,
\end{align*}
\]

where \( V_{f0} \) is an interaction potential [e.g., \( \Delta \varepsilon \) of Eq. (2.28)]. These equations can be numerically integrated to obtain \( C_0 \) and \( C_f \) at \( t \rightarrow \infty \) (e.g., McGrath and Johnson 1989). However, simple expressions are often useful.

If at \( t \rightarrow -\infty, C_0(t) = 1 \) and \( C_f(t) = 0 \), then the transition probability in Eq. (2.7) is

\[
P_{0 \rightarrow f} = |C_f(\infty)|^2.
\]

The Born approximation is the case \( |C_f(\infty)| \ll 1 \), so that Eq. (2D.8) yields

\[
P_{0 \rightarrow f} \approx \left| \int_{-\infty}^{\infty} V_{f0} e^{i\omega_{f0} t} \, dt \right|^2,
\]

where \( \hbar \omega_{f0} = \varepsilon_f^0 - \varepsilon_0^0 \). Using a straight line trajectory this is also equivalent to the interaction with a classical oscillator in Appendix 2C. Equation (2D.10) used in Eq. (2.7) also yields the Bethe-Born result above for the integrated cross sections.

For strong coupling \( C_f \) is not small. Equation (2D.8) can describe charge transfer when the momentum change of the electron is small. For symmetric resonance charge transfer \( \varepsilon_0^0 = \varepsilon_f^0 \) and the solutions to Eq. (2D.8) give

\[
P_{0 \rightarrow f} = \sin^2 \Delta \eta_{0f}
\]

\[
\Delta \eta_{0f} = \frac{1}{\hbar} \int_{-\infty}^{\infty} V_{0f} \, dt.
\]

Using \( \Delta \varepsilon \) in Eq. (2.28) for \( V_{f0}, \sigma_{0 \rightarrow f} \) can be integrated numerically. Firsov (e.g. Olson 1980) usefully approximates the integral by defining \( b_{ci} \) to be that value of \( b \) for which \( \Delta \eta_{0f} \sim 1/\pi \). This becomes, roughly,

\[
\Delta \varepsilon(b_{ci})(2\pi b_{ci} a)^{1/2}/\hbar \nu \sim 1/\pi.
\]
Using the form for $\Delta \varepsilon$ in Eq. (2.28) gives estimates of $b_\varepsilon$ and $\sigma_{0 \rightarrow f}$ for Eqs. (2.35) and (2.34). Smirnov (1964) gives a general very accurate expression for this cross section.

When $\varepsilon_j^0 \neq \varepsilon_0^0$ numerical integration is required to obtain $P_{0 \rightarrow f}$. However, the general form $P_{0 \rightarrow f}(b) \approx 2P_{0 \rightarrow f} \sin^2 \Delta \eta_{0f}$ has been used by a number of authors to calculate $\sigma_{0 \rightarrow f}$. Expressions for crossing and noncrossing states are given in the text.